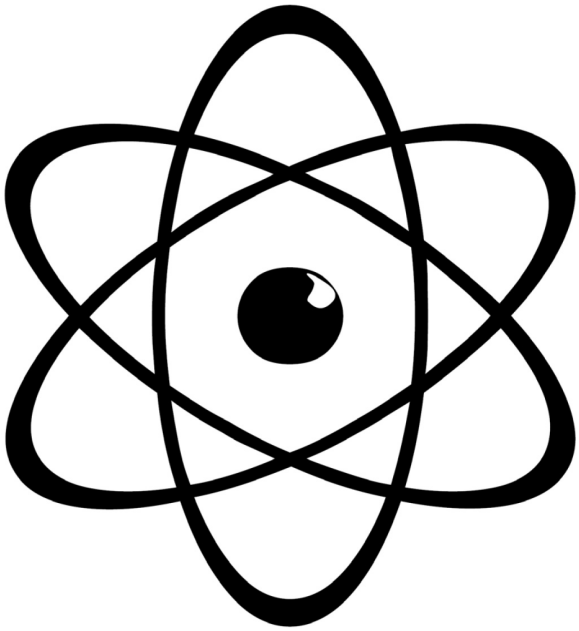
МІНІСТЕРСТВО ОСВІТИ І НАУКИ, МОЛОДІ ТА СПОРТУ УКРАЇНИ

ВІСНИК

ХАРКІВСЬКОГО НАЦІОНАЛЬНОГО УНІВЕРСИТЕТУ

імені В.Н. Каразіна

№ 1041



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DESCRIPTION AND PURPOSE OF THE JOURNAL

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ПРОФІЛЬ ЖУРНАЛУ ТА МЕТА ВИДАННЯ

"Вісник Харківського національного університету" (серія: фізична «Ядра, частинки, поля») є збірником наукових праць з фізики елементарних частинок, ядерної фізики, фізики плазми та плазмових технологій, фізики твердого тіла та радіаційної фізики. Збірник публікує наукові статті, короткі повідомлення, оглядові статті та рецензії на наукові видання.
Періодичність випуску збірника – 4 рази на рік.

Затверджено до друку рішенням Вченої ради Харківського національного університету імені В.Н. Каразіна (протокол № 2 від 22 лютого 2013 р.)

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**The articles are based on materials presented at the International Conference «Problems of modern physics», Kharkov, Ukraine, October 25-26, 2012, dedicated to the 50th anniversary of the Physics and Engineering Department, V.N. Karazin Kharkov National University.*

ЗМІСТ

**Статті грунтуються на матеріалі, представленому на Міжнародній конференції «Проблеми сучасної фізики», Харків, Україна, 25-26 жовтня 2012 р., присвяченої 50-річчю заснування фізико-технічного факультету Харківського національного університету імені В.Н. Каразіна.*

ALUMNI OF THE SCHOOL OF PHYSICS AND TECHNOLOGY - ITS MATTER OF PROUD

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Recently, V.N. Karazin Kharkiv National University celebrated two memorable events. 65 years ago, nuclear physicists graduated from the University for the first time. 50 years ago, School of Physics and Technology was established on the base of the Department of nuclear Physics. 2872 young people have graduated from the School since that time. If the alumni of the Department of Nuclear Physics are taken into account then total number of the nuclear alumni is 3428. 733 alumni graduated from the School with diplomas with distinction. 78 persons more graduated with such diplomas from the Department. Among the nuclear alumni there are over one thousand Doctors and Candidates of Science, 28 Academicians and Corresponding Members of the Academy of Sciences, Hero of Socialist Labor O.I. Pavlovsky, Hero of Ukraine V.G. Baryakhtar, authors of three inventions which were registered in the Soviet register of inventions, directors of the largest research institutions and enterprises, heads of physical laboratories all over the Ukraine and abroad, well-known political figures and managers of science. More than one hundred alumni are laureates of different prizes: State Prizes of USSR, Ukrainian and other Republics, Prizes of Academies.

What is the secret of such a high efficiency in educating the specialists? The answer is simple: the secret consists in so-called "fiztech" system of education that was introduced from the very first days of functioning of the Department of Nuclear Physics. This system is based on the fundamental education in Mathematics and Physics as well as on including of the students into real research carried out in physical institutions (first of all - national Science Center "Kharkiv Institute of Physics and Technology") for which the School prepares the specialists. Leading researchers of these institutes give lectures on special issues, supervise the students' research projects. Students start to carry out the research on the third-fourth year. Experimental equipment of the institutes is available for the students' research, for the BSc and MSc thesis preparation, for the industrial practice, etc.

In the paper below, one can find biographical data on the most outstanding alumni of the Department of Nuclear Physics and School of Physics and Technology, which had become Academicians. We hope, it will be interesting for those indifferent persons and, especially, for the youth.

AZARENKOV Mykola Oleksiyovych was born on December 15, 1951 in Kharkiv region in the village of Muravlynka, Novovodolazhsky district. In 1976, he graduated with honor from the School of Physics and Technology (SPhT), KhSU and was assigned to work at this University, to which he devoted all of his life. In 1980, he defended PhD thesis, and in 1991, he defended doctorate thesis. All these years, in parallel to the scientific activity, he teached. Since 1983, he worked as an assistant, since 1987 – associate professor, since 1992 – full professorship at the Department of General and Applied Physics. Since 1996, Professor M.O. Azarenkov headed the Department of Materials for Reactor Engineering. Since 1996 till 2005 he was a dean of the SPhT. Now he occupies the position of vice-rector of the University. In 2006, he was elected a corresponding member, and in 2012 - academician of the NASU. He actively participated in the establishing of new Computer Science School and School of Physics and Energy, and in establishing a new structure for the University - Institute of High Technologies, bringing together the three schools. He was the first director of this Institute.

Scientific work takes a special place in the work of Professor M.O. Azarenkov and has a breadth of scientific topics and scientific approaches. This is evident from his primary scientific activity: physics of limited plasma-like media, the physical basis of plasma-technological devices, parametric processes, nonlinear physics, semiconductor physics, radio physics, plasma electronics, material science, nanomaterials and their application for the development of new materials for nuclear power engineering, nanotechnology, and nuclear methods in materials. To each of these areas of scientific activity, together with his students and colleagues, he has made a significant contribution. With his students I. Denysenko and K. Ostrikov he developed the theory of linear antennas in magnetoactive plasma, which is called in the literature as the theory of ADO.

In 2008 he was awarded the honorary title of "Distinguished Professor of V.N. Karazin Kharkiv National University". In collaboration with colleagues, he has published more than 20 teaching materials, textbooks and monographs and over 500 papers. He has supervised 4 doctoral and 11 PhD theses. He is currently a member of the Coordinating Committee for the implementation of government agreements between Ukraine and the European Union on cooperation in the field of nuclear power engineering and in the field of controlled thermonuclear fusion.

Professor M.O. Azarenkov was awarded the distinctions of Ministry of Education and Science of Ukraine "Excellence in Education of Ukraine" (2000) and "For scientific achievements" (2010). In 2002, he was awarded the title "Honored Worker of Science and Technology of Ukraine". In 2005, he was awarded a Diploma of the NASU, and in 2010, honors of NASU "For scientific achievements". In 2010, he was awarded the K.D. Sinelnikov Prize of NASU (together with Prof. V.M. Voevodin and Prof. I.O. Girka).

AZHAZHA Volodymyr Mykhailovych (19.11.1931 – 23.12.2009) was born in the village of Velyki Sorochynci of Poltava region. In 1956, he graduated from the Department of Nuclear Physics (DNPh), School of Physics and Mathematics, Kharkov State University (KhSU). In January 1957 following the job assignment was sent at Institute of Physics and Technology, Academy of Science of Ukrainian SSR (at present - National Science Center "Kharkov Institute of Physics and Technology" -NSC KhIPhT), in which he was working all of his life, passing the scientific career from research assistant up to academician. He was a director of the Institute of Solid State Physics, Materials Science and Technology of NSC KhIPhT since 2004 till 2010. In 1964 he defended PhD thesis, and in 1986 – doctorate thesis.

V.M. Azhazha was well known scientist in solid state physics, material science and atomic energy. He was one of the founders of new scientific and technical area – vacuum and ultrahigh-vacuum metallurgy of ultra-pure metals and alloys with special physical features. He made a significant contribution to the development of physical bases, new methods and technology of producing the constructional alloys for atomic power engineering. He published more than 500 scientific papers, among them 5 monographs, 31 reviews, 36 inventions. He was scientific adviser of 5 doctorate and 15 PhD theses. He was a member of several specialized and coordinating councils, particularly, section “Rare Metals” of International association of Academies of Science, scientific council on chemistry and technology of ultra-pure matter of Russian Academy of Science, member of the bureau of the nuclear physics and power engineering of National Academy of Science of Ukraine (NASU). He was the editor of scientific journal series “Problems of Atomic Science and Technology”.

In 1982, V.M. Azhazha was awarded the State Prize of Ukraine in science and technology. In 1990, he was awarded the title of Professor. In 2003, he was elected a corresponding member of NASU, and in 2006 – academician of the NASU. In 2008, he was awarded the title "Honored Worker of Science and Technology of Ukraine". He was awarded the "Badge of Honor", medals "For Valiant Labor", "For long and dedicated work," "In honor of the 100th anniversary of Lenin's birthday", diploma of Council of Ministers of Ukraine and other marks of distinction. In 2009, he was awarded the title "Honorary Doctor" of V.N. Karazin Kharkiv National University (KhNU).

BAKAI Olexander Stepanovych was born on September 16, 1938 in Kharkiv city. He graduated from the DNPh, KhSU in 1961. In 1966, he defended PhD thesis, and in 1972, he defended his doctoral thesis. Since 1961, he has worked in NSC KhIPhT. He started as a research assistant passing to the head of the theoretical division (since 1981). In 1977-1999, he was a Professor of KhSU, and in 1994-1998 – professor of Belgorod Pedagogical University. His research areas are as follows: theoretical and mathematical physics.

He developed the theory of nonlinear multiwave phenomena in continuous media - plasma, ionospheric plasma, solid state; he developed the theory of moderate turbulence in plasma; he formulated the poly-cluster model of amorphous solids and studied the physical properties of poly-clusters; he built the structural phase diagrams of binary alloys under reactor irradiation; he heads the programs on the development and testing in experiments with irradiating the materials for the reactors of the fourth generation.

Professor O.S. Bakai is a member of the Shevchenko Scientific Society (2007), academician of NASU (2009), Soros Professor (1996), winner of K.D. Sinelnikov Scholarship (2003). Scientific work by professor Bakai on the theory of poly-cluster amorphous bodies was awarded the State Prize of Ukraine (1992), and the work on nuclear power was awarded the O.I. Leypunsky Prize of NASU (2008).

He was awarded the medals "For Valiant Labor", "In honor of the 100th anniversary of Lenin's birthday" (1970), "For Labor Valor" (1981), "Veteran of Labor" (1987). He was awarded the Gratitude of the Council of Ministers of Ukraine (2003), the honor of NASU "For scientific achievements" (2008). Among his students – 13 PhDs and 5 Doctors of Science. He has a portfolio of about 300 scientific papers and 5 monographs.

BAR'YAKHTAR Viktor Grygorovych was born on August 9, 1930. He graduated from the DNPh, KhSU in 1953. In 1959, he was awarded the title of PhD, and in 1965 – the title of Doctor of Physics and Mathematics. In 1972, he was elected a corresponding member of the Academy of Sciences of the Ukrainian Soviet Socialist Republic, in 1978, he was elected an academician.

In 1954-1973, he was a researcher, a head of the laboratory of theoretical division at KhIPhT, AS of Ukrainian SSR, led by academician O.I. Akhiezer; in 1973-82, he was a head of the department, deputy director for science at Donetsk Institute of Physics and Technology of the AS of Ukrainian SSR; and in 1985-89, he was a head of the department of theoretical physics and director of the Institute of Metal Physics, AS of Ukrainian SSR. In 1982-89, he was an academician-secretary of the department of physics and astronomy of the AS of Ukrainian SSR; in 1989-94, he was a vice-president of NASU; in 1994-98, he was a senior vice-president of NASU. Since 1995, he is a director of the Institute of Magnetism of the NASU and Ministry of Education and Science of Ukraine.

Professor V.G. Bar'yakhtar was actively involved in efforts to eliminate the consequences of the Chornobyl disaster. He was a chairman of the Committee on nuclear policy under the President of Ukraine, chairman of the commission on Chornobyl of the NASU.

Academician V.G. Bar'yakhtar is the author of over 500 scientific papers, including 16 monographs on physics and 5 monographs on eliminating the consequences of the Chornobyl disaster, co-author (with O.I. Akhiezer and S.V. Peletminsky) of discovery of "Magnetoacoustic resonance in ferro-, ferri- and antiferromagnetics" (1956).

Professor V.G. Bar'yakhtar gave lectures at KhSU, University of Donetsk, Taras Shevchenko Kiev National University and National Technical University of Ukraine "KPI". Among the students of professor Bar'yakhtar there are 25 doctors and more than 50 PhDs, six winners of the State Prize of Ukraine, the two heads of research institutes (V.N. Varyukhin and V.F. Klepikov), academician V.P. Seminozhenko, corresponding members of NASU V.F. Klepikov, B.A. Ivanov, and a member of the Academy of Pedagogical Sciences Yu.I. Gorobets.

Academician V. G. Bar'yakhtar is a founder and the first President of the Ukrainian Physical Society, a member of the American and the Italian Physical Societies, member of the Russian Academy of Arts, a member of the New York Academy of Sciences. The evidence of great public importance of the activity of academician V.G. Bar'yakhtar is rewarding him with three awards and honorary of President of Ukraine, as well as the medal of Pope John Paul II. In 2010, he was awarded the title "Hero of Ukraine".

DOVBNYA Anatoliy Mykolayovych was born on 12th of May in 1940 in Krasnograd, Kharkiv region. In 1962, he graduated from M. Gorky KhSU (DNPh). All his further work and scientific activities was closely associated with KhIPhT (now NSC KhIPhT). There he started to work as an intern-researcher, and nowadays he is a Director of the Science and Research Unit "Accelerator" and a Director of the Institute of High-Energy Physics and Nuclear Physics. He defended the PhD thesis in 1972, and in 1993, he was given a degree of Doctor of Science, then he became a Professor. Since 1979, he was a Head of the Laboratory. Further, since 1990 he was a Head of the Department of the Accelerator LEA 2 GeV, where all the works on improvement of the KIPT's linear electron accelerators were carried under his direct leadership. Since 1992, a new stage in his scientific and organizational activities has been started. It is the stage of development and constructing of the relatively small accelerator complexes and their applications for the solution of various fundamental and applied problems. A large number of researches for the medical isotopes production were carried out under A. Dovbnya's initiative. Ongoing developments will provide Kharkiv region with medical radionuclides, which are necessary both for diagnostics and for treatment of various diseases. A large complex of studies on the high-energy physics, the nuclear physics, the development of the charged particle detectors, the development of the computer technologies, the constructing of the complex of accelerators and storage rings were carried out under A. Dovbnya's leadership in the IHEPNP. A. Dovbnya is a famous scientist in the field of the accelerator physics, the nuclear and radiation physics. He is the author of more than 300 publications. He is a member of the Ukrainian and American Physical Society. He is the editor of the journal "Problems of Atomic Science and Technology". He is a Corresponding Member of NASU since 2006.

The fruitful work of A. Dovbnya was awarded by the government according to his deserts. He was awarded the Order "For Services" of III class by President of Ukraine. Also he was awarded the A.I. Leypunskiy Prize by NASU.

FOMIN Petro Ivanovych (**20.06.1930 – 05.10.2011)** was born in Zhikharevo village, Orel region. In 1952, he graduated from the DNPh, M. Gorky KhSU. After postgraduate study, Petr Fomin started to work as a Researcher at the O.I. Akhiezer Theoretical Department of the KhIPhT of AS of Ukrainian SSR (now NSC KhIPhT).

His science and creative activity inseparably connected with the Institute and the University for 21 years. There he grew up as a scientist. He defended the PhD thesis in 1957, and in 1972 he was given a degree of Doctor of Science. P. Fomin carried out the advanced researches on the theory of the radiative corrections to the electron bremsstrahlung in the external electromagnetic field. He determined the structure of the mass renormalization electron in quantum electrodynamics based on the adding the perturbation theory major terms in the renormalization group approach.

Without leaving off the quantum field theory research, P. Fomin began to investigate the fundamental problems of astrophysics and cosmology. The main task of it was the problem of the Universe origin. He proposed the theory of the Universe spontaneous creation from the vacuum due to its gravitational instability. In 1972, P. Fomin moved to Kiev, where he headed the Department of Astrophysics and Elementary Particles at the Institute of Theoretical Physics of the AS of Ukrainian SSR. P. Fomin developed the quantum-field theory of the quasars activity and the radio galaxies. The model of the spontaneous formation of the vacuum crystal-like structure at the Planck scales was proposed by him.

P.I. Fomin was an excellent educator as well as talented scientist. He lectured firstly at the KhSU and then at the Kiev University for many years. Since 1979, he was a Professor at the Kiev National University. He trained more than 20 PhDs, including 5 Doctors of Science. He was the author of more than 170 publications. He was a Corresponding Member of the NASU since 1990. He was the State Prize winner in Science and Technology of Ukraine, the Barabashov Prize of NASU. he was also a "Honored Worker of Science and Technology of Ukraine".

GNATCHENKO Sergiy Leonidovych was born on March 20, 1947 in Kupyansk city of Kharkiv region. In 1971, he graduated from the SPhT, KhSU. From the first years of his activity at Institute of Low Temperature Physics and Engineering which he joined after graduating from the University, the main focus of his scientific work was formed, i.e. the study by means of magneto-optical methods the low-temperature magnetic phase transitions and properties of domain structures, which are formed during these transitions in magnetic dielectrics. Further development of experimental studies of low-temperature magnetic phase transitions in antiferromagnetics and ferrimagnetics culminated in the formation of a new area - the study of the static and dynamic properties of magnetoinhomogeneous states formed during phase transitions in multisublattice magnetics. The second important area of his scientific activity is the study of photoinduced phenomena observed at low temperatures in magnetic materials and superconductors. The obtained results in this area are not only foreground and principal for low-temperature solid-state physics, but also are of great practical importance. S.L. Gnatchenko has written more than 100 scientific papers published in leading specialized journals. In 1987, S.L. Gnatchenko with his co-authors was awarded the joint prize of the AS of USSR and the Polish Academy of Science for the study of magneto-optical inhomogeneous states in magnetics. The series of his works on "New optical and magneto-optical phenomena in antiferromagnetics" was awarded the State Prize of Ukraine in the field of science and technology in 2004.

Professor S.L. Gnatchenko successfully combines his scientific study with a science management and training of young highly qualified researchers. For many years he headed the department of low-temperature magnetism, was the deputy director for research of B.I. Verkin Institute for Low Temperature Physics and Engineering (ILTPE) of the NASU, and now he heads this institute. Under the leadership of professor S.L. Gnatchenko 5 PhD students defended their theses in physics and mathematics.

He is the deputy chairman of the Scientific Council of NASU on the problem of "low-temperature physics and cryogenic technology," chairman of the specialized council for doctoral theses at ILTPE of the NAS of Ukraine, a member of the editorial board of "Low Temperature Physics" journal.

IVANOV Borys Oleksiyovych was born in 1948. In 1972, he graduated from SPhT, KhSU. After finishing the PhD course in 1974, he started to work at Institute for Low Temperature Physics and Engineering in Kharkiv as a Junior Researcher (1974-1978) and then as a Senior Researcher (1978-1983). After that, he was working in Institute for Physics of Metals NAS of Ukraine in Kyiv as a head of laboratory (1983-1992) and as a Leading Researcher (1992-1995). Since 1995, he has been working in Institute of Magnetism NASU and Ministry of Education in Kyiv as a Principal Researcher. He defended the PhD thesis "About the theory of magnetic domains" in 1974 under supervision of Academician V.G. Baryakhtar). He defended the doctoral thesis "Dynamical and topological solitons in magnetic" in 1983. In 2009, he was elected as a Corresponding Member of NASU. Under B.O. Ivanov's supervision 14 PhD students had prepared and defended their thesis successfully, three of them were given the Doctor of Science degree after that.

He is giving lectures on "Theoretical Mechanics", "Solid State Physics", "Selected Questions of Theoretical Physics", "Physics of Magnetism" in Taras Shevchenko National University of Kyiv.

The area of his scientific interests covers the solitons in solid state, the non-onedimensional solitons, the theory of magnetic domain structures, the magnetic relaxation, the macroscopic quantum phenomena, the magnetic nanoparticles.

He published 4 monographs, 8 reviews and more than 200 papers in referred scientific journals. Prof. Ivanov was awarded the O.S. Davydov Prize of NASU in 2005 for a series of works "Vortex dynamics of magnets" (shared with O.S.Kovalev and D.D. Sheka).

KARNAUKHOV Ivan Mikhailovych was born on January 19, 1937 in the village of Syrcevo of Ivnyansk district of Belgorod region. After graduating from the DNPh, KhSU in 1959 he was hired by KhIPhT of AS of Ukrainian SSR. Formation and development of scientific talent of I.M. Karnaukhov was held in the Institute (now NSC KhIPhT), where he started as a research assistant and rose up to the deputy director general for research (1997). Here, he defended his Ph.D. (1967) and doctorate (1982) thesis. In 1991, he was awarded the title of professor. In 2009, he was elected a corresponding member, and in 2012 - academician of the NASU. His academic research focuses on the physics of nuclei and elementary particles, radiation physics, physics of synchrotron radiation. Studies of polarized phenomena in double polarization experiments using the developed by him a complex of experimental setups with polarized proton and deuteron targets brought him worldwide fame. Designed and created by him experimental setups work in ErFI (Armenia), Institute of Nuclear Physics (Russia), JINR (Dubna, Russia) and in the Institute of Solid State Physics (Julich, Germany). Of particular interest is the work carried out by him to create electron storage ring in order to obtain high-power monochromatic collimated beams. The main equipment of the storage is installed and the study of how to run the installation is initiated. Professor I.M. Karnaukhov took the initiative to develop a safe clean nuclear energy in Ukraine, which is based on sub-critical assemblies that are driven by a powerful beam. He heads the finalization of the development of the conceptual project "Neutron source, based on the subcritical assembly controlled by linear electron accelerator" and initial stage on this project under the financial support from the Argonne National Laboratory (USA). With rich experience of working with powerful radiation fields, professor I.M.Karnaukhov actively participated in the formation and implementation of the proposed by NSC KIPT program to make the fourth unit of Chornobyl NPP an environmentally safe area. I.M.Karnaukhov is an author of 231 scientific papers and two monographs; he was a supervisor of eleven PhD and one doctorate theses. For many years he taught at the V.N. Karazin KhNU. Professor I.M. Karnaukhov is a member of International Advisory Committee "Synchrotron Radiation Instrumentation", and a member of the editorial board of the journal "Problems of Atomic Science and Technology." Scientific achievements and labor services of I.M.Karnaukhov was awarded the State Prize of Ukraine in science and technology (2002). he was awarded the marks "Veteran of Nuclear Energy and Industry of the Russian Federation" and "For the preparation of scientific generation" of NASU. He was awarded the Diploma of the Ministry of Education and Science of Ukraine for the significant contribution to the development of national science and fruitful scientific activity.

KHARCHENKO Mykola Fedorovych was born on October 21, 1939 in a family of teachers in rural farm village HTZ of Chutovski district of Poltava region. In 1960, he graduated from the DNPh, KhSU. In 1961, M.F.Kharchenko started to work at the ILTPE of the AS of Ukrainian SSR. Since then for more than 50 years, scientific activity of M.F Kharchenko is inseparably linked to this institute. There he was promoted from engineer to the head of the department. In 1969, M.F.Kharchenko defended his PhD, and in 1984 - his doctoral thesis. In 1995, he was elected a corresponding member of NASU, on the specialty "experimental physics," and in 2009 - a member of NASU.

M.F. Kharchenko is a renowned expert on magnetism and optics of magnetically ordered systems, whose works cover a wide range of physical problems. He obtained important results in scientific and technical aspects in various fields of physics of magnetism of solids that forever enter in the treasury of world science. Among the main results of M.F.Kharchenko there are the pioneering research of new magneto-optical effects, which are called "linear magneto-optical effect" and "quadratic magnetic rotation of the plane of polarization of light." M.F.Kharchenko was the first to realize the optical imaging of collinear antiferromagnetic domains, developed methods for switching collinear antiferromagnetic domains in the crystals with different magnetic symmetry and demonstrated the possibility of preparing the antiferromagnetic domain structure with a predetermined configuration.

He is a co-author of the monograph "Magnetic optics and spectroscopy of antiferromagnets," published by the publishing house "Naukova Dumka" and later reprinted by «Shpringer-Verlag». He is an author of over 150 scientific papers and reviews.

M.F.Kharchenko is a chairman of the Scientific Council of the ILTPE on the problem of "Low temperature magnetism and optics of ferroics", a member of the editorial boards of the journals "Low Temperature Physics" and «Ukrainian Journal of Physical Optics».

M.F. Kharchenko pays a great attention to teaching and training of scientific personnel. About 30 years, he is actively cooperating with the V.N. Karazin KhNU, where he teaches courses at the department of General Physics and acts as a head of the branch of the department at ILTPE. Six PhDs were prepared and defended under his supervision. Among the students of M.F. Kharchenko there are one academician of NASU and two doctors of sciences.

M.F. Kharchenko was awarded the K.D. Sinelnikov prize of AS of Ukrainian SSR (1985), prize of the AS of USSR and the Polish Academy of Sciences (1987) and the State Prize of Ukraine in science and technology (2004).

KLEPIKOV Vyacheslav Fedorovych was born in Kharkiv in 1949. In 1971, he graduated from the Department of Theoretical Nuclear Physics, SPhT, Maxim Gorky KhSU. During 1971-1990, he was working at KhIPhT NASU. During 1990-1992, he was organizing a new institution in NASU – Center of Electrophysical Machining (nowadays it is the Institute of Electrophysics and Radiation Technologies of NASU). He is a Director of the institute now.

The following main scientific results are obtained by V.F. Klepikov. The conditions of the giant amplification of the nuclear magnetic resonance in the thin magnetic films are predicted; the physical principles of the data storage devices with the record parameters, which can work under a radiation, are developed; the radiation methods of recovering the nuclear material properties are developed; the effects of the radiation stimulated superplasticity are predicted; the methods of the quantum electrodynamics are generalized for the cases of the non-local fields of matter, and they are applied for solving the problems of the electromagnetic interactions in nuclei; the methods of the modification and phase transformation using beams of the charged particle are proposed, and the new nuclear and radiation technologies, which are now widely implemented in practice, are developed; the new radiation technologies of diagnostics, safety control and lifetime prolongation for the nuclear reactors and other equipment of the NPPs are developed; the radiation technologies for medicine, agriculture and security are developed; the mechanism of the spontaneous breakdown of the discrete analog of the supersymmetry for the field theories with the highest derivatives is proposed; the particle spectra in the critical areas in the scope of the nonlinear field theories are studied..

His students prepared and defended 4 theses for Doctor of Science degree and 5 PhD thesis. For many years he is giving lectures at SPhT of V.N. Karazin KhNU. In 2003, he was elected as a Corresponding Member of NASU.

Since organizing the Division of the Nuclear physics and energy in NASU, V.F. Klepikov is a Deputy Academician-Secretary of the Division, and he has brought a lot in its formation and in organization of its activities. He is a Head of Expert Council on State Nuclear Program of Ukraine.

V.F. Klepikov is a Honoured Science and Technology Worker of Ukraine, and he was awarded the S. Pekar prize of NASU and M. Ostrovsky Prize.

MIROSHNYCHENKO Valentyn Ivanovych was born in Ivanovka village, Volchansk district, Kharkiv region on 21th of May in 1935. In 1958, he graduated from Maxim Gorky KhSU (DNPh). After graduation V. Miroshnychenko started to work at KhIPhT of AS of Ukrainian SSR (now NSC KhIPhT) as a Junior Researcher. In 1967, he defended his PhD thesis, and in 1989, he was given a degree of Doctor of Science. He has been a Senior Researcher since 1975.

Since 1995, he has been a head of the Electrostatic Accelerators Department at the Institute of Applied Physics, NASU, in Sumy. Since 2006, he has been a Deputy Director on Scientific Activities. He was elected a Corresponding Member of NASU in 2006. He is a "Honored Worker of Science and Technology of Ukraine" since 2009.

He is the author of the pioneer papers about the application of the relativistic electron beams for generating the short-wave electromagnetic radiation on the basis of the stimulated coherent scattering of electromagnetic waves by the relativistic electrons. He developed the free electron laser non-linear theory in the so-called Raman regime simultaneously with American scientists for the first time. He is one of the developers of the plasma free electron laser nonlinear theory. In this theory Langmuir wave excited in a plasma is the undulator. Another pioneer paper of V.I. Miroshnychenko is devoted to the studies of the plasma instability due to the ion-cyclotron heating. This study initiated a wide range of both theoretical and experimental works carried out at NSC KhIPhT for solving the problem of the controlled thermonuclear fusion. His scientific advances of the last decade are related to the development and construction of the analytical accelerating complex in IAP NASU for the study of the elemental composition and structure of the matter by the nuclear-physical methods. These investigations were finished by launching the scanning nuclear microprobe for the local non-destructive analysis of the matter structure and elemental composition. This microscope is the first in the CIS.

V.I. Miroshnychenko takes an active part in the young human resource development. He gives courses of lectures on the “Physical basis of the charged particle acceleration” and "Fundamentals of Plasma Physics" in Experimental and Theoretical Physics Department of the Sumy University, working part-time as a professor.

ORAEVSKY Viktor Mykolayovych (09.03-1935 – 23.11.2006) was born on March 9, 1935 in Poltava city. He graduated from the DNPh, KhSU in 1957. During 1958 – 1965, he was a senior laboratory assistant, associate researcher at the Institute of Nuclear Physics of the USSR Academy of Sciences. During 1965-1970, he was a senior scientist at the Institute of Physics of the AS of the Ukrainian SSR. From 1970 till 1974, he was a head of the department of the Institute of Nuclear Research, AS of the Ukrainian SSR. In 1974-1979, he was a head of the section of the SPA "Energy". From 1979 till 1989, he was a head of laboratory, head of the department of the Institute of terrestrial magnetism, ionosphere and radio wave propagation, AS of the USSR. In 1989-2003, he was a director of this institute. He was a head of international satellite projects. He was a doctor of physics and mathematics, professor, academician of the Academy of Natural Sciences (1996), a member of the International Informatization Academy, International Academy of Astronautics, the New York Academy of Sciences. He was awarded the title "Honored Worker of Science of Russia" (1996). He was a winner of the State Prize of the Ukrainian SSR, State Prize of the USSR (1987), the State Prize of Russia (1997). he was a foreign Member of the NASU in "space physics" (2003). He was a specialist in the theory and calculations of plasma processes.

PAVLOVSKY Olexander Ivanovych (27.06.1927-12.02.1993) was born in Zaporizhzhya city. In 1951, he graduated from the DNPh, KhSU. In the same year he was sent to work tt Arzamas-16. There under the supervision of A.D. Sakharov and Yu. B. Khariton he worked to develop the thermonuclear weapons. He was responsible for the creation of high-intensity neutron sources, neutron physics, and nuclear fission. At first O.I. Pavlovsky worked as a senior laboratory assistant, after a while headed the laboratory, and from 1960 he led a major research department of All-Russian Research Institute of Experimental Physics (VNIIEF). In 1953, O.I.Pavlovsky awarded the Stalin Prize. In 1971, he led the division of fundamental and applied research, and then became deputy and first deputy of supervisor of VNIIEF while leading the department. He was doing research in the field of neutron physics, pulse technology, physics and technology of accelerators, high energy density physics, and quantum electronics. He was one of the founders of a new direction in high energy density physics - magnetic

cumulation. Under his leadership, cumulative phenomenon was studied and powerful pulsed sources of energy based on magnetocumulative generator, a device for generating ultra-high pulsed magnetic fields, was created. In 1963, Olexander Pavlovsky defended doctor thesis. In the same year he was awarded the Lenin Prize. In 1979, O.Pavlovsky was elected a corresponding member of the USSR AS (the department of nuclear physics). By the Decree of the Presidium of the Supreme Soviet of the USSR from 29.07.1966 O.I.Pavlovsky was awarded the title of Hero of Socialist Labor with awarding the Order of Lenin and the Gold medal "Hammer and Sickle" for his work in nuclear physics used in the interests of nuclear and thermonuclear weapons. In 1983, he became a laureate of the State Prize of the USSR. In 1988, he was awarded the title "Honored Scientist of the RSFSR." In 1991, O.I.Pavlovsky was elected an Academician of the Russian AS. In 1999, he was awarded the State Prize of Russia (posthumously) for outstanding results on generators of microwave radiation.

PELETMINSKY Sergiy Volodymyrovych was born on February 14, 1931 in urban village Tetkino of Kursk region. In 1953, he graduated from the DNPh, KhSU and was enrolled in graduate school to O.I. Akhiezer. In 1957, he started to work in KhIPhT (now NSC KhIPhT of the NASU). Here he went from a research assistant to the head of the laboratory of statistical physics. From 1989 till 1996, he was a head of theoretical physics department. In 1959, S.V. Peletminsky defended his PhD thesis, and in 1966 - his doctoral dissertation. In 1969, he was awarded the title of Professor. In 1978, Professor S.V. Peletminsky was elected a corresponding member, and in 1990, he was elected an academician of the AS of the Ukrainian SSR.

Research interests of S.V. Peletminsky are associated with the different areas of theoretical physics and are devoted to solving the fundamental problems of quantum field theory, statistical mechanics, the physics of quantum liquids and crystals, theory of magnetic phenomena in crystals. He owns a number of fundamental results, recognized by the international scientific community. Together with O.I. Akhiezer and V.G. Bar'yakhtar he predicted a new physical phenomenon, i.e. the "phenomenon of interaction of hypersonic and magnetic (spin) waves in ferro-, ferri-and antiferromagnetics (magnetoacoustic resonance)" registered as a discovery under the number No. 46 in 1956 year. Studies by S.V. Peletminsky, I.O. Akhiezer and V.G. Bar'yakhtar on the theory of high-frequency relaxation processes in magnetic materials have been awarded the K.D. Sinelnikov prize of AS of Ukrainian SSR in 1978. In his studies on statistical mechanics S.V. Peletminsky refers to the proposed by M.M. Bogolyubov method of reduced description of nonequilibrium processes. In a series of works by professor S.V. Peletminsky and his students, this method has been successfully used both for kinetic equations describing irreversible processes, and to find the asymptotic properties of the Green's functions of different physical systems. For the study of systems with spontaneously broken symmetry in 1986 year S.V. Peletminsky was awarded the N.M. Krylov prize of the AS of Ukraine. In the 80s years, professor S.V. Peletminsky and his students developed semi-phenomenological Fermi-liquid approach as applied to the description of superfluid systems. The proposed theory was the generalization for the superfluid system as a Landau-Silin normal Fermi liquid and for the BCS-Bogolyubov equations. In 1996, S.V. Peletminsky with a group of scientists was awarded the State Prize of Ukraine in science and technology for the set of works "Kinetic processes in quantum liquids and crystals". In 2002, he was awarded the M.M. Bogolyubov Prize of the NASU for the set of works "Field theory and the theory of disordered systems". S.V. Peletminsky has authored and co-authored over 250 scientific publications and 5 monographs published in Ukraine and abroad. S.V. Peletminsky pays a lot of attention to the training of researchers. He created the world famous school on statistical physics. Among his students there are twenty PhDs of physics and mathematics, twelve of which are doctors. Over 45 years, he gave lectures on quantum electrodynamics to the students of SPhT, KhSU. In 2001, S.V. Peletminsky was awarded the medal "Excellence in Education of Ukraine" for outstanding scientific achievements, selfless teaching career, and a great contribution to the development of the University. In 2004, he was awarded the title "Honorary Doctor of Kharkiv University."

SEMINOZHENKO Volodymyr Petrovych was born on June 9, 1950 in Kiev. In 1972, he graduated from the SPhT, KhSU. In 1974, he defended his PhD thesis, and in 1984 - his doctoral thesis. He is a Professor, corresponding member of the AS of Ukrainian SSR (1988), academician of the NASU (1992).

Until 1985, he worked as a senior research fellow at ILTPhE. In 1985, he was appointed a general director of SPA "Monokristallreaktiv." Since 1991, he has headed the STC "Institute for Single Crystals" NASU. Since 1992, he is a member of the Presidium of the NASU, chairman of the North-East Scientific Center of NASU and Ministry of Education and Science of Ukraine. Professor V.P. Seminozhenko is an author of more than 500 scientific papers, 80 patents and inventions. He is the editor in chief of the journals "Problems of Science" and "Functional Materials", the anthology of comparative studies "Ecumene", member of editorial board of several scientific

journals, including the scientific journal of the National Security and Defense of Ukraine "Strategic View", etc. He was thrice elected to the Parliament of Ukraine. In 1996-1998, he was a Minister of Science and Technology. In 1999 and 2001-2002 he was a Deputy Prime Minister of Ukraine. In 2003-2005 he was an Advisor to the President of Ukraine. In 2006-2007 he was an Advisor to the Prime Minister. In 2010, he was appointed a head of the State Agency for Science, Innovation and Informatization of Ukraine. V.P. Seminozhenko is twice winner of the State Prize of Ukraine in science and technology (1992, 2000), and the International Prize in nuclear physics (1999). He was awarded the Order "For Merit" I, II and III degrees, "Holy Prince Vladimir" IV degree, diplomas of the Council of Ministers and the Parliament of Ukraine, etc. he is a Honor Full Member (Academician) of the Academy of Arts of Ukraine. he is a Honorary doctor and president of the alumni association, faculty and friends of V.N. Karazin Kharkiv National University. He is a honorary Citizen of the city of Kharkiv (2010).

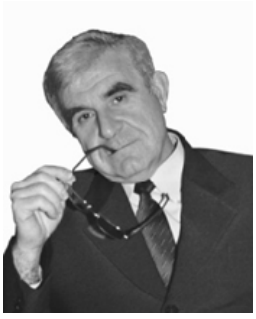
SHUL'GA Mykola Fedorovych was born on September 15, 1947 in Kharkiv. After graduating in 1965 with silver medal from high school, he enrolled to study at the SPhT, KhSU. After the graduating from KhSU in 1971, M.F. Shul'ga was drafted into the Soviet Army and served as an officer for two years in the city of Volgograd. From 1973 until the present time, he works at KhIPhT (now NSC KhIPhT). Within its walls, he defended his PhD in 1977 and doctoral thesis in 1985. In 2009, he was elected an academician of the NASU. Academician M.F. Shul'ga is one of the founders of the Institute for Theoretical Physics of NSC KhIPhT and is the first its director (1996).

Academician M.F. Shul'ga is a leading expert in quantum electrodynamics and high energy physics. The fundamental results obtained by him in these areas are well known and recognized throughout the world. Together with S.P. Fomin he predicted the suppression of bremsstrahlung in a thin layer of the material (this effect is called in the literature as the effect of Tarnovsky-Shul'ga-Fomin), and developed the quantitative theory of this phenomenon. Together with A.A. Grinenko, he predicted the stochastic slewing of the high-energy particle beams by bent crystals, thus opening up new opportunities for a relatively simple solution of the problem how to output beams of different charged particles from accelerators. On the initiative and with direct participation of M.F. Shul'ga a number of critical experiments were carried out to test the predicted pehnomena on the accelerators at CERN (Switzerland), SLAC (USA), MAMI and S-DALINAS (Germany), as well as at KhIPhT. In the late 90's, M.F. Shul'ga with O.I. Akhiezer have initiated the work in theoretical physics at KhIPhT on physics of fast neutron reactor, which operates in a wave of slow nuclear burning.

M.F. Shul'ga pays much attention to the education of decent scientists. For many years, M.F. Shul'ga gives lectures at V.N. Karazin KhNU on quantum electrodynamics at high energy in the matter. He is the head of a branch of the department of Theoretical Nuclear Physics of SPhT of V.N. Karazin KhNU at NSC KhIPhT. Among his students there are four doctors and eight PhDs in Physics and Mathematics.

M.F. Shul'ga is an author and co-author of over 250 scientific papers (including 8 monographs and monographic reviews). In 2000, the scientific work of M.F. Shul'ga was awarded the O.S. Davydov prize of NASU. In 2002, he was awarded the State Prize of Ukraine in science and technology. M.F. Shul'ga is a member of the Scientific Council of the NASU on the subject "Nuclear Physics and Nuclear Energy" and of the Scientific Council of the CIS countries on the application of nuclear physics methods in the interdisciplinary areas.

He is a member of the editorial boards of the "Ukrainian Physics Journal", "Problems of Atomic Science and Technology", "Journal of Kharkiv University," and enters a number of scientific councils of NSC KhIPhT and V.N. Karazin KhNU. In 2004, M.F. Shul'ga was elected a vice-president of the Ukrainian Physical Society.



SLYUSARENKO Yuriy Viktorovych was born on 24th of January in 1957 in Lesnoy village, Kirov region of Russia. In 1980, he graduated from the SPhT, Maxim Gorky KhSU. Since finishing the PhD course and till 1991, he was working at the laboratory of ion processes of KhSU. There he obtained the important theoretical results on the description of the interaction of the charged particles with the solid state surface. These results have been used for the statement and interpretation of the new experiments. In 1984, he defended the PhD thesis. Since March 1991 till present, he is working in O.I. Akhiezer Institute for Theoretical Physics, NSC KhIPhT. Now, he is a head of the Department of Statistical Physics and Quantum Field Theory. Due to his efforts, the method of the reduced description of the nonequilibrium states of the systems with a large correlation radius was developed. It gives a possibility to describe the kinetics and hydrodynamics of the long range fluctuations. In 1996 he defended the thesis for Doctor of Science degree.

Then his scientific interests were directed to studying and describing the Bose-Einstein condensation phenomenon.

In 1998 in co-authorship with Academicians O.I. Akhiezer and S.V. Peletminsky he carried out the pioneer investigation on the Bose-Einstein condensation of the particles with the integer spin in the external magnetic field. Recently he has developed the original scheme of the approximate method of the secondary quantization of the systems in the case of the bound states. This scheme can be used for the small kinetic energies of the particles.

He is managing the scientific projects of State Programs of NASU, and he is participating in the set of international projects. He published 120 papers in scientific journals. During many years he is giving lectures on "Kinetic Theory", "Quantum Statistics", "Probability Theory" and "Higher Mathematics", "Solid State Physics" at V.N. Karazin KhNU and Belgorod State University (Russia). In 2009, he was elected as a Corresponding Member of NASU.

SOLOSHENKO Igor Oleksandrovych (01.01.1942 – 29.04.2007) was born in Lugovka village of Sumy region in Ukraine. In 1963, he graduated from the SPhT, Maxim Gorky KhSU and started to work at the Institute of Physics AS of Ukrainian SSR in Kyiv. His entire science and job career was related with the institute, where he worked at positions from an engineer to a head of laboratory and a director. In 2000, he was elected as a Corresponding Member of NASU.

He worked in different areas of plasma physics, radiation physics and physics of intense ion beams, i.e. ion sources, interaction of ion beams with solid state surface, gas discharge in low-density gases and atmosphere. His most significant results were related with problems of the space charge compensation of the positive and negative ion beams; the oscillation excitation in the compensated ion beams; the long range transport of the ion beams. Due to the obtained results, the prediction of the intense ion beams behavior in various systems became possible, i.e. in the neutral beam injectors for the controlled nuclear fusion, in accelerators and other technological systems. Most of these works were carried out in 1970s and 1980s. These works founded the principles of the new branch of plasma physics, i.e. physics of ion-beam plasmas. It still excels the analogous works, which are carried out in other organizations worldwide.

The research of the plasma sources of the negative ions is widely known among specialists in Ukraine and abroad. In these works by I.O. Soloshenko the main mechanisms of the negative ion formation and breakdown are determined; the emission characteristics of the sources are calculated; the steady state source of the negative ions of hydrogen with the record parameters is constructed. His studies on the interaction of the ion fluxes with the metal surface were recognised. One of the most important work among applied works of the I.O. Soloshenko is the new technology of the cold sterilization of medical instruments based on the gas discharge plasma. This technology should replace the environmentally dangerous technology which is based on the use of the toxic gases. The innovation excels by its performance, universality and simplicity of usage. Now it has been successfully implemented to production in Ukraine and USA.

STEPANOV Kostyantyn Mykolayovych (24.03.1930 – 19.04.2012) was born in Leningrad. In 1952, he graduated from the DNPh, Maxim Gorky KhSU. After graduation, he started to work at KhIPhT (now NSC KhIPhT), where he carried out his researches at positions of Researcher, Senior Researcher (since 1959 года) and a head of a laboratory (since 1967). Since 1976, K.M. Stepanov headed newly arranged Department of Radiofrequency Heating and Plasma Theory at the Plasma Physics branch of KhIPhT (since 1993 Department of Plasma Theory at the Institute for Plasma Physics of NSC KhIPhT). In 1958, he defended PhD thesis, and in 1965 he defended the thesis for Doctor of Science degree. In 1961, he was given a degree of Senior Researcher, and in 1969, he was given a degree of Professor. In 1992, he was elected as a Corresponding Member of NASU.

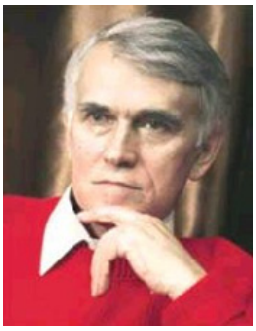
Main works of K.M. Stepanov are related to plasma physics and controlled nuclear fusion. In this area he obtained a set of fundamental results on the kinetic theory of propagation, absorption and mode conversion of the electromagnetic waves in the plasma in the external magnetic field; the theory of the charged particle fluxes and the strong electromagnetic fields interaction with the plasma in the external magnetic field; the theory of plasma stability in the magnetic traps.

He is one of the founders of the Plasma Electrodynamics in the magnetic field. He had proposed new effective methods of the radiofrequency plasma heating, which nowadays have become the basis for experiments on RF heating in the largest toroidal traps (tokamaks and stellarators). These methods are promising for tokamak-reactor.

K.M. Stepanov was an author and a co-author of more than 600 scientific works, including 5 monographs and 10

inventions, which were well-known to scientist worldwide. He had prepared 26 PhD and 14 Doctors of Science, among them D.G. Lominadze, who is an Academician and a Vice President of Georgian AS. More than 40 years, Prof. Stepanov carried out scientific and teaching work at V.N. Karazin KhNU. These activities were awarded by giving him the degree of Honorary Doctor of V.N. Karazin KhNU, the degree of Soros's Professor and by awarding him the sign "Excellent Education Worker of Ukraine".

For many years K.M. Stepanov was a member of the bureau of the United Scientific Council on Problems of Plasma Physics in AS of Ukrainian SSR, member of the bureau of the Plasma Physics Problem Council in AS of Ukrainian SSR, a member of the editorial boards of journals: "Plasma Physics Reports", "Problems of Atomic Science and Technology" Series: "Thermonuclear fusion" and The Journal of Kharkov National University (Physical series "Nuclei, Particles, Fields"), headed Scientific Council on Problems of Plasma Physics and Plasma Electronics in NASU. He was awarded by the Order of the Red Banner of Labour, Diploma of the Presidium of the Supreme Soviet of the Ukrainian SSR and medals, he was given the honorary degree "Honored Worker of Science and Technology of Ukraine" and State Prize in the Area of Science and Technology of Ukraine.



STORIZHKO Volodymyr Yukhymovych was born on October 26, 1935 in the village of Ol'hovatka of Kharkiv region in the family of rural intellectuals. In 1958, he graduated from the DNPh, KhSU. In 1962, he finished postgraduate studies at the department of experimental nuclear physics under the guidance of the eminent nuclear physicist academician Anton Karlovych Walter, and was hired in KhIPhT. Here he created a new direction - study of subbarrier reactions with protons by nuclei of medium atomic weight, which process analysis is based on a statistical model, or on the basis of the model-independent method for the angular correlations of aligned nuclei. This is a rapidly developing area and now it is supported by his students and followers. It has been shown in his works that to obtain the maximum information on the structure of atomic nuclei the measurements of angular correlations should be carried out near the reaction threshold, at which the maximum alignment of cores is achieved and where the data analysis is weakly dependent on the parameters of the optical potential. These studies identified the conditions under which the angular correlations are isotropic or anisotropic. In 1974, V.Yu. Storizhko successfully defended his doctoral thesis, and in 1978 he was awarded the title of professor.

Since 1988, professor V.Yu. Storizhko concentrates on establishing of the Institute of Applied Physics of the NASU, in Sumy city. And from 1991 till now, he is its director. The accelerator, complex physical installations and equipment, which are actively used in various areas of applied physics, are built in this institute. In 1992, V.Yu. Storizhko was elected a corresponding member, and in 1995 - a member of the NASU; he was awarded the title of "Honored Worker of Science and Technology of Ukraine".

V.Yu. Storizhko is an author and co-author of about 300 scientific works and inventions. He has supervised 2 doctors of science and 14 PhDs. He is a member of scientific councils of the NASU, member of the specialized councils of the V.N. Karazin KhNU and NSC KhIPhT.

At the same time professor V.Yu. Storizhko actively manifests itself as a statesman. From 1994 till 1998, he was a deputy of Parliament of Ukraine, member of the Presidium of the Parliament of Ukraine, Chairman of the Committee on Science and Education, Chairman of the State Committee for Science, Technology and Industrial Policy, chairman of Interstate committee for scientific and technological development, member of the bureau of the Department of physics and astronomy and the Division of nuclear physics and power engineering of the NASU.

STRUTINSKY Vilen Mitrofanovych (16.10.1929 – 28.06.1993) was born in Danilova Balka village, Ulyanovsk district Kirovograd region. In 1952, he graduated from M. Gorky KhSU (DNPh). After graduation, V. Strutinsky started to work to I.V. Kurchatov Institute of Atomic Energy (group of nuclear theory), where he worked since 1953 till 1970. In 1959, he defended the PhD thesis, and in 1965 he was given a degree of Doctor of Science. He underwent an internship in Niels Bohr Theoretical Physics Institute, Copenhagen, Denmark (1957-1958). In 1967, V. Strutinsky was invited to Niels Bohr Institute for development of his theory, and he worked there until 1970. After that he returned to Kiev. He was a Head of Nuclear Theory Department at the Institute of Nuclear Research of AS of Ukrainian SSR till 1991. Since 1992 till 1993 he was a Senior Researcher of Nuclear Theory Department of INR NASU.

The first research period of V. Strutinsky was related with development of new concepts of the complex nuclei structure, because of the discovery of its non-spherical shape. Using these concepts he specified the dependences of the alpha decay probabilities, known as Alagi's rules. The next series of studies were devoted to the classical interpretation of the quantum angular momentum, the additional

rules of the quantum angular momentums and correlation between orbital angular momentum of the particle and its motion direction. As a result, the simple expressions for angular distributions of the debris of the rotating nucleus (Halpern-Strutinsky formula), angular distributions of the particles emitted from the rotating compound nucleus (Erikson-Strutinsky formula) and the angular correlation in the processes of mixed type were obtained. V. Strutinsky carried out fundamental work, which was devoted to the quantitative description of the geometric shapes, which the nucleus undergo during its fission. In the following investigations of the nuclear fission theory he showed the equivalence of the liquid drop model of the deformed nuclei and the statistical models which are using the energy density functional. These studies had shown the need of the shell effect accounting in the nuclei deformation. And they became the basis for the method of calculating the net binding energy of a nuclei (the method of the shell corrections), which has been developed in 1965 - 1968's by V. Strutinsky, and which received his name further. V. Strutinsky theory gave a possibility to explain many known features of the nuclear fission process as well as to predict its new properties, which were unexpected from the point of view of the traditional concepts of the Niels Bohr theory. The theoretical conclusions of V. Strutinsky were confirmed completely by the following intensive researches and experiments. For the first time his theory has provided the ability to predict the nuclear masses, and many properties of the fissionable nuclei, in particular, the stability of the superheavy nuclei. The theory has been widely spread and it took place in the principles of nuclear physics.

A significant place in investigations of V. Strutinsky and his colleagues is occupied by the theory of the collective motion in nuclei under the high amplitudes and the finite value of the velocity. They obtained fundamental results, which were important for developing the quantitative theory of such nuclear processes. New theoretical model for the dynamics of the collective processes in heavy nuclei, namely the gas-liquid drop model (GLM) was proposed and developed by them. Such expressions as "the Strutinsky energy theorem", "the Strutinsky shell correction method", "the Strutinsky double-peak fission barrier" widely entered to the world scientific literature on the nuclei theory and nuclear physics.

The phenomenon of the shell structure existence in the strongly deformed nuclei and formation of the intermediate metastable state during the nuclear fission, predicted by V. Strutinsky, were registered as a discovery in the USSR (the State Register of Scientific Discoveries of the USSR № 200, 1977).

A large number of specialists were trained under his supervision. Many of his students were given a degree of PhD and Doctor of Science, became Professors. V.M. Strutinsky was an Alexander von Humboldt Science Prize winner (1991), and he was given the T. Bonner Award for Nuclear Physics of the American Physical Society. He was awarded a medal "For Labor Valor" (1983) and "In memory of the 1500th anniversary of Kiev." He was a Honorary Doctor of Sciences of Copenhagen University since 1979.

TERESHIN Volodymyr Ivanovych (17.01.1938 - 11.07.2010) was born in Donetsk. In 1960, he graduated from the DNPh, Maxim Gorky KhSU, and started to work at KhIPhT (now NSC KhIPhT). There he had started career at position Junior Researcher and finally became a Director of Institute for Plasma Physics in NSC KhIPhT. In 1968, V.I. Tereshin defended PhD thesis, and in 1992 he defended the thesis for Doctor of Science degree. In 2009, he was elected as a Corresponding Member of NASU.

Scientific interests of V.I. Tereshin were concentrated in the field of the experimental plasma physics. He studied the parametric resonance, which takes place in the rippled magnetic field with plasma fluxes, he spent a lot of time developing the complex plasma accelerator, which generates the plasma fluxes with suitable parameters for injection into stellarator magnetic traps; he developed the methods of the particle plasma diagnostics and the multichannel analyzers for measuring the energetic characteristics of the moving plasma (this work was awarded by Silver medal on the Exhibition of Achievements of the National Economy UdSSR and the invention certificate was obtained).

Under supervision of V.I. Tereshin, the constructing and the wide class of researches of quasi-stationary plasma accelerators had been started. As a result of these activities, the plasma fluxes with record parameters were obtained. These fluxes can be used in different areas of plasma physics and plasma technologies. In the framework of the international program on the tokamak-reactor ITER V.I. Tereshin in a close collaboration with German physicists had been involved in studies on the experimental simulation of the processes at the divertor plates in the reactor in the case of the extreme scenarios of operation. Immediately he launched the investigation of the surface modification of the structural materials under the strong plasma fluxes in order to improve their physical and chemical characteristics.

V.I. Tereshin was a Professor of the Department of Physical Technologies at SPhT, V.N. Karazin KhNU, where he was giving lectures on Plasma Dynamics, supervising the diploma studies of students and PhD students. Under his supervision, 6 PhD theses were defended, and he was a scientific consultant in one work for Doctor of Science degree. He published more than 300 scientific papers. Besides that several inventions were developed. In 2007, he was awarded the State prize in the field of Science and Technology.

TOLOK Volodymyr Tarasovych (25.12.1925 – 11.12.2012) was born in Uman city of Cherkasy region. In 1951, he graduated from the DNPh, Maxim Gorky KhSU and started to work at KhIPhT (now NSC KhIPhT). He was starting his scientific activities at the laboratory of accelerator equipment. In 1957, V.T. Tolok defened the PHD thesis. His scientific advisor was Academician K.D. Sinelnikov.

Since 1958, on recommendation of K.D. Sinelnikov V. Tolok started new in that time area of physics, i.e. plasma physics and controlled thermonuclear fusion. These work has just launched at the institute, and he was involved in studying the constant and alternate fields' interaction with plasma and gases. Besides that, he dealt with the developing of the plasma heating methods, and took part in the constructing of the sources of the energetic plasma fluxes. In 1960, on the recommendation of K.D. Sinelnikov and on the direct instructions of Academician I.V. Kurchatov he was entrusted to head the new scientific program related with developing of principles of the controlled thermonuclear fusion reactor.

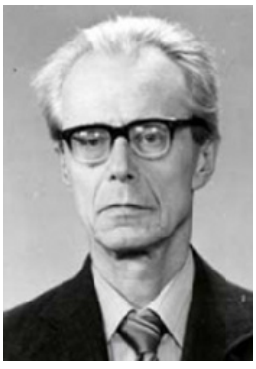
Since 1966, he was entrusted to head the whole stellarator program at KhIPhT. As a result of activities carried out for many years at the institute, a set of stellarators were constructed starting from Sirius, Uragan-1 and then Uragan-2 and much later Uragan-2M. The milestone in the upgrowth of the Plasma branch at KhIPhT was constructing the torsatron Saturn for the first time in the world in 1970. The new concept of the magnetic system of the device was proposed by a physicist of the Institute V.F. Aleksin. In 1982, the largest at that time torsatron Uragan-3 was constructed. Its modification Uragan-3M was launched with the magnetic system placed in the vacuum vessel.

In the early 1970s, the study of the non-equilibrium plasma chemistry with high energies was started on the V.T. Tolok's initiative. As a result the new technology of the vacuum-plasma coatings was developed (condensation with ion bombardment). It gave an opportunity to increase the endurance of the cutting tools up to several times, and to rise the reliability and service life of the mechanism docking assembly with friction. This new technology got a wide spread in our country as well as abroad (in 1982 the license on this technology was sold to the American company Multyarcs for the first time in the history of KhIPhT and of Ministry of Medium Machine-Building Industry).

V.T. Tolok started to work at the Kharkiv university since the end of 1966, when he had headed the Department of Plasma Physics on the invitation of G.A. Milyutin - the dean of the SPhT. The Department was arranged by K.D. Sinelnikov. V.T.Tolok headed the Department till the beginning of 1971. Since that time he maintained a close relations with the Department and the SPhT constantly. In 1988, V.T. Tolok with the help of the university administration organized the vacuum-plasma laboratory at the university.

In last his years, V.Tolok paid much attention to the popularization of the science and technology achievements. He published a lot in different editions including the university journal Universitates, which is published by the V.N. Karazin KhNU Association of Alumni, Tutors and Friends. At the apogee of these activities the book 'Physics and Kharkiv' was published in 2009.

V.T. Tolok was awarded by the Order of the October Revolution, the Order of the Patriotic War of the 2nd class, the Order of the Badge of Honour, the Order For Courage of the 3rd grade and numerous medals. On 2nd of November in 2012 V.T. Tolok was awarded the medal and the diploma of the Honored Doctor of the V.N. Karazin KhNU.



VOLKOV Dmitry Vasylyovych (03.07.1925 – 05.01.1996) was an outstanding physicist theoretician, academician of the NASU, a major specialist in the field of elementary particles, quantum electrodynamics, nuclear physics, quantum field theory, condensed matter physics.

He was born in Leningrad. In 1943 he was drafted into the Soviet Army. In 1947, he joined the school of physics of Leningrad University. In 1951, he moved to study in Kharkiv, where he graduated from the DNPh, KhSU in 1952. After completing his graduate studies at the University under the supervision of academician O.I. Akhiezer and his defense of PhD in scalar quantum electrodynamics in 1956, D.V. Volkov was assigned to work for the theoretical department of KhIPhT headed by O.I. Akhiezer. There for nearly forty years, he has made a career from researcher to the head of the laboratory, to the academician. In 1959, he proposed a new scheme of field quantization - the so-called parastatistics or statistics of Green-Volkov, which was the important instrumental in the development of concepts of the quark structure of hadrons. The discovery of a new type of symmetry – supersymmetry (in 1972, co-authored by V.P. Akulov) and built upon it the supergravity theory, which generalized Einstein's theory of gravitation (in 1973, co-authored by V.A. Soroka) brought V.D. Volkov the international fame. In 1968, he defended his doctoral thesis. In 1976, he was elected a corresponding member of the AS of Ukrainian SSR, was awarded the Order of the Red Banner of Labor. In 1977, he received the title of Professor. In 1988, he was elected an Academician of NASU. He was awarded the title of "Honored Worker of Science and Technology of Ukraine". In 1997 (posthumously), he was awarded the International

W. Thirring Prize for the discovery of supersymmetry and supergravity, and in 2010 (posthumously), he was awarded State Prize of Ukraine in Science and Technology.

VOYEVODIN Victor Mykolayovych was born in Kharkiv on 24th of April in 1946. In 1970, he graduated from Maxim Gorky Kharkiv State University (klhSU) (School of Physics and Technology (SPhT)). After its graduation, V.M. Voyevodin started to work at the KhIPhT (now NSC KhIPhT). He started to work there as an intern-researcher, and nowadays he is a Director of Institute for Solid-State Physics, Materials Science and Technologies. In 1984 he defended the PhD thesis, and in 1995 - the doctoral degree. In 2012, he has been elected a Corresponding Member of the NASU.

V.M. Voyevodin is a known specialist in the experimental radiation material science and nuclear energy. The main area of his scientific interests is the material science of fuel and constructional materials of nuclear reactors (exploited ones and promising innovative concepts). He has carried out the cycle of researches on the features of the structure and composition of the zirconium alloys under irradiation in nuclear reactors. He is one of the founders of the environmentally-friendly method for simulating the reactor damage using particle accelerators.

He combines research and teaching activities successfully. During many years he gives a course of lectures on the "Radiation Material Science" at SPhT of the V.N. Karazin KhNU. Besides that he is a head of the branch of the department of Reactor Materials and Physical Technologies at NSC KhIPhT. Three PhD thesis were prepared and defended under his supervision. He is the author and co-author of more than 300 publications, reviews and patents including 3 monographs.

He was the winner of the Prizes of the Committee on the Peaceful Uses of Atomic Energy of the USSR for the best work on the physics of radiation damage in 1985 and in 1989. He is a Honorary Professor of NSC KhIPhT since 2003, and K.D. Sinelnikov prize of the NASU winner in 2010.

ZALYUBOVSKY Illya Ivanovych (15.06.1929 – 21.02.2013) was born in Butenki village, Kobelyatsky district, Poltava region. In 1954, he graduated from M. Gorky KhSU (DNPh). All his further life was closely associated with the University. In 1958, he defended the PhD thesis. In 1963—1965, he was a head of the group of scientists, who carried out a scientific work and trained highly qualified specialists in the Atomic Center of the United Arab Republic of Egypt. In 1966, he was given a degree of Doctor of Science, he was a Professor since 1967. Since 1965, he was a head of the Department of Experimental Nuclear Physics, and since 1967, he was a Vice-President on Scientific Activities at the University. In 1968, he took part in the scientific research and gave a course of lectures in Manchester (former Rutherford) laboratory in England. He was a Corresponding Member of NASU since 1988. From the beginning of his scientific activities, I. Zalyubovsky carried out the investigations on the accelerated particle interaction processes with atomic nuclei and their structure.

For the first time in our country the problem of atomic nuclei static electromagnetic moments measuring was formulated and solved by I. Zalyubovsky together with Academician A.K. Walter using the method of the perturbed angular correlations. This work has been received further development on modern accelerators. In 1983, the series of these investigations was awarded the K.D. Sinelnikov Prize by Ukraine's Academy of Sciences.

The effect of the radio-frequency emission of the wide air showers of the cosmic rays was discovered under the leadership of I. Zalyubovsky, and then a detailed experimental study of its formation mechanism was carried out. Obtained experimental results are interesting for the theory development and understanding the radio emission, as well as for the development of new methods of the detecting the cosmic rays with ultrahigh energies. In 1971, the series of these works was awarded the State Prize of Ukraine. Under the leadership of I. Zalyubovsky, a new areas of study were opened and successfully developed. They were the acoustic phenomena in the interaction process of radiation with matter; a set of the nuclear-physical methods of the solid state physics. The series of works on complex research of the atomic nuclei and the processes of interaction of particles, nuclei and radiation with various energies with matter was awarded by the Yaroslav Mudry Prize in 1994. I. Zalyubovsky contributed significantly to the organization and development of School of Physics and Technology (SPhT) in V.N. Karazin KhNU. He was the first dean of SPhT. He was the author and co-author of more than 400 publications, including 5 monographs, "Nuclear Physics" and "Nuclear Spectroscopy" textbooks for university students. The fourth edition of the "Nuclear Physics" textbook was awarded the State Prize of Ukraine in 1993.

I. Zalyubovsky organized the scientific school, he trained the hundreds highly skilled professionals. Among his students there are 8 Doctors of Science and 40 PhDs.

He gave much energy to the organizational and social work. He was a Chairman of the Science Expert Council of

Ministry of Education and Science of Ukraine, a member of the Council of the State Prize of Ukraine in Science and Technology, a member of the Scientific Council of NASU on nuclear physics and high energy physics. For many years, he presented the government of Ukraine in the Joint Institute of Nuclear Research (Dubna, Russia).

I. Zalyubovsky was a "Honored Worker of Science and Technology of Ukraine". He was awarded two Orders of the Red Banner of Labor (1976, 1986), the Orders of Merit of III, II and I grades (1998, 2004, 2008.). In 2007 he was awarded by title of “Honorary Citizen of Kharkov”.

ZELENSKY Viktor Fedotovych was born on February 18, 1929 in the village of Globunivka of Novopokrovsky district of Saratov region. In 1951, he graduated from the DNPh, KhSU. Since 1951, all of V. Zelensky's life is connected with KhIPhT (now NSC KhIPhT). He was a graduate student and part-time laboratory technician, junior researcher, senior researcher, head of the laboratory of VM-2, MR department head, head of section, deputy director. Since 1980 till 1997 he was a director of the KhIPhT and then a director of NSC KhIPhT.

He defended PhD thesis in physics and mathematics in 1956, and doctoral thesis in technical sciences - in 1966. Topics of his work were related to the problems of the Soviet nuclear program. In 1978, V.F. Zelensky was elected a corresponding member of the AS of the Ukrainian SSR. In the same year, he was awarded the title "Honored Worker of Science and Technology of Ukraine". In 1988, he was elected an academician of the NASU.

He is a famous scientist, his main research interests lie in the fields of radiation damage physics, nuclear technology and radiative study of materials. he was an initiator of research in the new scientific field devoted to the development of rapid diagnostic methods of radiation damages of the materials of nuclear and fusion reactors by means of irradiation of these materials at the accelerators of multi-charged ions and electrons. In 1971, V.F. Zelensky has initiated a research program of the USSR on radiation physics and radiation material science and supervised the implementation of this program over 20 years. He is the author of the world's first heavy ion material testing accelerator (1973), which operates up to this day. Together with I.M. Neklyudov he made a decisive contribution to the scientific basis of the method of forecasting the reactor damages of steels and alloys. In co-authoring with O.S. Bakai he developed a new theory of the creation of steel and alloys, which are stable under radiation exposure. Under his leadership, the work was carried out in the area of nuclear materials, i.e. the study of the nature of instability of uranium fuel in industrial and power reactors and the search for ways to eliminate this instability, the creation of steel resistant to swelling, development of heat-resistant magnesium-beryllium "pseudoalloys", creation of high temperature reactor heat-generating element with a gas-coolant and other studies.

V.F. Zelensky is an author of several monographs and more than 400 original research papers and 60 inventions. For many years he was teaching at KhSU. Among his students there are about 30 PhDs and doctors of science. He is a laureate of the State Prize of the USSR (1972), the State Prize of Ukraine (2007). He was awarded the Orders of the USSR, Czechoslovakia and Ukraine.

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NANOSTRUCTURAL MATERIALS IN THE NUCLEAR ENGINEERING

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A brief review of research findings, pilot projects and application of nanomaterials in the nuclear power industry and engineering is presented. Examined are the prospects of creation of nanostructural materials and coatings for building blocks in NPPs and future fission reactors with a view to improving mechanical properties, increasing radiation resistance. Also, investigated are the main problems arising from development of methods for nuclear fuel modification, development of dispersion-hardened steels.
KEY WORDS: nanomaterials, nanotechnologies, nuclear fuel cycle, radiation resistance and corrosion resistance

НАНОСТРУКТУРНЫЕ МАТЕРИАЛЫ В ЯДЕРНОЙ ЭНЕРГЕТИКЕ

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Представлен краткий обзор результатов исследований наноматериалов для ядерной энергетики. Рассмотрены перспективы применения наноматериалов в ядерной энергетике, связанные с созданием наноструктурных материалов и покрытий конструкционных элементов АЭС и будущих ТЯР для увеличения показателей твердости и прочности, повышения радиационной стойкости. Также рассмотрены основные проблемы, возникающие при разработке методов модифицирования ядерного топлива, разработке дисперсно-упрочненных сталей.
КЛЮЧЕВЫЕ СЛОВА: наноматериалы, нанотехнология, ядерный топливный цикл, радиационная и коррозионная стойкость

НАНОСТРУКТУРНІ МАТЕРІАЛИ В ЯДЕРНОЇ ЕНЕРГЕТИЦІ

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Представлено короткий огляд результатів досліджень наноматеріалів для ядерний енергетиці. Розглянуто перспективи використовування наноматеріалів в ядерний енергетиці, які пов'язано з створенням наноструктурних матеріалів і покриттів конструкційних елементів АЕС і наступних ТЯР для збільшення показників твердості та міцності, підвищення та радіаційної стійкості. Також розглянуто основні проблеми які виникають при розробці методів модифікування ядерного палива, розробці дисперсно-зміцнених оксидами сталей.
КЛЮЧОВІ СЛОВА: наноматеріали, нанотехнології, ядерний паливний цикл, радіаційна і корозійна стійкість

Nuclear power is a major source of electric and heat energy in Ukraine. In Ukraine, many nuclear fuel cycle (NFC) elements are already available, and for their further successful operation and development, it is necessary to carry out intensive fundamental and applied research [1, 2]. In nuclear power engineering, the issue of upgrading fuel and constructional materials for the reactor core is of critical importance. The fuel materials include a wide range of uranium and transuranium elements and their compounds. The nuclear reactor constructional materials include austenic, ferritic, ferritic-martensitic and other steels, graphite and carbon materials, zirconium alloys and various ceramic materials.

Therefore, one of the tasks is to develop basic and applied research in the field of radiation materials science and radiation technologies, creation of new fuel and constructional/engineering/structural materials, as well as new methods for analysis and control of materials. Over the last decades nanotechnologies have been used practically in all areas of advanced technologies, and in fact have turned into an interdisciplinary field of science and engineering. In the nuclear sector, nanotechnologies had been used even before the word 'nano' became popular with researchers because newly created heat and structural materials were largely based on qualitative changes in materials properties which occurred when going down to the nanometric size range [3-5].

The purpose of this paper is to present a summary of outcomes of the last research and developments in the area of application of construction and functional nanostructural materials in the nuclear power industry and engineering.

STATUS OF NANOMATERIALS IN THE NUCLEAR POWER INDUSTRY

Nanomaterials in nuclear power engineering

Among the top priorities in R&D support for creation of NFC constructional materials one can note research works aimed to ensure design and beyond-design (30-60 years) operational life of nuclear units, as well as development of improved constructional/engineering/structural materials for thermal neutron reactors, increase of the depth of nuclear fuel burnup. The areas of application of nanotechnologies in the nuclear power industry are rather diverse and cover practically the whole range of problems relating to the nuclear fuel cycle and created fusion fuel cycle [6-33]:

- Creation of a new high-density nuclear fuel with nano-sized additives, fuel compositions for fuel assemblies of the NPP reactor core (active zone of nuclear reactors). Creation of a new class of mixed uranium-plutonium mixed oxide (MOX) fuel. Development of the torium-uranium cycle [7].
- Creation of nano-disperse construction and functional materials (zirconium alloys for nuclear fuel elements, oxide dispersed strengthened (ODS) ferritic-martensitic steels or nano-dispersed ODS steels.
- Research and development of materials for quick neutron reactors and future Generation IV reactors. Research of irradiation-induced microstructure. Microstructure grounds for a possibility to extend operational life of reactor elements: vessel excluding swelling.
- Development and production of fast-quenched solder alloys for high-temperature flux-free soldering of zirconium alloys, corrosion-resistant steels, transition joints of steel-zirconium and steel-titanium, and other dissimilar materials providing a preset level of radiation and corrosion resistance of soldered joints.
- Creation of nano-membranes and nano-filters for spent nuclear fuel (SNF) and radioactive waste (RAW) conversion technologies, ceramic materials for afterburning of radiolytic hydrogen.
- Development of metrological assurance for application of constructional and functional units based on nanomaterials for nuclear facilities.
- Multi-scale simulation of nanostructures, materials and processes.
- Nanogages and nanosensors for NPP management and control systems.
- Research and development of materials for future nuclear fusion reactors. Nanostructural materials for the ITER blanket and first wall. Nanostructural low- and high-temperature superconductors for ITER magnets.

In the process of solution of the above-listed tasks, experimental-industrial technologies are developed to obtain functional materials and products with application of nanotechnologies and nanomaterials for nuclear, thermonuclear, hydrogen and conventional fuel power production, as well as pharmaceutical drugs. Let us look at some of the results obtained in the course of research and development of nanostructural materials in the nuclear power industry.

Nuclear fuel with nanometric additives

The Ukrainian energy strategy stipulates gradual introduction of new MOX fuel nuclear power technologies with nuclear fuel cycle closure. Further development of the nuclear power industry requires inclusion of fast neutron reactors into the NPP capacity structure. Out of all types of such reactors only sodium loop reactors (BN) are commercially manufactured. The BN-600 reactor, which has been working at the Beloyarsk NPP (Russia) since 1980, may serve as an example of such reactors. In 2012, there is a plan to launch the 4-th power generating unit of the Beloyarsk NPP with a BN-800 reactor, set up MOX fuel production and implement a closed fuel cycle based on this reactor. One of the pre-requisites for higher NPP efficiency is an increase of the depth of nuclear fuel burnup. To ensure a deep fuel burnup, there is a need to create nuclear fuel macrocrystalline structures with controlled porosity. Nuclear fuel macrocrystalline structures confine gaseous and volatile fission products, prevent transportation of fission fragments on grain boundaries towards the fuel element jacket, which results in considerably lower level of damageability of the fuel element jacket. To obtain a macrocrystalline state, when the fuel ceramics is being pressed from UO_2, (U, Pu)O_2, (U, Pu)N) it is being added ultradispersed powder UO_2 with nano-crystals of a size of ~40 nm. As a result, the fuel ceramics sintering temperature goes down to ~ 200 degrees, ceramics density increases, and the grain size increases up to 35÷40 μm without degradation of other characteristics. Activation of the sintering process due to nano-additives may become one of the trends in creation of technologies for new types of uranium-plutonium oxides and nitrides for the nuclear fuel of the fast reactors nuclear power industry (Fig. 1).

These trends are as follows:

- modification of nuclear fuel;
- creation of complex carbonitride doped with nanodiamond UZrCN;
- fine tuning and modernization of the pilot plant project for production of MOX fuel for BN-800;
- development of a model of solid structures formation on the solid-liquid boundary (solid-melt interface) of reactor materials;
- investigation of interaction of prototypes of melted materials in the reactor core with the reactor vessel;
- study of the mechanism of explosion of liquid metal drops;
- large-scale simulation of reactor core (RC) materials.

Paradoxically, the process of application of ultradisperse additives in fuel ceramics manufacturing lies in utilization of nano-additives to produce a structure which is close to monocrystalline (syngle-crystalline).

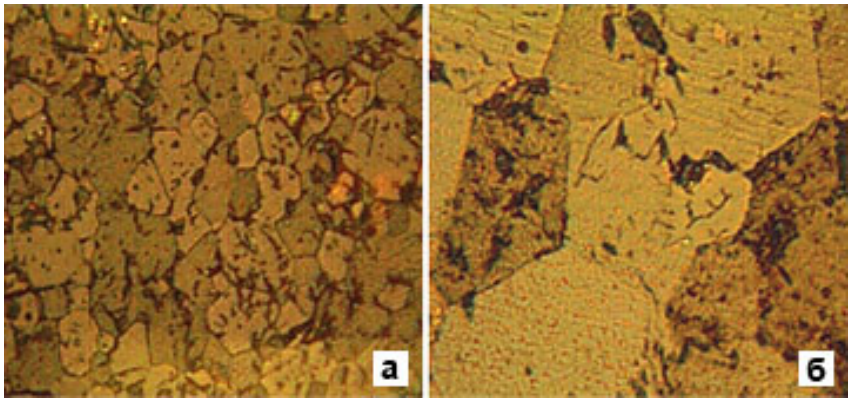


Fig. 1. Microstructure of nuclear fuel.
a - standard microstructure, b - microstructure obtained with application of nano-additives

Oxide dispersion strengthened ferritic-martensitic steels. Nano-dispersed ODS steels

Application of nanomaterials and nanostructures becomes more wide and efficient, particularly in development of ODS steels. ODS steels are various chromiferous steels of the ferritic-martensitic class, strengthened with nano-sized oxide particles. The chromium content in steels is in the range of 9÷18 wt. %, while content of other alloying elements (Al, W, Mo, Nb, Ti, Zr etc.) may be at a level of a few percents and less. The main strengthening oxide particle with a size of <10 nm is Y_2O_3 (down at 0.5 wt. %). Along with yttrium oxides, also used are oxides of aluminum, titanium and other metals. Increase in performance efficiency and length of operational life of prospective fast neutrons reactors requires first of all increase in burnup fraction up to 18-20% without degradation in performance of heat-carrying medium. Solution of these problems is inseparable from development of radiation resistant constructional/engineering/structural materials. These materials are to be exploited in fast neutron reactor cores (E > 0.1 MeV) in fluencies up to $2 \cdot 10^{16}$ n/(sm^{2}s) with damaging doses 160…180 dpa at temperatures 370...710 °C. Radiation resistance of constructional materials in fast neutrons reactors is defined by swelling, creep, high- and low-temperature embrittlement, as well as stability of the material structure properties in the neutron irradiation field. Similar problems arise in creation of radiation resistant constructional/engineering/structural materials for the first wall and blanket of the ITER (International Thermonuclear Experimental Reactor). Solution of this problem requires creation of a new class of radiation resistant metallic materials strengthened with nanoparticles of metal oxides. These materials should have the following properties [14-19]:

- low creep at temperatures up to 970 K and dimensional stability, long operational life ~9 years;
- high radiation resistance to neutron irradiation with irradiation doses ~250 dpa;
- combination of radiation resistance and increased heat resistance;
- high mechanical properties: high rupture resistance of >300 MPa at 970 K, creep rupture strength of >120 Mpa at 10^4 hrs at 970 K, percentage of elongation of >1%;
- high corrosion resistance compared to heat-carrying medium under an elevated temperature and chemical compatibility with the fuel;
- high chemical compatibility when in contact with the fuel and sodium flow.

One of the ways to solve this problem is to create and use a new class of ferritic-martensitic radiation resistant steels strengthened with nano-sized oxide particles (ODS steels).

One should note that this task is an element of the global development of constructional/engineering/structural materials strengthened with high-disperse non-metallic particles (nanoparticles) and designed for reactor core elements in prospective nuclear reactors. This line of research is being intensively developed in countries which have developed nuclear power ITER structures (Russia, USA, Japan, China, France, Ukraine) [20-29]. Radiation swelling is the main criterion for selection of prospective nuclear reactor constructional/engineering/structural materials. Dose dependencies of swelling for materials of austenite and ferritic-martensitic classes are considerably different. Swelling and creep strains of EP-450 cladding from high burn-up fuel assemblies in BOR-60 fre presented on Fig. 2. Currently available data to ~163 dpa imply that the void swelling rate of EP-450 is very low. It is reasonable to assume that the swelling rate will always be low, especially at dose levels not yet reached in reactors. Ion bombardment can be used to explore swelling at very high dpa levels. A dpa rate of 10^{-2} dpa/sec is available on accelerator.

At present there is a great variety of ODS steel grades and types grouped according to their producer countries:
Belgium: DT2906 (Fe - 13Cr – 1.5Mo – 2.9Ti – 0.6 O_2); DT2203Y05 (Fe – 13Cr – 1.5Mo – 2.2Ti – 0.3O – 0.5 Y_2O_3
USA: MA957 (Fe – 14Cr – 0.9Ti – 0.3Mo – 0.25Y2O3); 12CrY1 (Fe – 12.4Cr – 0.25Y_2O_3); 12CrYWTi (Fe – 12.3Cr – 3W – 0.39Ti – 0.25 Y_2O_3)
Europe: ODS EUROFER (Fe – 9Cr – 1.1W – 0.2V – 0.14Ta – 0.3 (0.5) Y_2O_3)

China: K7 (Fe – 13Cr – 1.1Ti – 0.2Mo – 2W – 0.39Y_2O_3)
Japan: Fe – 9Cr – 0.12C – 2W – 0.20Ti – 0.35Y_2O_3
Fe – 12Cr – 0.3C – 2W – 0.3Ti – 0.23Y_2O_3

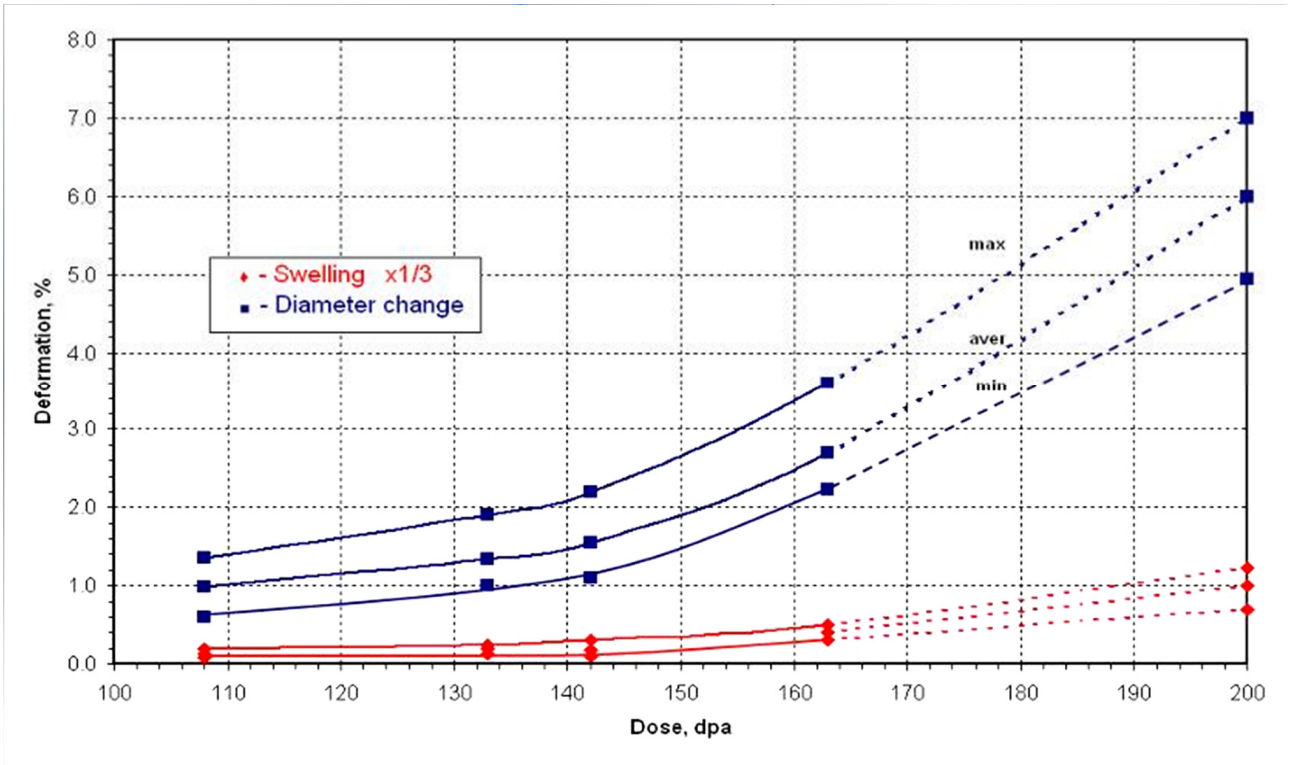


Fig. 2. Dose dependencies of for different swelling. Swelling and creep strains of EP-450 cladding from high burn-up fuel assemblies in BOR-60. Povstyanko et al., 2011 [33]

On this background, stand out chrome-rich (up to 22%) steels with Al additives (up to 4.5 %). 9Cr-ODS steels developed for sodium-cooled fast neutron reactor shells turned out to be unpromising for super critical water cooled fast reactors (SCWFR) and liquid bithmuth energetic fast reactors (LBEFR) due to high corrosion levels.

Table.

OD Steels of Russia			
Steel	Y_2O_3 Content (wt. %)	Ti Content (wt. %)	$MgAl_2O_4$ Content (wt. %)
EP450	0.5	-	-
EP450	0.25	0.3	-
EP450	-	-	1
F1 (18%Cr)	0.25	0.3	-
EK181	1	1	-
EK181	0.25	0.3	-
C+S68	0.25	0.3	-
AISI 316 (waterdispersed)	0.25	0.3	-

The structure of ODS steel is characterized by precipitation of oxide phase particles of various sizes, composition and distribution density against the matrix background (Fig. 4).

Presence of nano-oxide particles substantially improves mechanical properties, e.g. significantly changes thermal creep parameters (Fig. 4). The main results of earlier studies of oxide dispersion strengthened ferritic steel [27-29] and

developed powder ferritic steels (based on Cr13 steel for the whole class of ferritic stainless steels) [30] after strengthening them with high-dispersion oxides drive us to the following conclusion: under all irradiation conditions (in a heavy-iron accelerator, in VVR-M and BN-600 reactors) embrittlement of material is not observed. In fluencies of up to $2.6 \cdot 10^{23}$ n/sm^2 swelling of material makes 0.25%, residual plasticity is 3…4%.

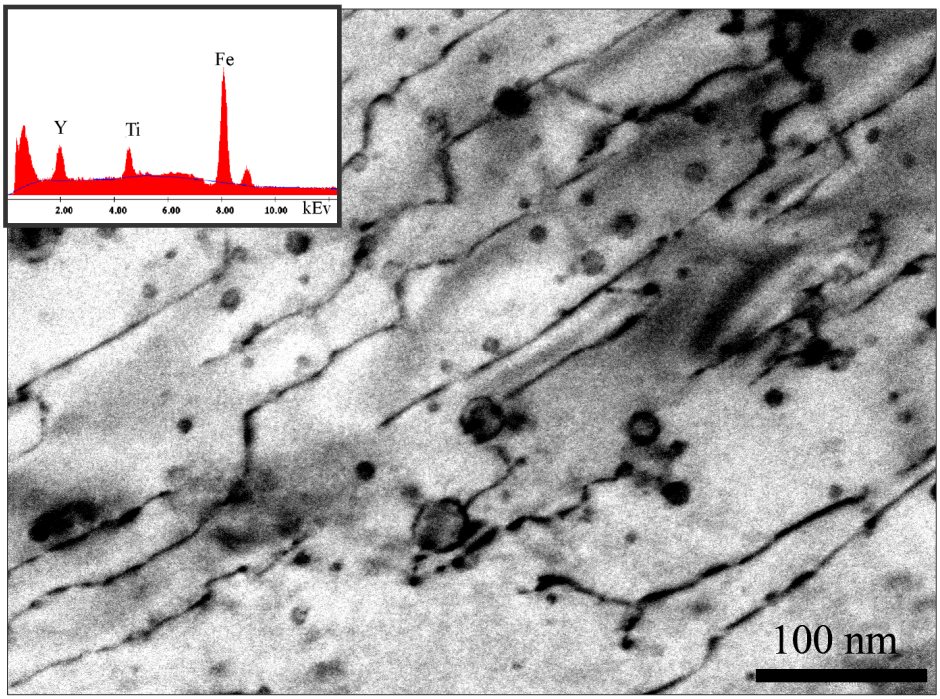


Fig. 3. Nano-oxides in steel EP450 ODS

Corrosion resistance of dispersion strengthened steels in liquid lithium, lithium-lead eutectics, cesium and tellurium vapors is equal or somewhat higher than it is for the best industrial reactor steels. The steel has a sufficient heat resistance at 970 K, high radiation and corrosion resistance in liquid metal environments and fission products. In spite of the above named facts, powder technology does not ensure sufficient homogeneity of products. Over the last years, Russian researchers have developed a number of ODS ferritic-martensitic steels for fast neutron nuclear reactors, including those based on steel EP450 (Fe-13Cr-2Mo-Nb-V-B-O, 12C) which is used as operational material of BN-600 reactor fuel assembly [14, 33].

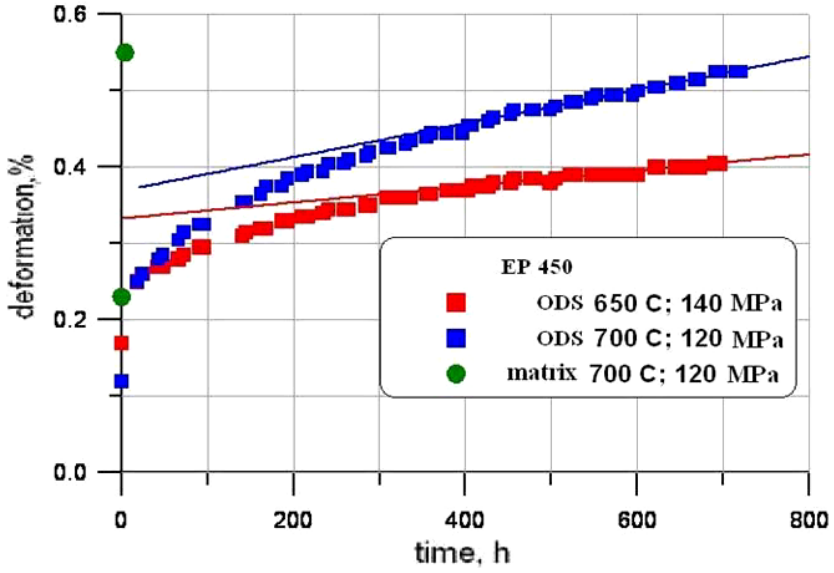


Fig. 4. Thermal creep of EP450 (matrix) and EP450 ODS steels.

Fig. 5 shows that in transition from scale 50 nm to scale 5 nm the particles structure displays an order with a hexagonal or octaedric symmetry (Fig. 6).

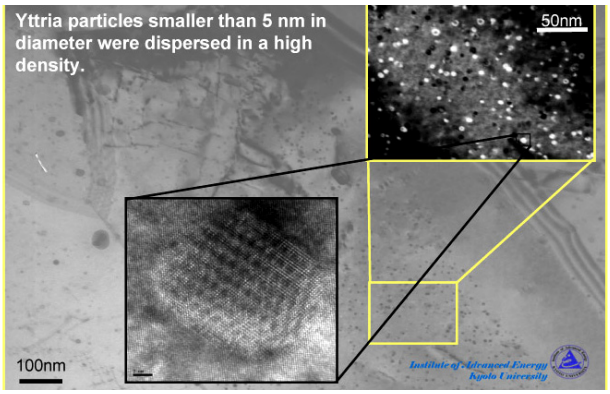


Fig. 5. Nanoscale oxide dispersion: Y_2O_3 particles have the size of less than 5 nm in diameter and are disperse distributed with high density (bottom left corner). (Data according to Kyoto University)

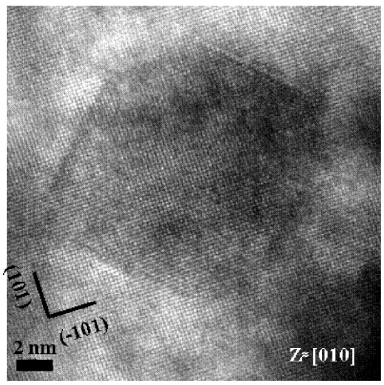


Fig. 6. Structure of precipitates in SOC steels

The best creep resistance characteristics (Fig. 7) are obtained in formation of the maximum amount of evenly distributed nanoclusters with the size of 1-2 nm (Fig. 8).

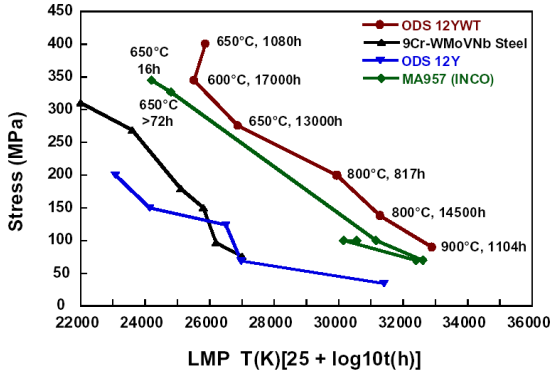


Fig. 7. Creep resistance characteristics of ODS steels

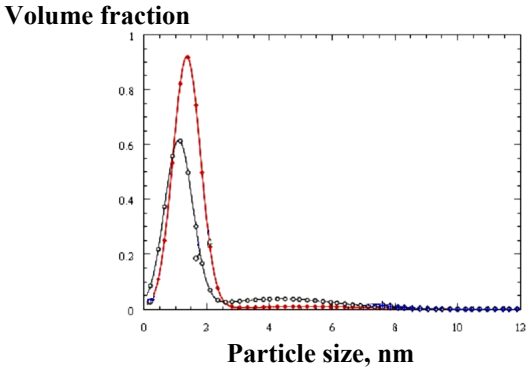


Fig. 8. Distribution of nanoparticles in the strongest steels (Fig. 5).

In the process of additional alloying with zirconium, dispersion of oxide yttrium particles shifts towards smaller sizes, close to optimal (Fig. 9). High density of particles enriched in Ti, Y and O (Fig. 10) is observed. The mean size and concentration of oxide particles in initial and annealed samples of 12YW and 12YWT ODS steels (alloyed with titanium) are also close to values of 2-3 nm at a high mean concentration.

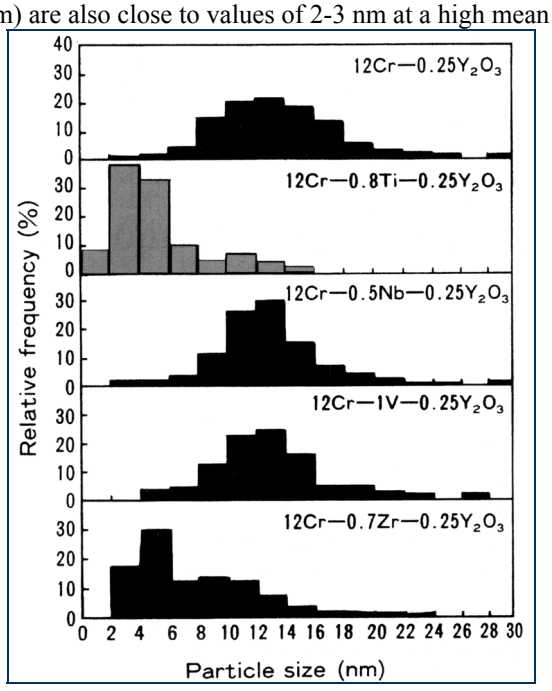


Fig. 9. Size distribution of Y_2O_3 particles in ODS ferritic steel alloyed with Ti, Nb, V and Zr.

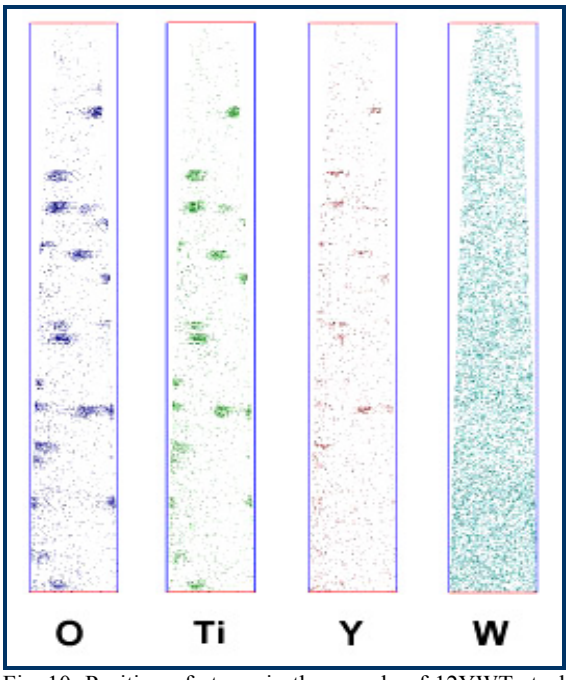
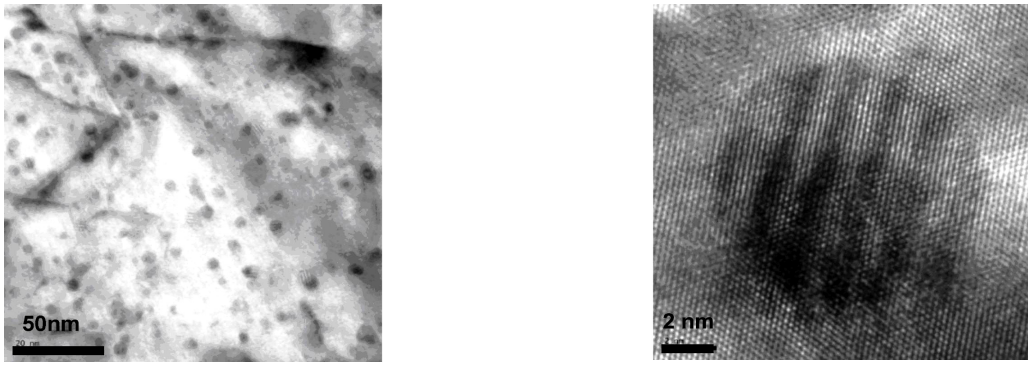


Fig. 10. Position of atoms in the sample of 12YWT steel annealed at 1300°C.

Besides, MA K3-ODS steel contains mostly $Y_4Al_2O_9$ (YAM) particles with a monocline structure (Fig. 11a). Fig. 11b shows another type of ordered oxide structure at a scale of 2 nm.



a b

Fig. 11. Disperse oxide particles in SOC-1 steel without irradiation Z=[111]
a - general view of the microstructure, b - nanostructure of ordered oxide particle

ODS STEELS: IRRADIATION

Radiation swelling of ODS steels of different compositions was intensely investigated in neutron irradiation, as well as in one-beam, two-beam (metal, gas) and three-beam irradiation. When analyzing irradiation results, various models of oxide nanoparticle formation mechanism are used.

Formation of nanoparticles is done in three stages:

1) Fragmentation of moving Y_2O_3 particles at the early stages of globe mill processing.
2) Clasterization and solid-state amorphization of Y_2O_3 fragments mixed with matrix components at later stages of globe mill processing.
3) Clystallization of amorphous agglomerates of a size less than 2 nm to form oxide nanoparticles with a nuclear shell structure at the steel consolidation stage.

Nanoclasters of a size of less than 2 nm remain amorphous (disordered) or have a crystal structure similar to the matrix. These nanoclusters play a critical role in ODS steel radiation resistance.

The irradiation results given below (Fig. 12) show that a substantial change in the steel structure takes place with doses of 65 dpa and at T=700 C.

On the other hand, an important element which characterizes irradiated ODS steels is formation of voids in nanoclusters. Electron microscope investigations allowed to study the crystal structure and density of oxide particles in the ODS ferritic steel, investigate the density and distribution of radiation-induced voids in original steel Fe-14Cr (without oxide strengthening) and in ODS steel Fe-16Cr-4Al-2W-0.3Ti-0.3Y_2O_3. Partial inputs of the crystal matrix and oxide nanoparticles nucleus/shell structure have been defined.

Preliminary results have shown that the swelling process slows down due to increase of oxide particles density in ODS steels. Complex oxides ensure stability of the structure after ion irradiation of up to 60 dpa at 650 °C. Given below is an example of an irradiated area in SOCP-1 steel, 300 °C, 60 dpa. An evident contrast of damage caused by ion irradiation as well as dense dislocations in irradiated and non-irradiated areas are observed. Synergy effect of He and H was clearly demonstrated in triple ion beam (Fe3+ He+ H+) irradiation. Average swelling in F82H steel was considerably accelerated under the influence of triple ion beam irradiation. To create more sophisticated irradiated conditions, researchers of the NSC KIPT (Kharkiv, Ukraine) apply irradiation in a triple ion beam mode on the basis of the ESUVI accelerator with Cr, Cr+He, Cr+H, Cr+He+H ions.

The study of irradiated K3-ODS steels shows that: there are voids formed in nanoclusters; a homogeneous distribution of voids filled with helium in the matrix of K3-ODS steel similar to high-density disperse nanoclusters is observed; nanoclusters enhance heterogeneous bubble nucleation near the clusters which results in retardation of transformation of bubbles into pores.

Analysis of chemical properties of nanoclusters in ODS steels is an important issue. Experiments on homogeneous saturation of ODS materials with He atoms have been conducted at different temperatures on the RRC KI cyclotron. Fast helium ions stop in targets forming profiles of radiation-induced damage, degradation and development of which result in homogeneous saturation of ODS materials with helium. Mechanical tests of irradiated and non-irradiated ODS materials have shown presence of helium embrittlement in irradiated ODS steels at T=450°C. Helium bubbles are observed in irradiated ODS materials at C_{He} = 500 appm at 300°C and 450°C.

The structure and composition of oxide/matrix boundaries which depend on the size of $Y_4Al_2O_9$ particle for Super ODS steels are shown. Incoherent particles beecome larger much quicker due to the higher boundary energy leading to changes in the strength of flows which take up pin holes and helium bubbles. A large precipitate (of size > 15 nm) is characterized by an incoherent boundary with the matrix associated with/ the spherical -shaped shell. In The small precipitates (of size < 10 nm) with a semi-coherent boundary associated with/ the facets.

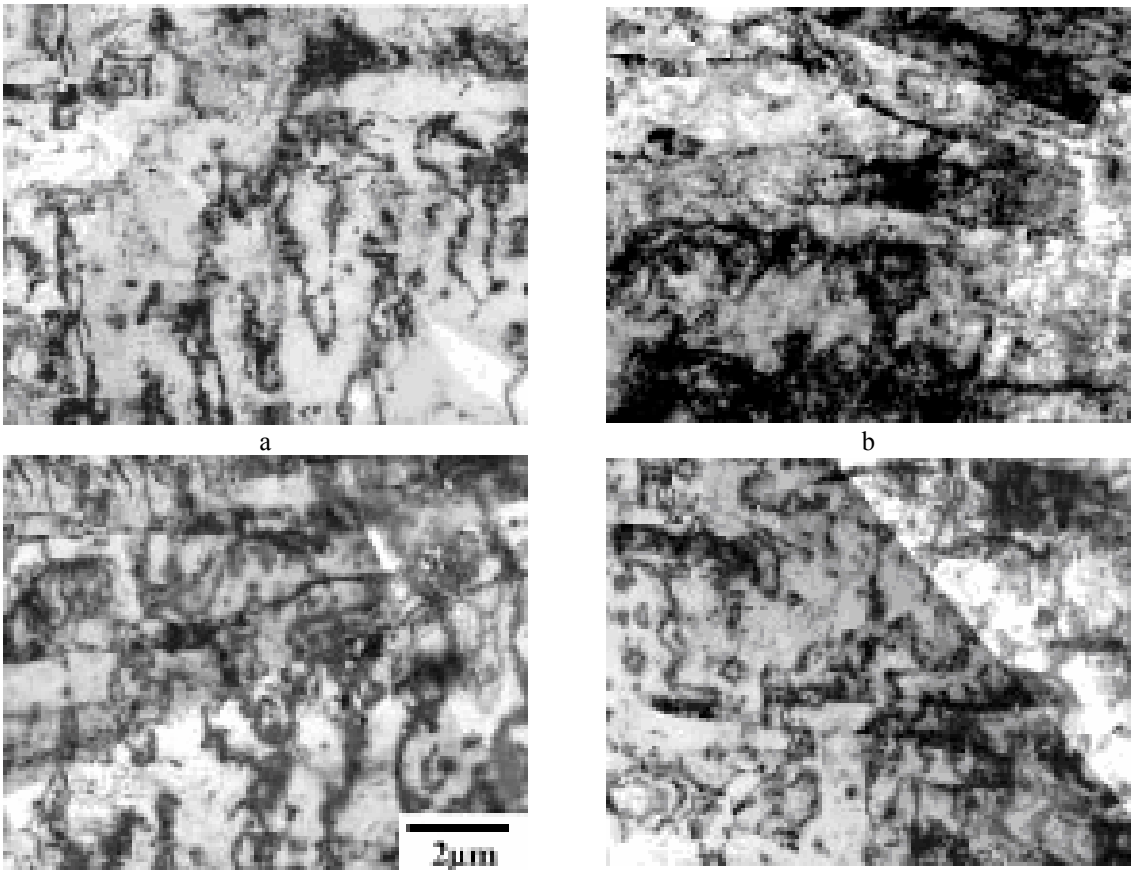


Fig. 12. Structure of MA957 (Fe -14Cr – 1 Ti - 0.3 Mo – 0.25 % Y_2O_3) after irradiation in reactor JOYO
a - without irradiation, b - 65 dpa, 500°C; c - 101 dpa 710°C, d - 101 dpa, 500°C

CONCLUSIONS

One can see from the quoted results that nano-structural materials take on an important role in the nuclear power industry as construction and functional materials which are being used in practically all stages of the nuclear fuel cycle. Extremely important is formation in irradiated nano-structural materials of an ordered nanostructure composed of new phases with a period of a few nanometers. This structure facilitates retention of materials properties in high-dose irradiation. The discovered phenomenon may initiate development of a new trend in the radiation materials science – creation of structural materials "positively" responding to radiation exposure. The prospect of application of nanotechnologies in the nuclear power industry is related to the opportunity of creation of structural and functional elements of nuclear and thermonuclear facilities with the required complex of mechanical, corrosion and radiation resistance properties. Impressive characteristics of ODS steels make it possible to plan application of this kind of materials in the thermonuclear power industry as materials for first wall and blanket. Transition to nanostructural materials will make it possible to create materials with new, game-changing properties for the nuclear power industry and set up create new departures in development of power generating equipment. This is why the crucial task is to accelerate development of projects in the field of nanotechnologies and nanomaterials to ensure economic stability and innovative industrial transformations.

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SURFACE VIBRATIONS IN SEMI-INFINITE CHAINS WITH CONSIDERATION OF LONG-RANGE INTERACTION. SURFACE VIBRATIONS IN CUBIC CRYSTALS

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Vibrations within infinite and semi-infinite monoatomic and diatomic chains in approximation of nearest and next nearest neighbors have been considered. Phonon dispersion relations in an infinite and a semi-infinite cubic crystal have been studied. Calculations have been carried out using a unitary methodology based on solving the difference equations. The following methodology is of broad generality and can be used for studying of both continuous and discrete spectrum in crystal models close to real systems. For cubic crystals volume vibrations zones and localized states representing surface waves have been calculated.
KEY WORDS: phonons, localized state, surface waves, force constants matrix, adsorbed monolayer, long-range interaction.

ПОВЕРХНОСТНЫЕ КОЛЕБАНИЯ В ПОЛУОГРАНИЧЕННЫХ ЦЕПОЧКАХ С УЧЕТОМ ДАЛЬНОДЕЙСТВИЯ И В КУБИЧЕСКИХ КРИСТАЛЛАХ

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Изучены колебания в бесконечных и полуограниченных одно- и двухатомных цепочках в приближении первых и вторых соседей. Исследованы законы дисперсии фононов в кубическом бесконечном и полуограниченном кристалле. Вычисления проведены с помощью единой методики, основанной на решении разностных уравнений. Используемая методика обладает широкой общностью и может быть использована в моделях, близких к реальным системам, для изучения как непрерывного, так и дискретного спектра колебаний кристалла. Для кубических кристаллов найдены зоны объемных колебаний и вычислены локализованные состояния, соответствующие поверхностным волнам.
КЛЮЧЕВЫЕ СЛОВА: фононы, локализованное состояние, поверхностные волны, матрица силовых постоянных, адсорбированный монослой, дальнодействие.

ПОВЕРХНЕВІ КОЛИВАННЯ У НАПІВОБМЕЖЕНИХ ЛАНЦЮЖКАХ ІЗ УРАХУВАННЯМ ДАЛЬНОДІЇ ТА У КУБІЧНИХ КРИСТАЛАХ

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Розглянуто коливання, що виникають у безкінечних та напівбезкінечних одно- і двоатомних ланцюжках із урахуванням взаємодії між першими і другими сусідами, а також при урахуванні дальнодії. Досліджено закони дисперсії фононів у кубічному безкінечному та напівбезкінечному кристалі. Розрахунки було проведено за допомоги єдиної методики, що основана на розв'язанні різницевих рівнянь. Використана методика має широку спільність і може бути використана у моделях, близьких до реальних систем, для вивчення як безперервного, так і дискретного спектру коливань кристала. Для кубічних кристалів знайдено зони об'ємних коливань та вирахувано локалізовані стани, що відповідають поверхневим хвилям.
КЛЮЧОВІ СЛОВА: фонони, локалізований стан, поверхневі хвилі, матриця силових констант, адсорбований моношар, дальнодія.

The main purpose of the article is the use of one-dimensional models, as it is of definite interest, since they can be used to find out the basic properties of more complex physical objects close to reality. And, in addition, to provide a solution in closed form, which can be used to control the interpretation of the approximate and numerical solutions obtained in the expansion of real systems.

ATOMIC VIBRATIONS IN MONOATOMIC AND DIATOMIC CHAINS

A necessity of comparison the results with some reference physical models often rise in a process of studying the excitation spectra of different quasiparticles in real crystalline structures. In this connection the exactly solvable models can be used (for example, one-dimensional atomic or molecular chain) [1]. On one hand, these one-dimensional models are of academic interest, since they may be used for studying of the basic properties of more complex physical objects that are close to real systems. On the other hand, such model systems are also help to carry out the exact solutions used

for comparison and interpretation of the approximate and numerical solutions obtained for real systems.

In this section we consider vibrations which take place in monoatomic and diatomic chains when considering the nearest and the next nearest neighbours interaction. When taking into account an influence of the next nearest neighbours a situation may occur when α_2 constant corresponding the next neighbour interaction is of different sign with α_1 which is for interaction between nearest neighbours. This situation may be applied to so-called metamaterials simulation [2]. Presence of a negative constant α_2 leads to a problem of solutions stability which can be resolved by setting the restriction on the force constants. Consider now possibility of consideration a long-range interaction within such chains. In this connection we use a model representation of force interaction close to the real one. Account of the long-range interaction solves a problem of solution instability which arises when the long-range interaction is not considered.

Acoustic vibrations in a monatomic chain within approximation of first and second neighbours

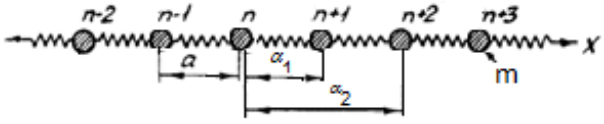

Fig. 1. The monoatomic chain model.

Consider an infinite one dimensional monatomic chain which consists of atoms connected with each other by means of force elastic interaction (Fig. 1). Consider a to be the interatomic distance, α_1 is a force constant corresponding for nearest neighbour interaction and α_2 is for the next nearest one.

The motion equation for the displacement of any n-th lattice-point atom within approximation of first and second neighbours is as follows:

$$m\ddot{u}_n = \alpha_1(u_{n-1} + u_{n+1} - 2u_n) + \alpha_2(u_{n-2} + u_{n+2} - 2u_n). \quad (1)$$

The equation (1) is sought in the form of plane waves

$$u_n(t) = u_0 \exp\{i(nka - \omega t)\}. \quad (2)$$

Here u_0 is a plane wave amplitude, ω and k are frequency and wave number correspondently.

After substituting (2) into (1) we receive

$$m\omega^2 = 2\alpha_1(1 - \cos ka) + 2\alpha_2(1 - \cos 2ka) \quad (3)$$

The dispersion equation (3) can be rewritten as:

$$\frac{m\omega^2}{\alpha_1} = 4\sin^2\frac{ka}{2} + 4\frac{\alpha_2}{\alpha_1}\sin^2 ka \quad (4)$$

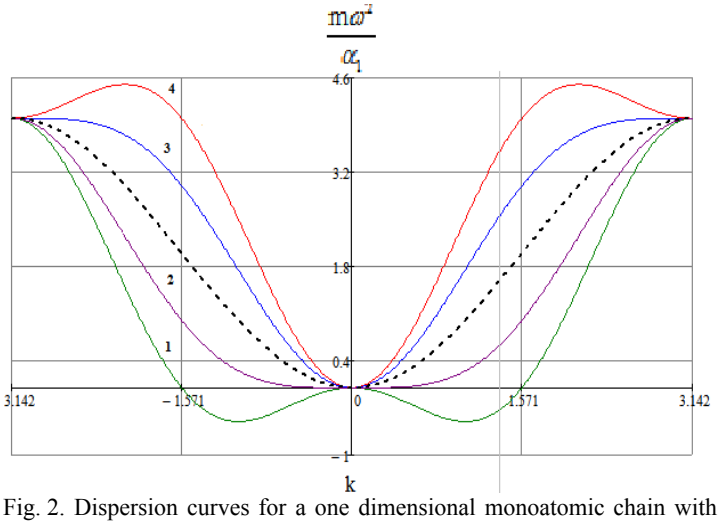

Fig. 2. Dispersion curves for a one dimensional monoatomic chain with accounting of nearest and next nearest neighbours (p = -1\2, -1\4, 0, 1\4, 1\2).

Introduce a designation $p=\alpha_2/\alpha_1$. Dispersion curves for a monatomic chain in approximation of nearest neighbours (p = 0, dashed curve) and second nearest ones (p = -1\2, curve 1; p = -1\4, curve 2; p = 1\4, curve 3; p = 1\2, curve 4) are shown in Fig. 2. An instability solution takes place at negative values of Here the condition of instability of negative values of, $\alpha_2/\alpha_1 \prec -1/4$ which is also represented at Fig. 2 (curve 1, p = -1\2). This situation can be applied in the simulation of metamaterials. The system considered is stable if $\alpha_2/\alpha_1 \prec -1/4$ (ω_2 is positive, (4)).

In case of an oscillating (alternating) interaction a restriction imposed on force constants comes out.

On considering interaction between the third neighbours, the dispersion equation transforms as following:

$$\frac{m\omega^2}{\alpha_1} = 4\sin^2\frac{ka}{2} + 4\frac{\alpha_2}{\alpha_1}\sin^2 ka + 4\frac{\alpha_3}{\alpha_1}\sin^2\frac{3ka}{2}. \quad (5)$$

Existence condition of a stable solution to implement in equation (5) is:

$$1 + 4\frac{\alpha_2}{\alpha_1} + 9\frac{\alpha_3}{\alpha_1} > 0. \tag{6}$$

Thus, when considering oscillatory (alternating) interactions a problem of system stability arises. It demands particular restriction on force constants connection.

Acoustic oscillations in the one-dimensional monatomic chain with long-range interaction

It is of high interest to take into account an interaction that exponentially decays with distance increasing (i.e., long-range interaction). This fact was shown in [3,4]. Therefore, consider interaction between all the atoms in an infinite chain. Motion equation is as follows

$$m\ddot{u}_n = \sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(u_{n+m'} - u_n\right) \tag{7}$$

The solution of equation (7) is sought in the form of plane waves (3). Thus,

$$m\omega^2 = \sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(1 - e^{im'k\alpha}\right). \tag{8}$$

From symmetrical reasoning $\alpha_{-m'} = \alpha_{m'}$, and we have

$$m\omega^2 = 2\sum_{m'=-\infty}^{+\infty} \alpha_{m'} \left(1 - \cos im'k\alpha\right). \tag{9}$$

Otherwise,

$$m\omega^2 = 4\sum_{m'=-\infty}^{+\infty} k_{m'} \sin^2 \frac{m'ka}{2}, \qquad k_{m'} = \alpha_{m'} / \alpha_1, \quad k_1 = 1. \tag{10}$$

The given equation cannot be solved without choosing of an appropriate model of force constants $\alpha_{m'}$ changing. The further the interacting atoms are situated the weaker the interaction is.

Consider the following model

$$\alpha_{m'} = \alpha_1 q^{m'-1}, \ |q| < 1, \tag{11}$$

which is an analog of RKKI exchange interaction which simplified obtaining of the magnetic materials excitation spectra [5]. It allows one to take into account when solving the problem of finding the excitation spectrum of the infinite-dimensional chain, the impact of long-range. Since in the model allows the existence of alternating force constants, it can be used to solve problems in physics metamaterials.

Substituting (11) into (10) and summing the expression, we get:

$$\frac{m\omega^2}{\alpha_1} = 2\frac{1+q}{1-q} \cdot \frac{1-\cos ka}{1-2q\cos ka+q^2}. \tag{12}$$

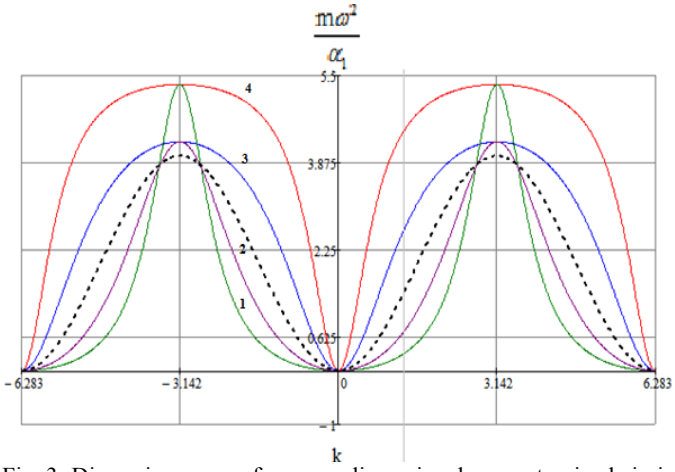

Fig. 3. Dispersion curves for a one dimensional monoatomic chain in approximation of nearest neighbours and when considering long-range interaction (q = -1\2, -1\4, 0, 1\4, 1\2).

Dispersion curves for a monatomic chain in approximation of nearest neighbours (q = 0, dashed curve) and for long-range interaction (q = -1\2, curve 1; q = -1\4, curve 2; q = 1\4, curve 3; q = 1\2, curve 4) are shown in Fig. 3. Account of the long-range interaction removes the problem of solution instability which appears when considering a finite number of neighbours.

Stability analysis of the equation (12) leads to the conclusion that solutions within the whole q range of definition are stable. When interaction between second and third neighbours is not considered a stability solution range narrows. As for only second neighbours consideration p should be p = [-1/4; 1]. Thus, consideration of the long-range interaction (when $|q| < 1$) allows removing the restrictions imposed upon the stability range of

dispersion equation solution.

Acoustic vibrations in an infinite monoatomic chain having a point defect

Consider an infinite chain consisting of atoms with m masses (Fig. 4) and a point defect with m' one within approximation of nearest neighbours interaction α. Maximum value of a square frequency for monoatomic ideal infinite chain is:

$$\omega_m^{\,2} = \frac{4\alpha}{m} \tag{13}$$

Let us study conditions of appearing and characteristics of so-called local vibrations.

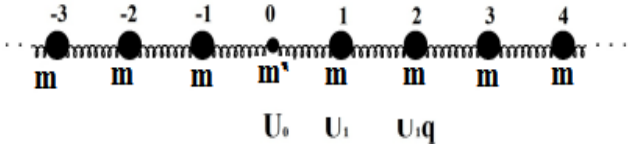

Fig. 4. An infinite atomic chain within which there is an impurity atom.

Without losing generality suppose that a defect atom is located in the grid origin. Solution is sought in the following form

$$\begin{cases} m'\ddot{u}_0 = -\alpha(u_1 + u_{-1} - 2u_0) \\ m\ddot{u}_1 = -\alpha(u_2 + u_0 - 2u_1) \\ m\ddot{u}_{-1} = -\alpha(u_0 + u_{-2} - 2u_{-1}) \end{cases}.$$

As for the other motion equations, they correspond those of the volume atoms (located far from the impurity one). We seek the solutions that coordinate the amplitudes decreasing on the sides of the defect atom, i.e.

$$\begin{cases} u_2 = u_1 q, \\ u_{-2} = u_{-1} q, \end{cases} \quad |q| < 1. \tag{14}$$

In (11) we had q for interaction decreasing parameter and in (14) it is an amplitude displacement parameter. Considering (14) we obtain a system below (we should take into account that $u \sim \exp(-i\omega t)$, see eq.(2))

$$\begin{cases} m'\omega^2/\alpha \cdot u_0 = \{2u_0 - u_1 - u_{-1}\}, \\ m\omega^2/\alpha \cdot u_1 = \{2u_1 - u_0 - u_1 q\}, \\ m\omega^2/\alpha \cdot u_{-1} = \{2u_{-1} - u_0 - u_{-1} q\}, \end{cases}$$

which has nontrivial solution if

$$\begin{pmatrix} (m'\omega^2/\alpha) - 2 & 1 & 1 \\ 1 & (m\omega^2/\alpha) - 2 + q & 0 \\ 1 & 0 & (m\omega^2/\alpha) - 2 + q \end{pmatrix} = 0. \tag{15}$$

Equation (15) is an equation for q expressed in terms of $m\omega^2$. Besides of it, we need the following equation to find q:

$$m\omega_л^2 = \alpha\left\{2 - \frac{1}{q} - q\right\}. \tag{16}$$

Hence,

$$q = \varepsilon/(\varepsilon - 2), \tag{17}$$

where $\varepsilon = m'/m$. From (17) it is obvious that $|q| < 1$ if $m'/m \prec 1$ which means that local vibrations appear without a threshold.

After substituting q into (16) we have:

$$\frac{m\omega_л^2}{\alpha} = \frac{4}{\varepsilon(2-\varepsilon)}. \tag{18}$$

Ratio of local and maximum frequencies (13) is:

$$\frac{\omega_л^2}{\omega_m^2} = \frac{1}{\varepsilon(2-\varepsilon)} \succ 1. \tag{19}$$

Dependences of $\omega_л^2/\omega_m^2$ on ε and q on ε are given in Fig. 5 (a and b respectively).

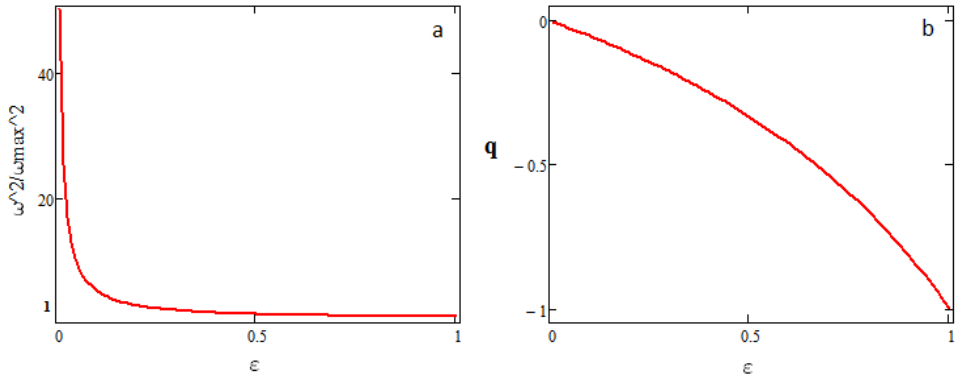

Fig. 5. Dependence of $\omega_л^2/\omega_m^2$ on ε (a) and of q on ε (b).

Local vibrations in one-dimensional semi-infinite chain having an impurity boundary atom

Consider a one-dimensional semi-infinite atomic chain consisting of atoms with m masses (Fig. 6) and one impurity m' boundary atom. Let us assume that $m' \prec m$. Similarly to the discussed above case of an infinite chain, local excitations will take place in the considered model. These local states are an analogue of the surface waves in one-dimensional system.

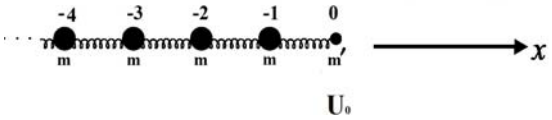

Fig. 6. A semi-infinite monoatomic chain having an impurity boundary atom.

We have obtained the following system in the given model

$$\begin{cases} m'\ddot{u}_0 = -\alpha\{u_{-1} - u_0\}, \\ m\ddot{u}_{-1} = -\alpha\{u_{-2} + u_0 - 2u_1\}, \\ m\ddot{u}_{-2} = -\alpha\{u_{-3} + u_{-1} - 2u_{-2}\}. \end{cases}$$

As we did in (14) let us rewrite this system in a following form

$$\begin{cases} m'\omega^2/\alpha \cdot u_0 = \{u_{-1} - u_0\}, \\ m\omega^2/\alpha \cdot u_{-1} = \{u_{-1}q + u_0 - 2u_{-1}\}, \end{cases} \tag{20}$$

which has a non-trivial solution on a condition that

$$\begin{pmatrix} (m'\omega^2/\alpha) - 1 & 1 \\ 1 & (m\omega^2/\alpha) - 2 + q \end{pmatrix} = 0. \tag{21}$$

For the second atom we have $m\ddot{u}_{-2} = \alpha\{u_{-3} + u_{-1} - 2u_{-2}\}$.

Hence,

$$m\omega^2 = \alpha\left\{2 - \frac{1}{q} - q\right\} \tag{22}$$

and

$$q = \frac{\varepsilon}{\varepsilon - 1}, \quad |q| \prec 1. \tag{23}$$

So, we can see that q is negative at $\varepsilon = m'/m \prec \frac{1}{2}$. It is also obvious that local vibrations arise if mass of an impurity boundary atom is twice lighter than the host one [6].

After substituting q into (22) we have:

$$\frac{m\omega_л^2}{\alpha} = \frac{1}{\varepsilon(1-\varepsilon)}. \tag{24}$$

Its maximum value is:

$$\omega_m^2/\alpha = 4/m. \tag{25}$$

Ratio of local and maximum frequencies is:

$$\frac{\omega_л^2}{\omega_m^2} = \frac{1}{4\varepsilon(1-\varepsilon)}. \tag{26}$$

Dependences of $\omega_л^2/\omega_m^2$ on ε (a) and q on ε are given in Fig. 7 (a and b respectively).

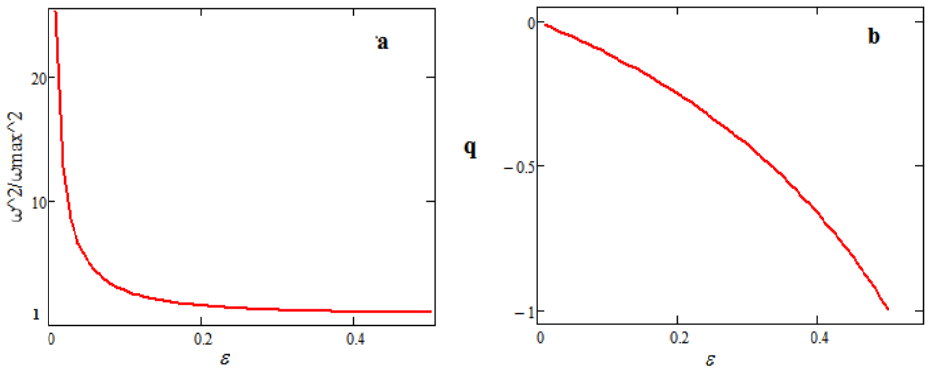

Fig. 7. Dependence of $\omega_л^2/\omega_m^2$ on ε (a) and of q on ε (b).

Diatomic infinite chain in model of the second-neighbour interaction

Consider a diatomic chain (Fig. 8). Assume the even numbers to be those of atoms with M masses and the odd numbers to be those with *m* ones.

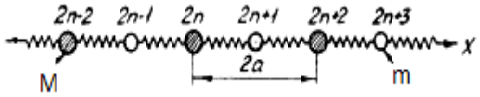

Fig.8. A diatomic chain.

$$\begin{cases} \text{m}\ddot{u}_{2n} = \alpha_1(u_{2n-1} + u_{2n+1} - 2u_{2n}) + \alpha_2(u_{2n-2} + u_{2n+2} - 2u_{2n}), \\ \text{M}\ddot{u}_{2n+1} = \alpha_1(u_{2n} + u_{2n+2} - 2u_{2n+1}) + \alpha_2'(u_{2n-1} + u_{2n+3} - 2u_{2n+1}). \end{cases} \tag{27}$$

The system equations are sought in the form of plane waves

$$\begin{aligned} u_{2n} &= u_1 \exp\{i(2nka - \omega t)\}, \\ u_{2n+1} &= u_2 \exp\{i([2n+1]ka - \omega t)\}. \end{aligned} \tag{28}$$

Substituting (28) into (27) we get

$$\begin{cases} \text{m}\omega^2 u_1 = 2\alpha_1(u_1 - \cos ka \cdot u_2) + 2\alpha_2(1 - \cos 2ka)u_1, \\ M\omega^2 u_2 = 2\alpha_1(u_2 - \cos ka \cdot u_2) + 2\alpha_2'(1 - \cos 2ka)u_2. \end{cases}$$

This system has non-trivial solutions for u_1 and u_2 if

$$\begin{vmatrix} 2\alpha_1 - \text{m}\omega^2 + 4\alpha_2 \sin^2 ka & -2\alpha_1 \cos ka \\ -2\alpha_1 \cos ka & 2\alpha_1 - M\omega^2 + 4\alpha_2' \sin^2 ka \end{vmatrix} = 0 \tag{29}$$

After evaluating a determinant obtained we get a dispersion relation for a diatomic chain.

$$\omega^4 - A(k)\omega^2 + B(k) = 0, \tag{30}$$

where

$$A(k) = \frac{2\alpha_1}{mM}(m+M) + 4\frac{m\alpha_2 + M\alpha_2'}{mM}\sin^2 ka,$$

$$B(k) = \frac{4\alpha_1^2}{mM}\sin^2 ka + 8\alpha_1\frac{\alpha_2 + \alpha_2'}{mM}\sin^2 ka + \frac{16\alpha_2\alpha_2'}{mM}\sin^4 ka.$$

Solutions of (29) are as follows

$$\omega_{\pm}^2(k) = \frac{1}{2}A(k) \pm \frac{1}{2}\sqrt{A^2(k) - 4B(k)}. \tag{31}$$

Dispersion curves for a diatomic chain in approximation of nearest neighbours (p = 0, dashed curve) and second nearest ones (p = -1\2, curve 1; p = 1\2, curve 2) are shown in Fig. 9. Here optical modes are marked with thin curves and acoustical ones are marked with thick curves.

Such plots demonstrate a condition of instability appearing for the acoustic vibrations within negative values of

$\frac{\alpha_2}{\alpha_1} \prec -\frac{1}{4}$ (p=-1\2). This result may be applied in simulation of metamaterials in acoustics.

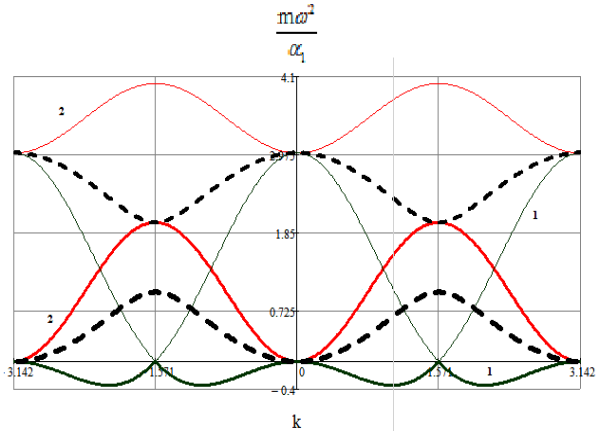

Fig. 9. Diatomic infinite chain with accounting of nearest and next nearest neighbours. (p=-1\2, 0, 1\2).

There are optical and acoustical vibrations in a diatomic chain (unlike a monoatomic one which doesn't have them). In our work we marked $\omega_+(k)$ as for optical modes and $\omega_-(k)$ as for acoustical ones. Solutions of (30) are stable if $A(k) > 0,\ \ 0 < B(k) < A^2(k)$.

Considering the form of *A(k)* and *B(k)*, these conditions bind both force constants and masses of various atoms. There is a gap between optical and acoustical excitations that appears in an infinite diatomic chain consisting of atoms of different type. The gap width can be estimated according to the dispersion curves form.

The lowest border is an optical mode which is $\omega^2_{+,\min} = \frac{m+M}{mM}$, and the upper one responds for acoustical vibrations $\omega^2_{-,\max} = \frac{1}{2}A(k) - \frac{1}{2}\sqrt{A^2_{\max} - 4B_{\max}}$.

Here $A_{\max} = \frac{2}{mM}(\alpha_1(m+M) + 2(m\alpha_2 + M\alpha_2'))$, $B_{\max} = \frac{4}{mM}(\alpha^2_1 + 2\alpha_1(\alpha_2 + \alpha_2') + 4\alpha_2\alpha_2')$ if accounting the next nearest neighbours.

Infinite diatomic chain with taking a long-range interaction into account

As for two types of atoms we have the following equations of motion:

$$\begin{cases} m\omega^2 u_1 = 2u_1 \sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska)) + 2\sum_{r=0}^{\infty} \alpha_{2r+1}(u_1 - u_2\cos[(2r+1)ka]), \\ M\omega^2 u_2 = 2u_2 \sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska)) + 2\sum_{r=0}^{\infty} \alpha_{2r+1}(u_2 - u_1\cos[(2r+1)ka]). \end{cases} \quad (32)$$

It is convenient to make a replacement

$$\begin{cases} m\omega^2 u_1 = F(ka)\cdot u_1 + G(ka)\cdot u_2, \\ M\omega^2 u_2 = G(ka)\cdot u_1 + F(ka)\cdot u_2, \end{cases} \quad (33)$$

where $F = 2\sum_{s=1}^{\infty} \alpha_{2s}(1-\cos(2ska))$, $G = 2\sum_{r=0}^{\infty} \alpha_{2r+1}(1-\cos[(2r+1)ka])$.

Equation system (33) has non-trivial solutions for u_1 and u_2 if

$$\begin{vmatrix} F(ka) - m\omega^2 & G(ka) \\ G(ka) & F(ka) - M\omega^2 \end{vmatrix} = 0. \quad (34)$$

Thus, we obtain

$$\omega^4 - A(ka)\omega^2 + B(ka) = 0, \quad (35)$$

where $A(ka) = \frac{m+M}{mM}F(ka)$, $B(ka) = \frac{F^2(ka) - G^2(ka)}{mM}$. We get $F(ka)$ and $G(ka)$.

Hence,

$$F(ka) = \frac{2\alpha_1}{1-q} - 2\alpha_1\frac{(\cos 2ka - q^2)\cdot q}{1+q^4-2q^2\cos 2ka}, \quad G(ka) = 2\alpha_1\frac{\cos ka(1-q^2)}{1+q^4-2q^2\cos 2ka}.$$

Solution of (35) is

$$\omega^2_{\pm}(ka) = \frac{1}{2}A(ka) \pm \frac{1}{2}\sqrt{A^2(ka) - 4B(ka)},$$

A and B are presented above.

Dispersion curves for a diatomic chain in approximation of nearest neighbours (q = 0, dashed curve) and second nearest ones (q = -1\2, green curve; q = 1\2, red curve) are shown in Fig. 10. Here optical modes are marked with thin curves and acoustical ones are marked with thick curves.

Account of the long-range interaction removes the problem of solution instability which appears when considering a finite number of neighbours. Long-range interaction takes away a restriction that $\alpha_2 < 0$.

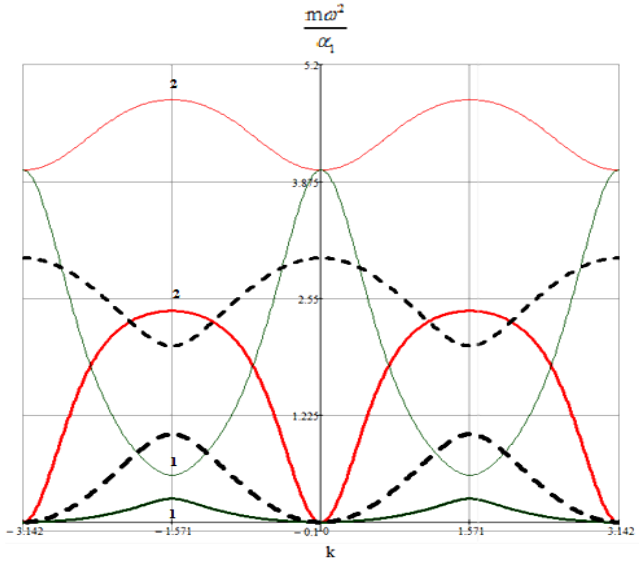

Fig.10. Diatomic infinite chain with accounting of nearest and next nearest neighbours. (q=-1\2, 0, 1\2).

INFLUENCE OF SURFACE PLANE ORIENTATION ON DYNAMICS OF VIBRATIONAL STATES IN A SEMI-INFINITE CUBIC CRYSTAL

Different theoretical and experimental studies of surface states of various nature (including elastic surface waves) cause deep interest both in the context of fundamental studies and technological applications. Pure shear surface waves having a horizontal polarization are of special interest. Such waves depend on surface characteristics much stronger than waves possessing Rayleigh polarization, for example [7, 8]. This comes from the fact that penetration depth of purely shear surface wave exceeds that of the Rayleigh wave within the long wavelength limit. If geometry of a studied crystal is of sufficiently high symmetry, pure shear surface waves split from the Rayleigh waves then.

Thus, without losing generality it is possible to study such surface waves using the so-called scalar models characterized by one displacement direction. For example, spin waves in magnetically ordered systems in the magnon approximation are described using this model.

In our paper we studied dispersion relations of phonons in a cubic crystal. For our calculations we used methodology stated in [9, 10]. The following methodology is of broad generality and can be used for studying of both continuous and discrete spectrum in crystal models close to real systems.

In a microscopic assumption we have studied zones of volume vibrations and properties of the single-component surface waves split off the volume zone, depending on surface orientation, direction of two-dimensional wave vector and its values in a two-dimensional Brillouin zone.

Volume vibrations

The equation of atomic motion for an ideal crystal in scalar model in harmonic approximation is as follows [11]:

$$m\ddot{u}(n,t) = -\sum_{n'} \hat{\Phi}(n,n')u(n',t). \tag{36}$$

Here $u(n,t)$ is a time-dependent displacement of the atom in the $n = (n_1, n_2, n_3)$ site from its equilibrium position, $\hat{\Phi}(n,n')$ is a force matrix and m is an atomic mass. Solution of (36) is sought in the form

$$u(n,t) = u(n_3) \cdot e^{i(k_\alpha n_\alpha - \omega t)}. \tag{37}$$

Here k_∞ are the components of a three-dimensional wave vector along a_1, a_2, a_3 (the unit vectors), $\alpha = 1,2,3$; ω is the wave frequency.

In order to study the surface waves, we examine first the situation where the chosen orientational plane is located deep in the crystal. Consider (001), (110) and (111) orientational planes. With (1) and (2), dispersion relations for each of the orientational planes in SC, FCC and BCC can be obtained.

- ***Simple cubic:***
  - *(001) plane*

$$\frac{m\omega_V^2}{\alpha} = 6 - 2\cos[k_1 a_0] - 2\cos[k_2 a_0] - 2\cos[k_3 a_0]. \tag{38}$$

Let us construct a diagram for volume vibration zone as a function of two-dimensional wave vector $\chi(k_1, k_2)$ at fixed k_3 (see Fig. 11, shaded area). For SC crystal lower and upper borders are as follows

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 2\cos[k_1] - 2\cos[k_2] - 2,$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 - 2\cos[k_1] - 2\cos[k_2] + 2. \tag{39}$$

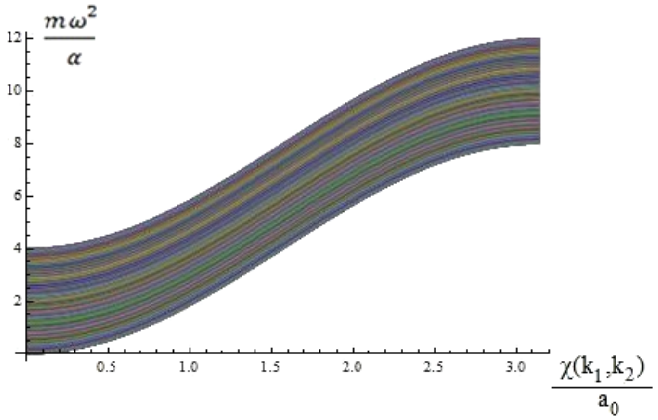

Fig. 11. A diagram of volume vibrations (shaded area) for (001) surface orientational plane in SC crystal.

Similarly, it is possible to find volume vibration zones for any other orientational plains.

- *(110) plane*

Equation for volume vibrations is

$$\frac{m\omega_V^2}{\alpha} = 6 - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_3\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0]. \tag{40}$$

And, hence, for lowest and highest boundaries we have (see Fig. 14, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 4\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 + 4\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2 a_0]. \tag{41}$$

- *(111) plane*

As for (111) orientational plane we have

$$\frac{m\omega_V^2}{\alpha} = 6 - 2\cos[K_3\frac{a_0}{\sqrt{3}} - K_2\frac{a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}} + K_3\frac{a_0}{\sqrt{3}}], \tag{42}$$

and (Fig. 12, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 6 - 2\cos[K_2\frac{a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}}],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 6 + 2\cos[K_2\frac{a_0}{\sqrt{6}}] + 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0}{\sqrt{6}}]. \tag{43}$$

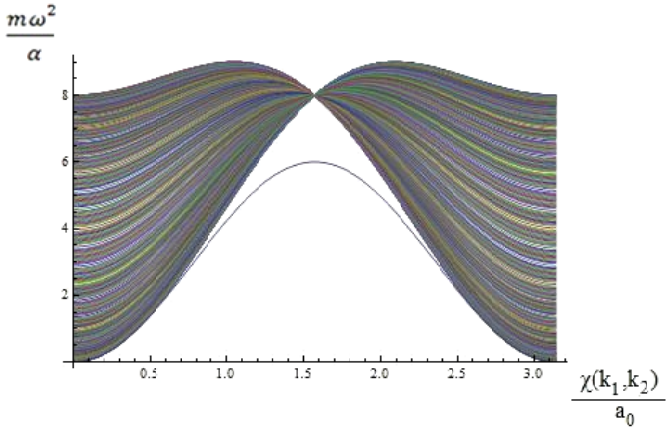

Fig. 12. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in BCC crystal.

- ***Face-centred cubic:***
  - *(001) plane*

Similarly to what was calculated for simple cubic crystal, for FCC with (001) orientational plane we have

$$\frac{m\omega_V^2}{\alpha} = 12 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] - 4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}] - 4\cos[k_2\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}]. \quad (44)$$

The lowest and the highest boundaries are as follows (Fig. 13, shaded area):

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 2 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] - 4\cos[k_1\frac{a_0}{\sqrt{2}}] - 4\cos[k_2\frac{a_0}{\sqrt{2}}],\\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 2 - 4\cos[k_1\frac{a_0}{\sqrt{2}}] * \cos[k_2\frac{a_0}{\sqrt{2}}] + 4\cos[k_1\frac{a_0}{\sqrt{2}}] + 4\cos[k_2\frac{a_0}{\sqrt{2}}].\end{aligned} \quad (45)$$

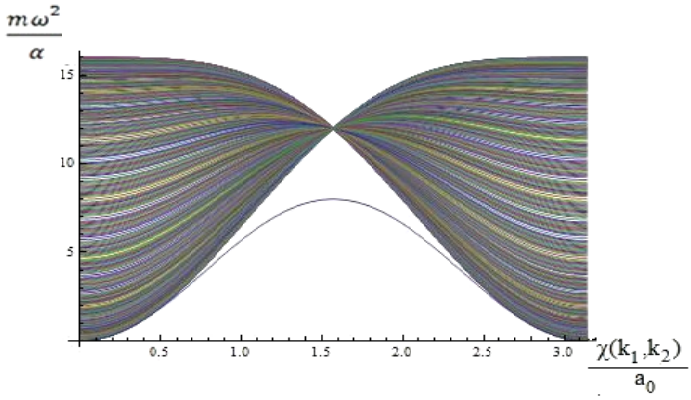

Fig. 13. A diagram of volume vibrations (shaded area) and surface wave for (001) surface orientational plane in FCC crystal.

  - *(110) plane*

$$\frac{m\omega_V^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] - 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}]\cos[K_3\frac{a_0}{2}], \quad (46)$$

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] - 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}],\\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[k_2\frac{a_0}{2\sqrt{2}}] + 8\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}].\end{aligned} \quad (47)$$

The corresponding diagram is shown in Fig. 14, shaded area.

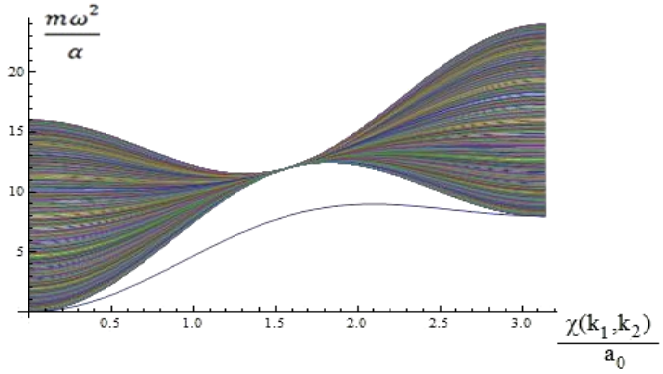

Fig. 14. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in FCC crystal.

  - *(111) plane*

In this case equations for volume vibrations are

$$\frac{m\omega_V^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[(\frac{K_2}{\sqrt{2}} + K_3)\frac{a_0}{\sqrt{3}}] - 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[(K_2\frac{a_0\sqrt{2}}{4} - K_3a_0)\frac{1}{\sqrt{3}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}] \quad (48)$$

and (see Fig. 15, shaded area):

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[\frac{K_2 a_0}{\sqrt{6}}] - 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[K_2\frac{a_0}{2\sqrt{6}}] - 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}],$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[\frac{K_2 a_0}{\sqrt{6}}] + 4\cos[K_1\frac{a_0\sqrt{2}}{4}]\cos[K_2\frac{a_0}{2\sqrt{6}}] + 4\cos[K_1\frac{a_0}{\sqrt{2}}]\cos[K_2\frac{a_0\sqrt{6}}{4}]. \quad (49)$$

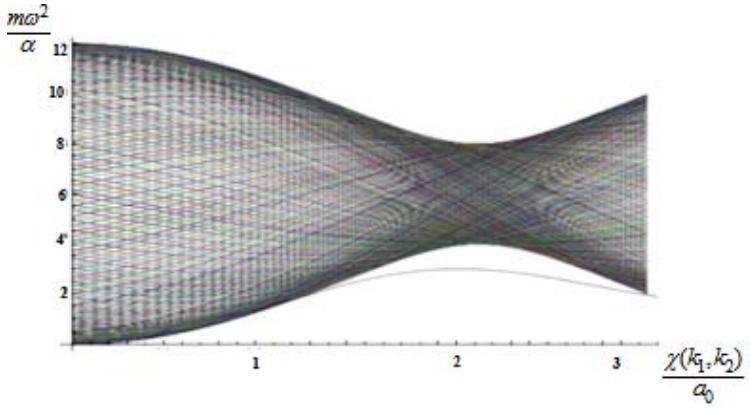

Fig. 15. A diagram of volume vibrations (shaded area) and surface wave for (111) surface orientational plane in SC crystal.

- ***Base-centred cubic:***
  - *(001) plane*

As for BCC, we have

$$\frac{m\omega_V^2}{\alpha} = 8 - 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}]\cos[k_3\frac{a_0}{\sqrt{2}}]. \quad (50)$$

Thus, dispersion equations for the lowest and the highest boundaries are as follows (see Fig. 16, shaded area)

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 8 - 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}]$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 8 + 8\cos[k_1\frac{a_0}{\sqrt{3}}]\cdot\cos[k_2\frac{a_0}{\sqrt{2}}] \quad (51)$$

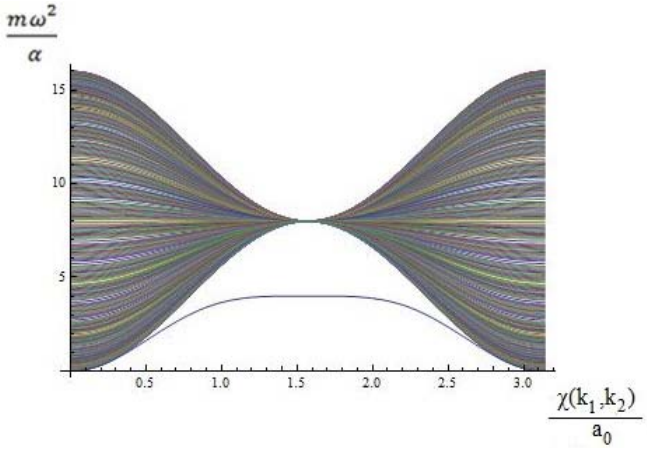

Fig. 16. A diagram of volume vibrations (shaded area) and surface wave for (001) surface orientational plane in BCC crystal.

  - *(110) plane*

Similarly,

$$\frac{m\omega_V^2}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2}]\cos[K_3\frac{a_0}{2\sqrt{2}}], \quad (52)$$

$$\frac{m(\omega_V^2)_{\min}}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2}]$$
$$\frac{m(\omega_V^2)_{\max}}{\alpha} = 8 - 4\cos[K_1\frac{a_0}{2}]\cos[K_2\frac{a_0}{2\sqrt{2}}] + 4\cos[K_1\frac{a_0}{2}] \quad (53)$$

The following diagram is shown in Fig. 12, shaded area.

- *(111) plane*

In the following case, we have

$$\frac{m\omega_V^2}{\alpha} = 8 - 4\cos[\frac{2}{9}K_1a_0] - 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})]\cos[\frac{\sqrt{2}}{9}K_3a_0] \tag{54}$$

and (Fig. 17, shaded area)

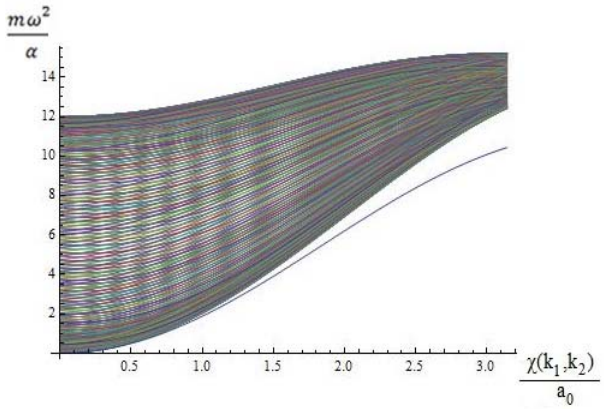

Fig. 17. A diagram of volume vibrations (shaded area) and surface wave for (111) surface orientational plane in FCC crystal.

$$\begin{aligned}\frac{m(\omega_V^2)_{\min}}{\alpha} &= 8 - 4\cos[\frac{2}{9}K_1a_0] - 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})] \\ \frac{m(\omega_V^2)_{\max}}{\alpha} &= 8 - 4\cos[\frac{2}{9}K_1a_0] + 4\cos[\frac{2}{9}a_0(K_1 - \frac{K_2}{\sqrt{2}})]\end{aligned} \tag{55}$$

Surface waves in cubic crystals

We use a Lifshitz Rosenzweig model [12] for describing a surface. In an infinite crystal we lay a plane that corresponds the needed orientation and then just "throw away" one of the halves of our crystal.

From (1) and (2) for surface plane we get

$$m\omega^2 u(n_3) = \sum_{n_3'} \hat{\Phi}(n, n_3'; n_1, n_2), \tag{56}$$

Here $\hat{\Phi}(n, n_3'; n_1, n_2)$ is a reduced dynamic matrix. Equation (56) are linear equations in finite differences of order $2s$ which set a sequence of $U(n)(n = 0,1,2,\ldots)$. It follows from the theory of finite difference equations [13] that, beginning from $n = N, U(n)$ can be presented as a sum of geometric progressions

$$u(n) = \sum_{j=1}^{2s} V_j q_j^n, \tag{57}$$

Here V_j are amplitudes of $2s$ partial waves, characterized by q_i parameters which determine degree of decrease (increase) of the partial wave with penetrating into crystal depth. q_i are solutions of the algebraic equation of $2s$ degree (in scalar model):

$$m\omega^2 - \sum_{n=-s}^{2s} \hat{\Phi}^0(n,k) q^n = 0 \tag{58}$$

As for $0 \prec n \prec N + s$ atomic motion equations for atoms situated in defect and intermediate layers (see (57)) play the role of boundary conditions and are used to determine relationship between the V_j and atomic vibrational amplitudes in defect layers. There are s summands left in (58) in case of SC, $|q| \prec 1$ for all of them. It was interesting for us to determine values of q and $m\omega^2/\alpha$ for different orientational surfaces.

Boundary conditions (motion equations for defect and intermediate layers) form a system of $N + s$ homogeneous linear equations for V_j and $u(n)(n = 0,1,\ldots N-1)$. The number of equations and unknowns are equal. Equating the determinant of this system to 0, we arrive to the equation for SC structure dispersion relation. Mathematically, the matter is to solve an algebraic equation and there is no need in integration over a continuous spectrum.

dispersion relations for phonons in cubic crystal with different orientational surface have been studied. So let us illustrate the technique used on some specific models.

(001) plane

- ***Simple cubic structure (SC).***

There are one defect $n=0(s=1)$ and one intermediate planes $n=1(N=1)$ for (001) surface plane in a SC crystal. Surface wave may be presented in the form of $u(n)=Vq^n$. For a $n=1$ intermediate layer and a $n=0$ surface defect layer equation system (58) transforms into:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6-2\cos[k_1a_0]-2\cos[k_2a_0]-(q+\frac{1}{q}),\ n\geq 1, \\ \frac{m\omega_s^2}{\alpha} = 5-2\cos[k_1a_0]-2\cos[k_2a_0]-q,\ n=0. \end{cases} \tag{59}$$

Here V is an atomic vibrational amplitude; s is a solution for a SC structure and ω_s is its frequency. From the expression for $n=0$ it's obvious that surface atoms have 5 neighbours, while those situated in any other layer inside the crystal have 6 neighbours.

An equation for $n=0$ in (59) plays the role of a boundary condition for surface waves. From (59) we obtain:

$$\begin{cases} q=1 \\ \frac{m\omega_s^2}{\alpha} = 4-2\{\cos[k_1a_0]-\cos[k_2a_0]\} \end{cases} \tag{60}$$

Thus, for the considered surface orientation equation $\omega_s(k)$, a surface wave corresponds the lowest boundary of volume vibration zone (see (38)). For such a situation we have $q=1$ which means that there are no surface vibrations for (001) orientational plane in SC. It is illustrated in Fig. 11.

A splitting value $\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}$ is a difference between dispersion relations for volume and surface vibrations. As for the considered situation it equals $\Delta=0$, as $\frac{m\omega_s^2}{\alpha}=\frac{m(\omega_V^2)_{\min}}{\alpha}=4-2\cos[k_1a_0]-2\cos[k_2a_0]$

- ***Face-centred cubic structure (FCC).***

Consider unit translation vectors and a two-dimensional vector o be as follows, respectively: $A_1=A_2=a_0/\sqrt{2}$, $k_1=k_2$. Then, we get:

$$\begin{aligned} &\frac{m\omega_s^2}{\alpha} = 12-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-2(q+\frac{1}{q})\{\cos[k_1\frac{a_0}{\sqrt{2}}]+4\cos[k_2\frac{a_0}{\sqrt{2}}]\},\ n\geq 1 \\ &\frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-2q\{\cos[k_1\frac{a_0}{\sqrt{2}}]+4\cos[k_2\frac{a_0}{\sqrt{2}}]\},\ n=0 \end{aligned} \tag{61}$$

Values for $m\omega_s^2/\alpha$ and q are obtained from (61):

$$\begin{cases} q=\frac{1}{2}(\cos[k_1\frac{a_0}{\sqrt{2}}]+\cos[k_2\frac{a_0}{\sqrt{2}}]) \\ \frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{2}}]\cos[k_2\frac{a_0}{\sqrt{2}}]-\cos^2[k_1\frac{a_0}{\sqrt{2}}]+\cos^2[k_2\frac{a_0}{\sqrt{2}}] \end{cases} \tag{62}$$

In Fig. 16 the line beneath the shaded area corresponds to a surface wave. For (001) orientational plane in FCC crystal we have the following splitting value: $\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}=4(1-q)^2,$ which shows that a surface wave exists in such an orientation.

- ***Base-centred cubic structure (BCC).***

For defect $n=0$ and intermediate $n=1$ layers we have:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 8-4\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}](q+\frac{1}{q}),\ n\geq 1 \\ \frac{m\omega_s^2}{\alpha} = 8-4q\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}],\ n=0 \end{cases} \tag{63}$$

$$\begin{cases} q=\cos[k_1\frac{a_0}{\sqrt{3}}]\cos[k_2\frac{a_0}{\sqrt{3}}] \\ \frac{m\omega_s^2}{\alpha} = 4-4\cos^2[k_1\frac{a_0}{\sqrt{3}}]\cos^2[k_2\frac{a_0}{\sqrt{3}}] \end{cases} \tag{64}$$

In Fig. 13 a curve beneath the shaded reach corresponds to a surface wave. The splitting value is: $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 3(1-|q|)^2$.

(110) plane

- ***SC structure.***

As for (110) surface orientational plane in simple cubic crystal we choose unit transition vectors as follows: $A_1 = a_0/\sqrt{2}\,(1\bar{1}0), A_2 = a_0(001)$. The two-dimensional wave vector will have the following components then: $K_1 = k_0/\sqrt{2}\,(1\bar{1}0), K_2 = k_0(001)$. Number of defect and intermediate layers are $s = N = 1$. Equations for atoms in $n \geq 1$ and $n = 0$ are

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6 - 2\cos[K_1\frac{a_0}{\sqrt{2}}](q+\frac{1}{q}) - 2\cos[K_1 a_0],\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 4 - 2q\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_1 a_0],\ n = 0 \end{cases}. \quad (65)$$

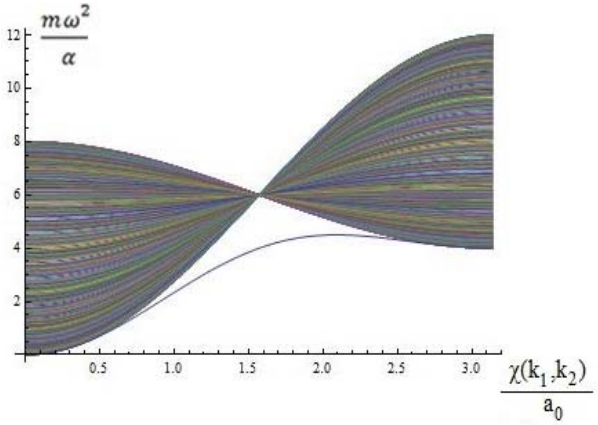

Fig. 18. A diagram of volume vibrations (shaded area) and surface wave for (110) surface orientational plane in SC crystal.

A solution for (65) is

$$\begin{cases} q = \cos[K_1\frac{a_0}{\sqrt{2}}] \\ \frac{m\omega_s^2}{\alpha} = 4 - 2\cos^2[K_1\frac{a_0}{\sqrt{3}}] - 2\cos[K_2 a_0] \end{cases}. \quad (66)$$

From (66) it follows that there is a surface wave for such a surface orientational plane. The penetration depth of the wave considered varies from a minimum value in $K_1 = k_0/\sqrt{2}\,\overline{(110)}$ direction up to infinity when spreading in $K_2 = k_0(001)$ direction. In Fig. 18 a curve beneath the shaded area corresponds to a surface wave. The splitting value is: $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 2(1-q)^2$.

- ***FCC structure.***

From the equations for $n \geq 1$ and $n = 0$:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 12 - 2\cos[K_1\frac{a_0}{2\sqrt{2}}] - 2\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}](q+\frac{1}{q}),\ n \geq 1, \\ \frac{m\omega_s^2}{\alpha} = 8 - 2\cos[K_1\frac{a_0}{\sqrt{2}}] - 2\cos[K_2\frac{a_0}{2\sqrt{2}}] - 4q\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{a_0}{2\sqrt{2}}],\ n = 0 \end{cases}. \quad (67)$$

We get values of ω_s

$$\begin{cases} q = \cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{a_0}{2\sqrt{2}}], |q| \prec 1, \\ \frac{m\omega_s^2}{\alpha} = 8 - 2\cos[K_1 \frac{a_0}{\sqrt{2}}] - 2\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] \end{cases}. \quad (68)$$

Splitting of a surface wave from the continuous spectrum is shown in Fig. 14 and equals $\Delta = \frac{m(\omega_V^2)_{\min}}{\alpha} - \frac{m\omega_s^2}{\alpha} = 4(1-q)^2$.

- ***BCC structure.***

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 8 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2\cos[K_1 \frac{a_0}{2}](q + \frac{1}{q}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 6 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2q\cos[K_1 \frac{a_0}{2}],\ n = 0 \end{cases} \quad (69)$$

For unit translation vectors $A_1 = a_0/2(001), A_2 = a_0/2\sqrt{2}(1\bar{1}0)$ we obtain the following equation system for defect $n=0$ and intermediate $n=1$ layers:

Hence,

$$\begin{cases} q = \cos[K_1 \frac{a_0}{2}], \\ \frac{m\omega_s^2}{\alpha} = 6 - 4\cos[K_1 \frac{a_0}{2}]\cos[K_2 \frac{a_0}{2\sqrt{2}}] - 2\cos^2[K_1 \frac{a_0}{2}] \end{cases} \quad (70)$$

In Fig. 12 a curve beneath the shaded area corresponds to a surface wave. The splitting value is:

$$\Delta = \frac{m(w_V^2)_{min}}{\alpha} - \frac{mw_s^2}{\alpha} = 2(1-q)^2$$

which shows that a surface wave exists in such an orientation.

(111) plane

- ***SC lattice.***

In case of SC crystal with (001) orientational surface we choose the following unit vectors in coordinate and impulse spaces: $A_1 = a_0/\sqrt{2}(1\bar{1}0), A_2 = a_0/\sqrt{6}(1\,1\bar{2})$; $K_1 = k_0/\sqrt{2}(1\bar{1}0), K_2 = k_0/\sqrt{2}(\bar{1}\bar{1}0)$. The dynamic equations for atoms located in defective ($n=0$) and intermediate ($n=1$) layers are as follows, respectively:

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 6 - 4qe^{iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{-3iK_2\frac{a_0}{\sqrt{2}}}) - \frac{1}{q}e^{-iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{3iK_2\frac{a_0}{\sqrt{2}}}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 3 - qe^{iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{-3iK_2\frac{a_0}{\sqrt{2}}}),\ n = 0 \end{cases} \quad (71)$$

Dispersion relation and q values are as follows then

$$\begin{cases} q = \frac{1}{3}e^{-iK_2\frac{a_0}{\sqrt{2}}}(2\cos[K_1 \frac{a_0}{\sqrt{2}}] + e^{3iK_2\frac{a_0}{\sqrt{2}}}), \\ \frac{m\omega_s^2}{\alpha} = \frac{4}{3}(2 - \cos^2[K_1 \frac{a_0}{\sqrt{2}}] - \cos[K_1 \frac{a_0}{\sqrt{2}}]\cos[K_2 \frac{3a_0}{\sqrt{6}}]) \end{cases}. \quad (72)$$

The surface wave is shown in Fig. 15 as a curve splitting from continuous spectrum.

- ***FCC lattice.***

Having $A_1 = a_0/2\sqrt{2}(1\bar{1}0), A_2 = a_0/2\sqrt{6}(1\,1\bar{2})$ we get

$$\begin{cases} \frac{m\omega_s^2}{\alpha} = 12 - 2\cos[K_1 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{3a_0}{2\sqrt{6}}] - qe^{-iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{3iK_2\frac{a_0}{2\sqrt{6}}}) - \\ -\frac{1}{q}e^{-K_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{-3iK_2\frac{a_0}{2\sqrt{6}}}),\ n \geq 1 \\ \frac{m\omega_s^2}{\alpha} = 9 - 2\cos[K_1 \frac{a_0}{2\sqrt{2}}] - 4\cos[K_1 \frac{a_0}{2\sqrt{2}}]\cos[K_2 \frac{3a_0}{2\sqrt{6}}] - qe^{-iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1 \frac{a_0}{2\sqrt{2}}] + e^{3iK_2\frac{a_0}{2\sqrt{6}}}),\ n = 0. \end{cases} \quad (73)$$

From (73) we obtain

$$\begin{cases} q = e^{iK_2\frac{a_0}{2\sqrt{6}}}(2\cos[K_1\frac{a_0}{\sqrt{2}}]+e^{-3iK_2\frac{a_0}{2\sqrt{6}}}), \\ \frac{m\omega_s^2}{\alpha}=\frac{16}{3}(2-\cos^2[K_1\frac{a_0}{2\sqrt{2}}]-\cos[K_1\frac{a_0}{2\sqrt{2}}]\cos[K_2\frac{3a_0}{2\sqrt{6}}]) \end{cases} \quad (74)$$

Splitting of a surface wave from the continuous spectrum (Fig. 17) equals $\Delta=\frac{m(w_V^2)_{min}}{\alpha}-\frac{mw_s^2}{\alpha}=2(1-q)^2$.

Cubic crystals having an adsorbed surface monolayer

Consider a cubic crystal that has a simple cubic lattice and (001) surface orientational plane of the (001). Consider now an adsorbed monolayer which consists of impurity atoms and is situated on the top of the surface layer. Equation (38) allows one to write the dispersion relations for the adsorbed surface monolayer ($n=0$) and a boundary layer located below it ($n=1$):

$$\begin{cases} \frac{m_0\omega_s^2}{\alpha}U_0=(5-2\cos[k_1a_0]-2\cos[k_2a_0])U_0-U_1 \\ \frac{m\omega_s^2}{\alpha}U_1=(6-2\cos[k_1a_0]-2\cos[k_2a_0])U_1-U_0-U_1q \end{cases}. \quad (75)$$

Here m_0 is a mass of an impurity atom and m is a mass of a host one. We had the dispersion relation for $n\succ 1$ layer given above (see (59)). From (75) we find the following determinant:

$$\begin{vmatrix} \frac{m_0\omega_s^2}{\alpha}-5+A & 1 \\ 1 & \frac{m\omega_s^2}{\alpha}-6+A+q \end{vmatrix}=0. \quad (76)$$

Hereinafter we introduce the following notation $A=2\cos[k_1a_0]+2\cos[k_2a_0]$. Equations (59), (76) are a system of two equations having two unknowns, q and $m\omega_s^2/\alpha$. For q in general case we have

$$q=\frac{-[m_0(6-A)-m(5-A)]\pm\sqrt{[m_0(6-A)-m(5-A)]^2+4m_0(m-m_0)}}{2(m-m_0)}. \quad (77)$$

A boundary transition should be hold: $q=1$ at $m_0=m$ (see (51), a (001) surface orientational plane in SC crystal). Denominator equals 0 then, so take a limit of (77). Let us set $X=[m_0(6-A)-m(5-A)]$, $Y=4m_0(m-m_0)$. Hence,

$2(m-m_0)=\frac{Y}{2m_0}$ and $q=\lim_{Y\to 0}2m_0\frac{-X\pm\sqrt{X^2+Y^2}}{Y}\approx -2m_0\frac{-X\pm(X+\frac{Y}{2X})}{Y}$. Since $|q|\prec 1$, only a positive root matches, and we get:

$$q=\frac{m_0}{X}=\frac{m}{X}=1. \quad (78)$$

Thus, the boundary condition is satisfied. It is easy to obtain $m\omega_s^2/\alpha$ knowing q.

Consider a situation when impurity atoms are lighter than the host ones $m_0\prec m$. Consider also a situation of heavy impurity atoms $m_0\succ m$.

For light impurity atoms $(m_0\prec m)$. In this connection $\frac{m_0}{m}=\frac{1}{2}$ and $\frac{m_0}{m}=\frac{1}{5}$ have been studied.

$$\frac{m_0}{m}=\frac{1}{2}: \quad \begin{cases} \frac{m\omega_s^2}{\alpha}=6+A+\sqrt{A^2-8A+20} \\ q=\frac{4-A-\sqrt{A^2-8A+20}}{2} \end{cases}. \quad (79)$$

At such ratio between masses of host and impurity atoms a surface wave splits off just from the highest boundary of the continuous spectrum (see Fig. 19).

$$\frac{m_0}{m}=\frac{1}{2}: \quad \begin{cases} \dfrac{m\omega_s^2}{\alpha}=\dfrac{105-20A+5\sqrt{16A^2-152A+377}}{8} \\ q=\dfrac{19-4A-\sqrt{16A^2-152A+377}}{8} \end{cases}. \tag{80}$$

Note that in both cases $q \prec 0$. Let us determine a splitting value now. From Fig. 19 it is obvious that a surface wave splits off the highest boundary of the continuous spectrum, so:

$$\Delta=\frac{m\omega_s^2}{\alpha}-\frac{m(\omega_V^2)_{\max}}{\alpha} \succ 0, \tag{81}$$

$$\frac{m_0}{m}=\frac{1}{2}: \Delta=8-A-2q \succ 0, \tag{82}$$

$$\frac{m_0}{m}=\frac{1}{5}: \Delta=17-4A-5q \succ 0. \tag{83}$$

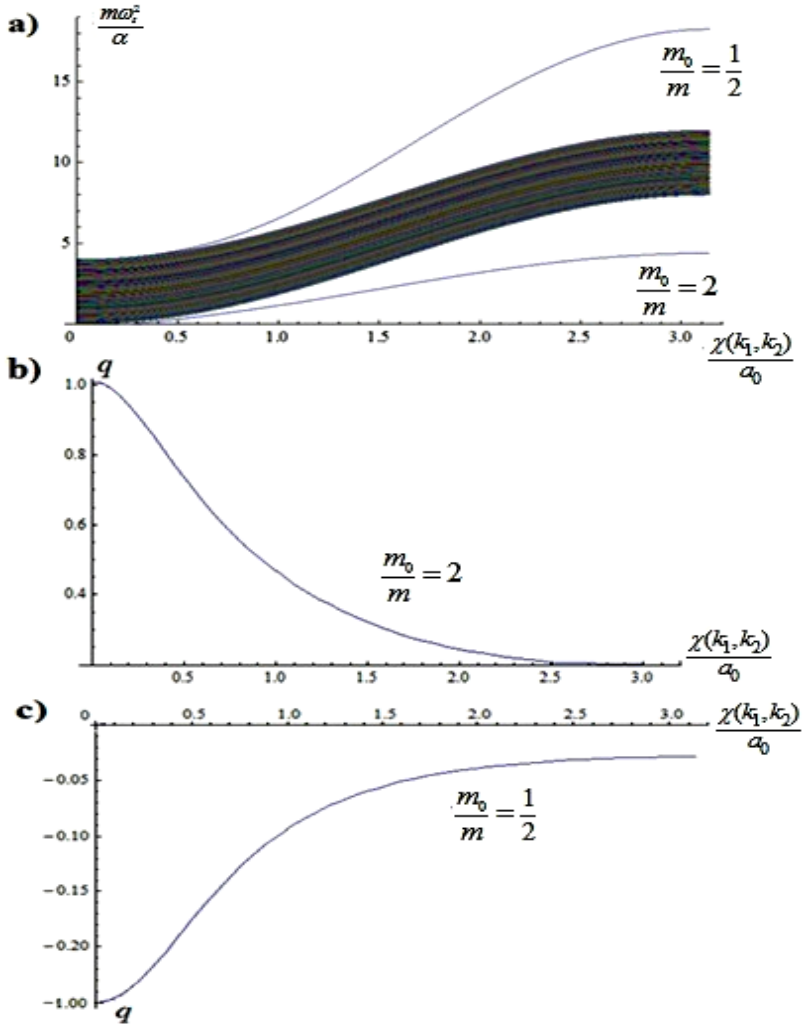

Fig. 19. A diagram of volume zone vibrations and surface waves for $m_0/m=1/2$ and $m_0/m=2$ (a); dependence of q on a two-dimensional wave vector if $m_0/m=2$ (b) and $m_0/m=1/2$ (c). All considered for a (001) adsorbed surface monolayer in a SC crystal.

Here q are the coefficients presented in (79) and (80) for each of the ratios. It's obvious that in both cases $\Delta \succ 0$ because . $q \prec 0, |q| \prec 1$ and A changes from -4 to 4 depending on the value of two-dimensional wave vector $\chi(k_1,k_2)=[0,\pi]$.

For heavy atoms ($m_0 \succ m$). Here $\frac{m_0}{m}=2$ and $\frac{m_0}{m}=5$ have been considered.

$$\frac{m_0}{m}=2:\begin{cases}\dfrac{m\omega_s^2}{\alpha}=\dfrac{3-A+\sqrt{A^2-14A+41}}{4}\\ q=\dfrac{7-A-\sqrt{A^2-14A+41}}{2}\end{cases}, \tag{84}$$

$$\frac{m_0}{m}=5:\begin{cases}\dfrac{m\omega_s^2}{\alpha}=\dfrac{15-4A+\sqrt{16A^2-200A+545}}{20}\\ q=\dfrac{25-4A-\sqrt{16A^2-200A+545}}{8}\end{cases}. \tag{85}$$

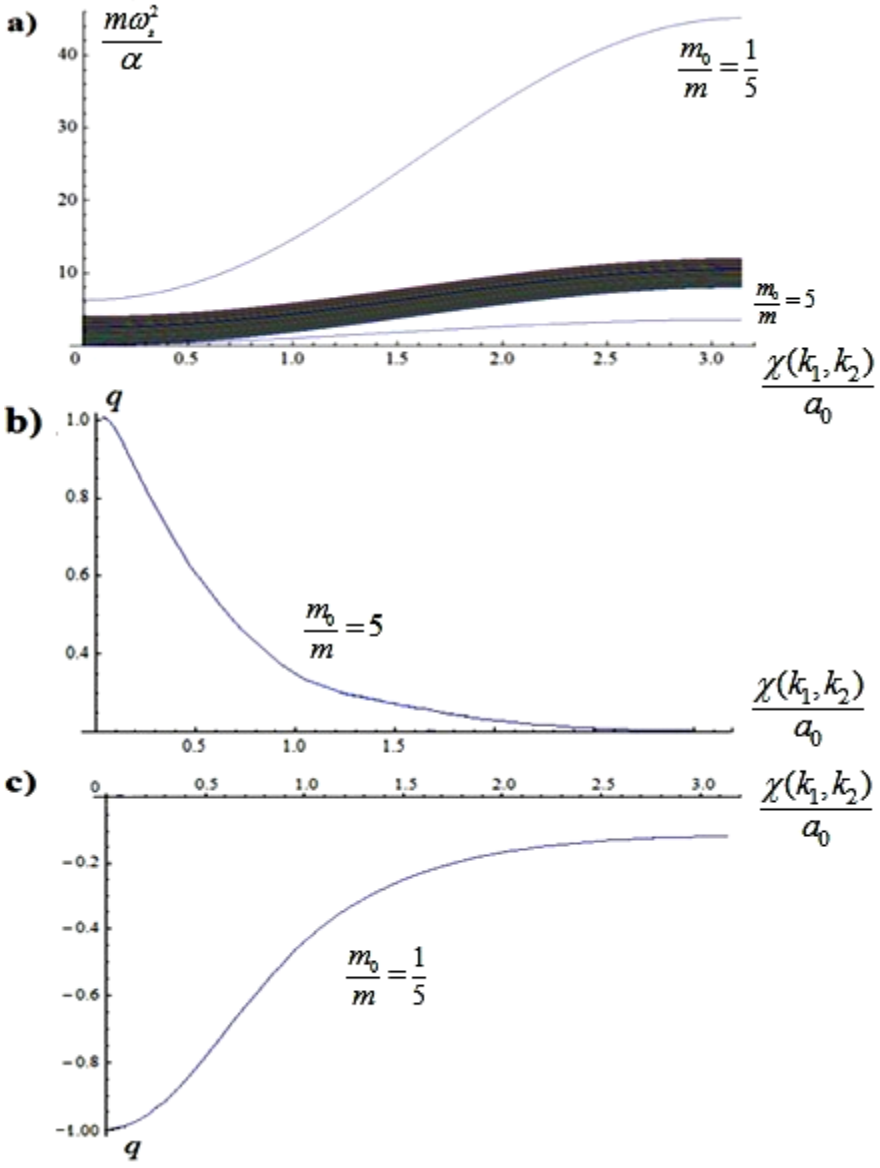

Fig. 20. A diagram of volume zone vibrations and surface waves for $m_0/m=1/5$ and $m_0/m=5$ (a); dependence of q on a two-dimensional wave vector if $m_0/m=5$ (b) and $m_0/m=1/5$ (c). All considered for a (001) adsorbed surface monolayer in a SC crystal.

A surface wave splits off the lowest boundary of the continuous spectrum (Fig. 20), so the splitting value is as follows:

$$\Delta=\frac{m(\omega_V^2)_{\min}}{\alpha}-\frac{m\omega_s^2}{\alpha}\succ 0. \tag{86}$$

For $m_0/m = 2$ we have $\Delta = \dfrac{3 - A + q}{2}$

From the form of (86) it isn't clear if $\Delta \succ 0$ as A varies from -4 to 4. However, in case of $\chi = 0$ and $A = -4$ we have $q = 1$ and $\Delta = 0$. With increasing of χ from 0 to $\pi/2$, q value decreases, and $\Delta \geq 0$ will always be true. Therefore,

$$\Delta = \frac{3 - A + q}{2} \geq 0. \tag{87}$$

As for $m_0/m = 5$ we get

$$\Delta = \frac{10 - 3A + 2q}{5} \geq 0. \tag{88}$$

q are given in (84) and (85). Similarly to $m_0/m = 2$ we find out that $\Delta \geq 0$ is realized for any χ. Based on the above stated, we conclude that, both in the cases of lights and heavy impurity atoms a surface wave splitting off the continuous spectrum exists. Diagrams for the continuous spectrum and surface waves splitted are shown in Fig. 20.

With decreasing of impurity atoms mass a splitting value increases. However, when averaged over all three values of wave vector $\vec{k}(k_1, k_2, k_3)$ the surface waves frequency gets into continuous spectrum. However, there is a sufficiently light impurity mass for a gap between volume zone and surface wave to appear. Let us find an appropriate ratio between impurity and host masses.

From Fig. 19 it's well seen that the lighter the impurity atoms are the greater the minimal surface wave frequency is. As for SC (001) $m(\omega_V^2)_{\max}/\alpha = 12$ (see Fig. 11). We need to find an appropriate m_0/m at which a gap exists, i.e. at which $m\omega_s^2/\alpha \succ m(\omega_V^2)_{\max}/\alpha$. We find q from:

$$m(\omega_V^2)_{\max}/\alpha = 12 = 2 - (q + 1/q) \tag{89}$$

$$q = -5 + \sqrt{24} \approx -1.101. \tag{90}$$

After substituting into (76) we get $m_0/m \approx 11$. Thus, a gap within spectrum appears if impurity atoms are lighter than the host ones in about 11 times.

CONCLUSIONS

The paper is dedicating to consideration of dispersion relations of an infinite and semi-infinite atomic chains consisting of similar and different types of atoms in approximation of the nearest neighbours. When taking to account the next nearest neighbours interaction it turns out that as for the model chosen both attractive ($\alpha_2 \succ 0$) and repulsive ($\alpha_2 \succ 0$) interactions take place. In the first case of problems with the stability of solutions arise. There are no stability problems for attraction, when there should be restriction imposed on α_2 in case of repulsion. In its turn, long-range interaction removes restriction at $\alpha_2 \prec 0$ .The same situation arises within diatomic chains. The features studied come up to the foreground when considering altering-sign chains within metamaterials (a sign before α_i alters)

Phonon and surface waves dispersion relations in cubic crystal are studied in the second section. Allowing for interactions between the nearest neighbors, dispersion relations of volume and surface vibrations for pure shear waves have been found in cases of (001), (110) and (111) surface orientations for simple cubic, face-centered cubic and body-centered cubic crystals. Method described in [14], has been used.

Furthermore, we have considered a monolayer adsorbed on crystal surface both having lighter atoms than those the crystal has, and having heavier ones. For the lighter atoms, consideration was given to $m_0/m = 1/2$ and $m_0/m = 1/5$; for heavier atoms we studied $m_0/m = 2$ and $m_0/m = 5$ (here m_0 is a mass of impurity atom in the adsorbed monolayer, m is a mass of one host atom). For light impurity atoms we have obtained splitting from the top edge of the continuous spectrum; for heavy atoms surface wave splits off from the lowest edge. Surface wave amplitude decreases monotonously in case of heavy atoms; in case of light ones amplitude decrease is oscillating (not monotonous). It has been shown that a gap within continuous spectrum and surface wave appears if $m_0/m \approx 11$.

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NUCLEAR BURNING WAVE REACTOR: SMOOTH START-UP PROBLEM

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The search for a smooth start-up method preventing the excessive increase of neutron flux and power production in the prospective fast reactor at the stage of establishing the self-sustained nuclear burning wave (NBW) regime is carried out. The problem is studied by means of numerical simulation of the initiation and evolution of NBW in such a reactor. For this simulation we use the deterministic approach based on solving the non-stationary neutron diffusion equation using the effective multi-group approximation together with a set of burn-up equations for fuel components and equations of nuclear kinetics for precursor nuclei of delayed neutrons. The special composition of the ignition zone composition that provides a smooth start-up of the NBW reactor is proposed. The features of the initial stage of the NBW reactor are studied in detail.
KEY WORDS: fast reactor, nuclear burning wave, smooth start-up method, intrinsic safety, non-stationary diffusion equation.

РЕАКТОР С ВОЛНОЙ ЯДЕРНОГО ГОРЕНИЯ: ПРОБЛЕМА ПЛАВНОГО ЗАПУСКА

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Проведен поиск методики плавного запуска перспективного быстрого реактора, работающего в режиме волны ядерного горения, избегая чрезмерного увеличения потока нейтронов и мощности реактора на начальном этапе до выхода на стационарный режим бегущей волны. Проблема изучается с помощью численного моделирования, основанного на решении нестационарного уравнения диффузии нейтронов совместно с системой уравнений выгорания для компонентов топлива и уравнения ядерной кинетики ядер предшественников запаздывающих нейтронов с использованием эффективного много-группового приближения. Предложена специальная композиция зоны запала, которая обеспечивает плавный запуск реактора. Исследованы особенности начального этапа работы реактора с волной ядерного горения в этом случае.
КЛЮЧЕВЫЕ СЛОВА: быстрый реактор, волна ядерного горения, плавный запуск реактора, внутренняя безопасность, нестационарное уравнение диффузии.

РЕАКТОР З ХВИЛЕЮ ЯДЕРНОГО ГОРІННЯ: ПРОБЛЕМА ПЛАВНОГО ЗАПУСКУ

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Проведено пошук методики плавного запуску перспективного швидкого реактора, що працює в режимі хвилі ядерного горіння, уникаючи надмірного збільшення потоку нейтронів і потужності реактора на початковому етапі до виходу на стаціонарний режим хвилі, що біжить. Проблема вивчається за допомогою чисельного моделювання, заснованого на рішенні нестаціонарного рівняння дифузії нейтронів разом із системою рівнянь вигоряння для компонентів палива й рівняння ядерної кінетики ядер попередників запізнілих нейтронів з використанням ефективного багато-групового наближення. Запропоновано спеціальну композицію зони запала, що забезпечує плавний пуск реактора. Досліджено особливості початкового етапу роботи реактора із хвилею ядерного горіння в цьому випадку.
КЛЮЧОВІ СЛОВА: швидкий реактор, хвиля ядерного горіння, плавний запуск реактора, внутрішня безпека, нестаціонарне рівняння дифузії.

After the Chernobyl accident, the ensuring of real safety of the operation of nuclear reactors has become a foreground requirement made to their construction. In this context a great interest has been shown in some new concepts of nuclear fission reactors with the so-called intrinsic safety, in which the development of uncontrolled chain nuclear reaction is impossible due to the physical principles of their operation.

One of such concepts is based on the phenomenon of self-sustained nuclear burning wave (NBW) in a fast reactor (FR), which was discovered and preliminary studied by Lev Feoktistov [1, 2]. The non-linear self-organizing regime of the NBW arises owing to a high conversion ratio from fertile to fissile materials in the FR. The main advantage of this type FR is that it does not require a reactivity control and therefore the initial fuel composition of the reactor will evolve according to neutron-nucleus processes without an external intervention and any refueling or fuel shuffling

during the full FR lifetime. The FR is automatically sustained in a state close to the critical one due to a specific type of the negative reactivity feedback, which is inherent to this regime ensuring the intrinsic safety of the NBW reactor.

Further, this concept was developed by several groups of investigators using different approaches and different names for this phenomenon: deflagration wave [3], criticality wave [4], CANDLE [5, 6], nuclear burning wave [7–11] etc. Lately, the most frequently used name is the Traveling Wave Reactor due to Bill Gates and TerraPower activity [12]. To simplify solving the essentially nonlinear non-stationary problem of neutron transport in such a system, Feoktistov [1, 2], as well as many authors later (see, e.g., [4–6]), considered a self-similar solution of this problem. This solution describes only a steady-state regime in the form of traveling NBW. This approach does not allow one to investigate the stability of the nuclear burning process in the reactor relative to different external perturbations, as well as to study the behavior of the FR in transient operation modes, such as the reactor start-up, emergency shutting down and restarting, partial coolant loss and so on.

In our previous works [7–11], a deterministic approach for describing the space-time evolution of the self-organizing regime of NBW in a critical FR has been developed in the framework of multigroup diffusion approximation. This approach is based on solving the non-stationary diffusion equation for neutron transport together with the burn-up equations for fuel components and the equations of nuclear kinetics for precursor nuclei of delayed neutrons, and has allowed us to simulate initiation of the NBW regime and to study its stability relative to distortions of the neutron flux as well as the mechanism of reactivity feedback inherent in this regime. In this approach, a number of studies of the NBW regime behavior were performed for the FR with metal fuel of U-Pu, Th-U and mixed Th-U-Pu cycles with taking account of typical volume fractions of fuel, constructional material (Fe) and different coolants (Na or Pb-Bi eutectic). In these studies, we used a rather simplified FR start-up scenario in which the NBW propagation in the breeding zone filled with the fertile material is initiated by an external neutron flux that irradiates a homogeneous ignition zone enriched with fissile isotopes. These calculations showed, in particular for the U-Pu metal fuel, a principal possibility of initiating the NBW, which then steadily propagates in the breeding zone during a long time period (decades). However, this simplified start-up scheme leads to an essential initial increase of the neutron flux in the ignition zone up to very high values that are unacceptable from the practical point of view and can even destroy the reactor. This initial neutron-flux increase develops slowly enough so that it could be prevented by means of conventional mechanisms of the reactor control in the ignition zone, but it is also interesting to elaborate a method of smooth start-up of this FR, which would include choosing a proper composition of the ignition zone that could ensure acceptable neutron flux values and a moderate power production. The aim of the present study is searching for such a method of smooth start-up of the NBW reactor with using the fuel of U-Pu cycle.

DESCRIPTION OF THE CALCULATION MODEL

In this research, we consider a critical FR of the cylindrical form with the metal fuel of U-Pu cycle in which the NBW would propagate along the cylinder axis (the axial direction). The FR under consideration consists of the ignition zone, that contains ^{238}U enriched with plutonium (the isotope composition of plutonium was ^{239}Pu : ^{240}Pu : ^{241}Pu : ^{242}Pu = 0.70 : 0.22 : 0.05 : 0.03) and the breeding zone adjacent to the ignition one, that is filled with the fertile ^{238}U isotope (see Fig. 1). The both zones also contain the constructional material Fe and the Pb-Bi eutectic coolant. In the simplified start-up scheme [7–11], both these zones are homogeneous with the sharp boundary between them. The initiation of the nuclear burning process in the system is done by an external neutron flux j_{ex}, that irradiates the end of the ignition zone. The initial configuration of the FR is chosen to be very close to the critical state by solving the corresponding criticality problem on reactor parameters that determine the variants of the size and the initial composition of the FR.

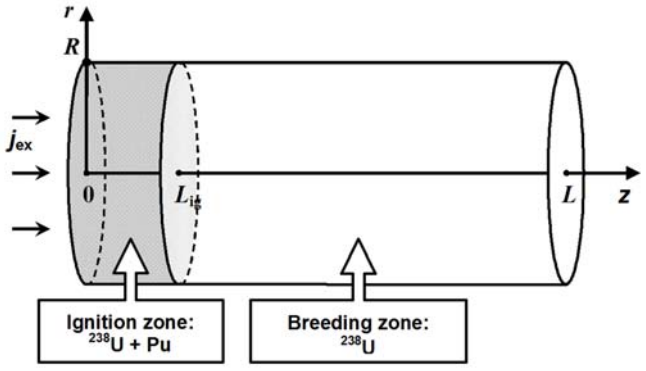

Fig.1. The initial critical assembly for the cylindrical FR with metal U-Pu fuel.

We solve the non-stationary problem under consideration in the so-called effective multigroup approach that was developed by us (see, e.g., [8, 10]). According to this approach, we can write down the one-group non-stationary diffusion equation with allowance for delayed neutrons and using the radial buckling concept in the following form

$$\frac{1}{v}\frac{\partial \Phi}{\partial t}+\frac{\partial V}{\partial z}+DB_r^2\Phi+\Sigma_a\Phi-(1-\overline{\beta})(\nu_f\Sigma_f)\Phi=\sum_l\sum_i\lambda_l^iC_l^i,\ V=-D\frac{\partial \Phi}{\partial z}, \quad (1)$$

where Φ is the scalar neutron flux; Σ_α, $\mathbf{\Sigma}_f$ are the effective macroscopic absorption and fission cross-sections and $D = 1/(3\Sigma_{tr})$ is the diffusion coefficient (Σ_{tr} being the effective macroscopic transport cross-section); $\nu_f\Sigma_f = \Sigma_l(\nu_f\sigma_f)_l$, where ν_f is the mean number of neutrons produced at a single nuclear fission event and l is the number of the fissioned nuclide; $\overline{\beta} = \mathbf{\Sigma}_l\beta_l(\nu_f\Sigma_f)_l / (\nu_f\Sigma_f)$ is the effective fraction of delayed neutrons, $\beta_l = \mathbf{\Sigma}_{li}\beta_l^i$, where β_l^i, C_l^i and λ_l^i are the fraction of delayed neutrons, the concentration and the decay constant of the precursor nuclei in the i-th group of the l-th fissioned nuclide, v is the one-group neutron velocity. The buckling coefficient is $B_r = 2.405 / (R + \delta_r)$, where δ_r is the extrapolation length. We use the value $\delta_r = 20$ cm, which corresponds to the case of a thick radial reflector of heavy material (U, Pb) [13].

The boundary conditions for the flux Φ at the FR ends ($z = 0$ and $z = L$) are:

$$\left(\Phi+2V\right)\Big|_{z=0}=2j_{ex},\quad \left(\Phi-2V\right)\Big|_{z=L}=0. \quad (2)$$

For all values of z in the interval $0 \le z \le L$, an initial distribution of the neutron flux at the moment $t = 0$ is specified, which is chosen as a small scalar neutron flux for the initial critical assembly.

The fuel composition in the FR changes with the time course according to the nuclear transformation chain of the U-Pu fuel cycle. In this transformation chain, we consider, as in [7–11], ten nuclides which are numbered as follows: 1 – ^{238}U, 2 – ^{239}U, 3 – ^{239}Np, 4 – ^{239}Pu, 5 – ^{240}Pu, 6 – ^{241}Pu, 7 – ^{242}Pu, 8 – ^{243}Am, 9 – ^{241}Am, 10 – fission products (FP). The concentrations of these nuclides obey the following burn-up equations:

$$\frac{\partial N_1}{\partial t}=-\sigma_{a1}\Phi N_1, \quad (3)$$

$$\frac{\partial N_l}{\partial t}=-\left(\sigma_{al}\Phi+\Lambda_l\right)N_l+\left(\sigma_{c(l-1)}\Phi+\Lambda_{(l-1)}\right)N_{(l-1)}+\sigma_{c3}\Phi N_3\delta_{l,5},\quad (l=2\div 8), \quad (4)$$

$$\frac{\partial N_9}{\partial t}=\Lambda_6N_6,\quad \frac{\partial N_{10}}{\partial t}=\sum_{l=1,3\div 7}\sigma_{fl}N_l\Phi, \quad (5)$$

where $\sigma_{al} = \sigma_{cl} + \sigma_{fl}$, σ_{cl}, σ_{fl} are the effective one-group microscopic cross-sections of absorption, neutron radiative capture and fission for the l-th nuclide; $\Lambda_l = \ln 2 / T_{1/2}^l$ and $T_{1/2}^l$ are the decay constant and the corresponding half-life for the l-th nuclide. Only the β-decay constants Λ_2, Λ_3 and Λ_6 are considered to be nonzero. At the initial moment, certain concentrations of nuclides are specified: $N_l(z, t = 0) = N_{0l}(z)$. In the calculations, we allow for the fission process for the nuclei with numbers 1, 3–7. Note that in our earlier studies we neglected the intermediate nuclide ^{239}Np burn-up, following [13]. The contribution of ^{239}Np burn-up can be essential for high values of the neutron flux. We use the kinetics equations for the concentrations of precursors of delayed neutrons in the approximation of one equivalent group of delayed neutrons (see, e.g., [7]). The method of solving the burn-up equations (3)–(5) and the nuclear kinetics equations is analogous to that described in [7].

The diffusion equation (1) is solved numerically using the conservative finite difference method (see, e.g., [14]) the implicit difference scheme by [15] with a variable time step, as is described in our previous works [7–11]. In the effective multigroup approach, at each time layer we also solve a multigroup stationary criticality problem with using the radial buckling concept for the assembly composition that changes with time according to the equations of fuel component burn-up. The calculations of the corresponding eigen functions are performed in the 26-group approximation, using the group neutron constant library [16]. The found group neutron fluxes are used to calculate the effective one-group microscopic cross-sections by the averaging procedure described in [13]. Thus, these cross-sections are corrected at each time step according to the neutron spectrum at each space mesh node. Solving the non-stationary problem in the effective multigroup approach with allowance for the mentioned alteration of neutron spectra can describe the evolution of the total (summed over groups) neutron flux accurately enough (see, e.g., [8]).

RESULTS OF CALCULATIONS

We have carried out a series of calculations of the space-time evolution of the NBW regime for different variants of the reactor parameters, which correspond to different compositions and geometrical dimensions of the initial critical FR assembly with using different variants of the ignition zone design. Below, we present the calculation results obtained for a variant of the NBW reactor with the simplified start-up scheme and, beside it, for the analogous FR with using the improved ignition zone design we found for a smooth start-up. First, let us discuss the results obtained for the simplified scheme. In Fig. 2*a* and *b* we present the axial distributions of some constituents of the composition of such a critical FR assembly and corresponding scalar neutron fluxes (normalized to the average energy release 20 W/cm^3). Calculations were performed in the 26-group and effective multigroup approximations for such geometrical dimensions of the reactor: the FR length $L = 500$ cm, the cylinder radius $R = 105$ cm, the axial size of the ignition zone

L_{ig} = 72.75 cm.

We have chosen the following values of the volume fractions of fuel, F_{fuel} = 44%, the constructional material Fe, F_{Fe} = 20%, and the Pb-Bi coolant F_{cool} = 36%. The value of the fuel void fraction p = 0.2. The concentration of plutonium in the ignition zone was chosen at 10%.

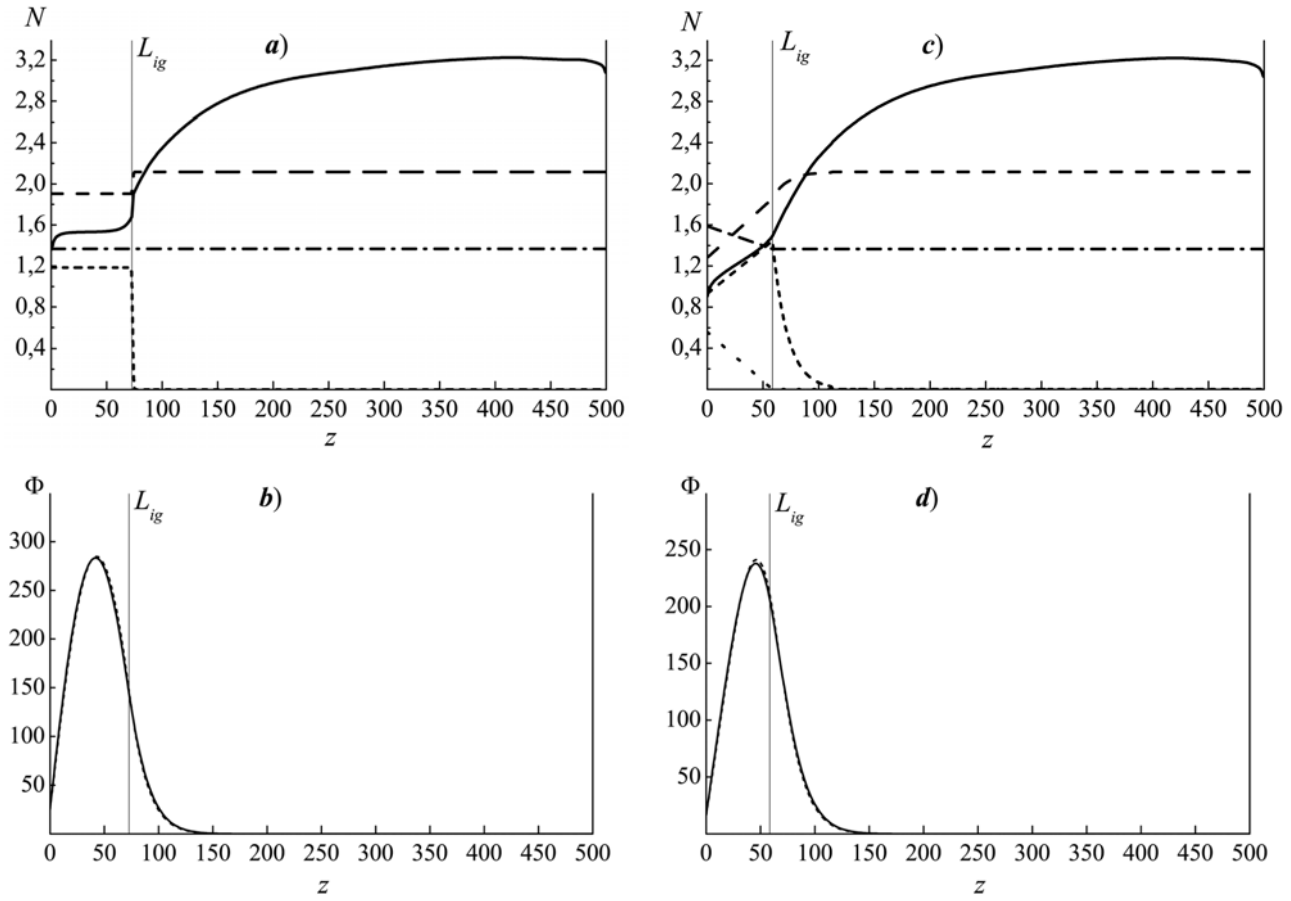

Fig. 2. Axial profiles (z in cm) for the initial critical FR compositions with the simplified (left) and improved smooth (right) start-up schemes.
a) and *c*) presents the concentrations N (10^{-3} $b^{-1}cm^{-1}$) of the actual N_4 (short dashes) and equilibrium N_{eq} (solid line) values for ^{239}Pu; and other values divided by 8: N_1 (dashes) for ^{238}U, $N_{\text{Pb-Bi}}$ (dash-dotted) for Pb-Bi and N_{Ta} (dots) for ^{181}Ta; *b*) and *d*) presents the neutron flux Φ ($b^{-1}day^{-1}$) in the effective multigroup approximation (dashes) and 26-group calculation (solid line).

The comparison of calculations of the neutron flux summed over 26 groups with the flux calculated in the effective multigroup approximation shows that the latter calculation reproduces the exact result in the multigroup approximation quite accurately. From Fig. 2b, it follows that in the simplified scheme the maximum neutron flux is reached approximately in the ignition zone center. The neutron flux on "the tail" of its axial distribution, which illuminates the breeding zone and determines the speed of isotope ^{239}Pu production near the border of the ignition and breeding zones, is not large enough. From Fig. 2a, one can see the ratio between the actual initial ^{239}Pu concentration and its equilibrium value, which is able to ensure, according to [1, 2], the self-sustained burning process and the NBW formation in this FR. The equilibrium value, $N_{eq} = \sigma_{c1}N_1 / (\sigma_{f4} + \sigma_{c4})$, is determined as the value of ^{239}Pu concentration to which it tends asymptotically with the time course under a constant irradiation of the fuel by a neutron flux [1, 2].

The chain reaction in this FR with the simplified start-up scheme is initiated by an external neutron flux with intensity $j_{ex} \approx 10^{13}$ cm^{-2} s^{-1} which is turned off at t = 30 days. As a result, after the initial period of approximately 2 years a stationary wave regime of nuclear burning is set in the FR under consideration. Figs. 3a,b present the corresponding time dependences for the NBW velocity V and the integral power of energy production P_I. Note that for the chosen FR radius and the breeding zone composition, the steady NBW regime has a rather small velocity of the wave (~ 0.05 cm/day) and a long reactor campaign (~ 20 years). The reactor power value at the stage of the stationary burning wave is ~ 3 GW. However, at the very beginning of the campaign, when the wave front is formed near the ignition zone border, there is a huge increase in the neutron flux in the ignition zone to values that are more than an order of magnitude higher than the flux value at the steady NBW stage, which is unacceptable from a practical point of view. In Fig. 3a, this effect is manifested by a sharp surge of the velocity V at $t \approx$ 150 days which is also accompanied

by a very high increase of the reactor power P_I up to values of ~ 30 GW (Fig. 3b).

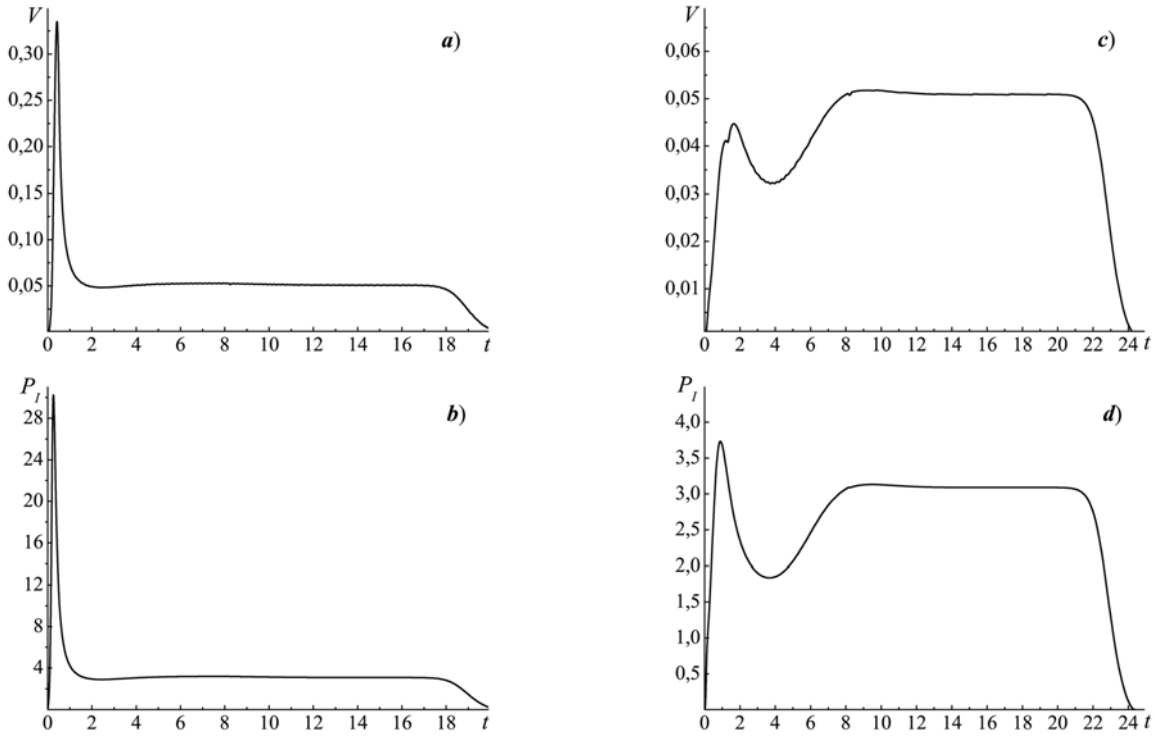

Fig. 3. The NBW velocity V (a, c; cm/day) and the total energy production power P_I (b, d; GW) versus time t (years) for the FR variants with the simplified (left) and improved smooth (right) start-up schemes, whose critical configurations are shown in Fig. 2.

For a better understanding of the process of forming the NBW front and the origin of the above-described unacceptable phenomena, in the left part of Fig. 4 we consider the space evolution of the axial distributions of the neutron flux and main fuel components at the initial stage of the nuclear burning in the FR with the simplified start-up at several time moments at regular intervals (40 days) during the first year of the FR operation. It is seen from Fig. 4a, that at $t < 150$ days (the moments: $t_1 - t_3$) a large increase of the flux Φ occurs, while the position of its maximum is almost the same. Then (the moments: $t_4 - t_8$), the Φ value gradually decreases to a level close to its value in the NBW and the position of the flux maximum gradually moves to the breeding zone, i.e. the wave starts to move. Fig. 4b shows that the time interval $t_1 - t_4$, during which the flux Φ has the largest values, corresponds to the most radical changes of the axial profile of the ^{239}Pu concentration, which consist in its rapid production in the breeding zone near the ignition zone. This leads to creating its distribution form characteristic of the wave front. Then, with a decrease of the flux Φ during the time interval $t_4 - t_8$, slower changes of the ^{239}Pu profile and the final formation of the wave front occur. From Fig. 4*c*, it is seen that during the time interval $t_1 - t_4$, the most rapid transformation and burning of the fertile ^{238}U isotope are observed, and at the interval $t_4 - t_8$ these processes are slower but the NBW front moves further into the breeding zone. From the above-mentioned facts, we can draw the following conclusions. For the simplified type of the ignition zone, a too radical rearrangement of the axial distribution profiles of the main fuel components is necessary to form the NBW front. However, the neutron flux fraction that irradiates the most important region of the ^{239}Pu production at the breeding zone border is rather small (Figs. 2a and 4a). A characteristic feature of the self-organizing process of nuclear burning in FR of this type is that the system itself adjusts in such a way that provides the neutron flux sufficient for the formation of NBW, which leads to its excessive growth.

The observed excessive increase of the neutron flux and energy production is rather slow, and it could be suppressed by a conventional system of external reactor control. However, this method would deprive this FR of its attractive features of self-regulation at the early stage of the NBW initiation, which would be prolonged for many years. Therefore, in this paper, we set the task to provide an acceptable passage of the initial stage of the FR operation without violating the self-regulating nature of the burning regime by choosing an optimal composition of the enriched ignition zone itself. When choosing the ignition zone structure, we aim, firstly, to provide the displacement of a large part of the neutron flux distribution to the breeding zone, and secondly, to facilitate the necessary rearrangement of the initial composition of the ignition zone during the NBW front formation.

It should be noted that in [17], to solve the problem of the smooth start-up of the CANDLE reactor, the authors tried to bring the initial reactor composition maximally close (in terms of k_{inf}) to the composition characteristic of the steady NBW stage. The calculation method, used in [17], is based on the self-similar solution of diffusion equation for neutron transport [5, 6]. This approach is quite sufficient for description of the steady NBW stage; however, it is unable

to describe the non-stationary processes at the initiation of the NBW regime adequately.

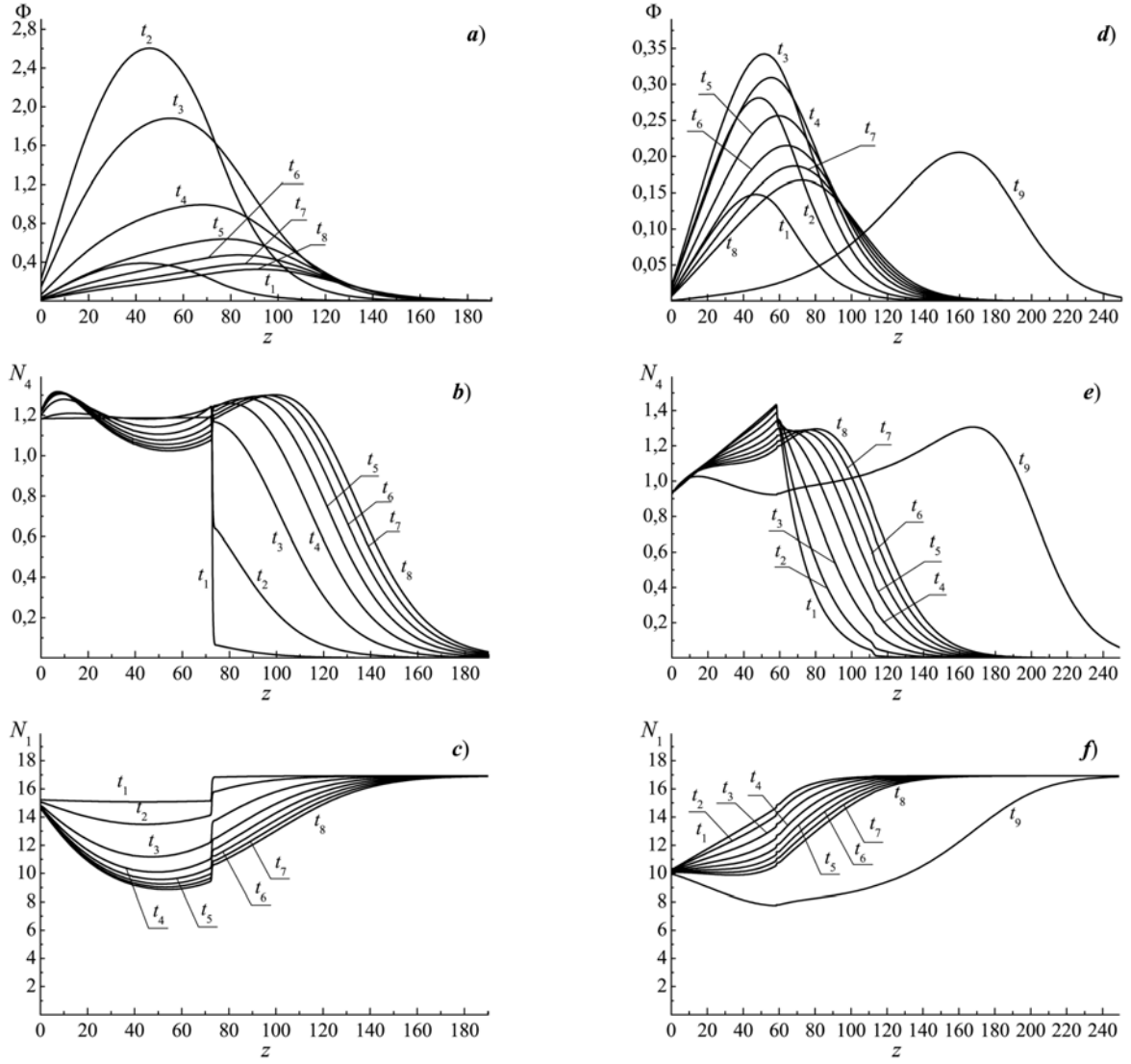

Fig. 4. Initial evolution of axial profiles (z in cm) near the ignition zone for the neutron flux Φ ($\times 10^{17}$ cm^{-2} s^{-1}) and the ^{239}Pu and ^{238}U concentrations N_4 and N_1 ($\times 10^{21}$ cm^{-3}) for the FR with simplified start-up scheme(left or *a*, *b*, and *c*) at the time moments $t_1 = 40$, $t_2 = 80$, $t_3 = 120$, $t_4 = 160$, $t_5 = 200$, $t_6 = 240$, $t_7 = 280$ and $t_8 = 320$ days, and with the improved smooth start-up (right or *d*, *e* and *f*) at the moments $t_1 = 100$, $t_2 = 200$, $t_3 = 300$, $t_4 = 400$, $t_5 = 500$, $t_6 = 600$, $t_7 = 700$, $t_8 = 800$ and $t_9 = 3000$ days.

In this paper, we have considered a number of possible variants for the ignition zone structure to optimize the regime start-up stage. On the basis of this analysis, we have proposed an improved ignition zone configuration for this FR, the use of which we consider below.

In the right part of Fig. 2, we present the characteristics of the initial critical FR assembly with the improved ignition zone of this type. The main parameters of the considered FR are the same as presented above, except the ignition zone. Now the plutonium content in the ignition zone is not constant, but varies by the linear law: $N_{\text{Pu}} = N_{\text{f}} [e_1 + z (e_2 - e_1) / L_{ig}]$, where N_{f} is the concentration of the fuel nuclides in the breeding zone, and the coefficients e_1 and e_2 characterize the fuel enrichment in the ignition zone. In the breeding zone, in the layer adjacent to the ignition zone, $L_{ig} < z < L_{ig} + 4\Delta$, we add an exponential "tail" enriched with plutonium: $N_{\text{Pu}} = N_{\text{f}} e_2 \exp[-(z - L_{ig}) / \Delta]$. This "tail" essentially facilitates forming the NBW front. The fuel volume fraction in the ignition zone varies linearly: $F_{\text{f}}^{(\text{ig})}(z) = F_{\text{f}} [u_1 + (1 - u_1) z / L_{ig}]$. The decrease of the fuel fraction in the ignition zone is chosen in such a way that the corresponding content of ^{238}U would ensure the equilibrium values N_{eq} being nearly at the level of the actual ^{239}Pu concentration (Fig. 2c).

The volume freed from the fuel is filled up with a mixture of the Pb-Bi alloy, which weakly absorbs neutrons, and ^{181}Ta that is used as an absorbing material in fast reactors [13]. The relative volume fraction of ^{181}Ta, $F_{\text{Ta}} = 0.58$, is chosen so that this mixture, in its absorption properties, could imitate the presence of fission products on the back side of the wave. An important effect of introducing this absorber in the ignition zone is shifting the maximum of the initial distribution of the neutron flux (Fig. 2d) in the direction of the breeding zone. Thus, an essential fraction of the flux

falls on the region of forming the NBW front in the breeding zone. The values of the above-mentioned parameters of the ignition zone used in the case under consideration are as follows: $L_{ig} = 58.5$ cm, $e_1 = 0.079$, $e_2 = 0.122$, $\Delta = 13.5$ cm, $u_1 = 0.687$.

Here, we also use a more effective scheme of bringing the initial neutron field in the FR to a chosen optimal level by using an additional absorbing ^{181}Ta regulator in the ignition zone. The initial configuration of FR is chosen with a little reactivity excess, $\rho \sim 10^{-4}$. The system is brought to a subcritical state by the additional tantalum absorber, which is gradually withdrawn from the system after turning the external neutron flux ($j_{ex} \approx 10^{11}$ cm^{-2} s^{-1}), until the neutron field in the FR reaches the chosen level. Note that in this case we can use a significantly lower value of j_{ex}. According to this, the additional concentration of ^{181}Ta varies with time as: $N_{\mathrm{Ta}}(t) = N_{\mathrm{Ta}}^{(0)}(T - t) / T$. In the presented calculation we put $N_{\mathrm{Ta}}^{(0)} = 2.5 \cdot 10^{-4}$ b^{-1}cm^{-1}, $T = 40$ days, and the neutron flux was brought to ~ 80% of its level in the NBW regime, after which the regulator withdrawal was stopped and j_{ex} was turned off.

In the right part of Fig. 3, we present the time dependencies of the NBW velocity V and total energy production power P_I during the reactor campaign for the FR with the above-described improved ignition zone. Fig. 3d shows that employing the improved start-up scheme allows us to prevent the exorbitant increase of the reactor power. There is no great surge of velocity value V (Figs. 3c and 3a), as well.

The NBW regime is formed slightly slower (for about 2.5 years) than in the case presented in the left part of Fig. 3. Note that the wave moves, at first, with a less velocity and a less power P_I than at the stage of the steady NBW regime, which, probably, is due to the influence of edge effects from the ignition zone residuals. Finally, the NBW reaches the steady regime in several years, which is not an essential disadvantage of the considered scheme, because at this stage the FR power should be adjusted according to current demands by some proper methods (e.g., by changing the radial reflector efficiency), which are not considered here.

In the right part of Fig. 4, we consider the space-time evolution of the distributions of neutron flux and main fuel components at the beginning of this FR campaign. We present the axial profiles of these quantities for several initial moments of time $t_1 - t_8$ of the reactor operation at regular intervals (100 days) and for the moment t_9, when the NBW has reached the steady regime. Unlike the left part of Fig. 4, here there is no excessive increase of the neutron flux, and the rearrangement of the system components and the formation of the wave front occur smoothly. During the interval $t_1 - t_8$, the maximum of the neutron flux gradually shifts toward the breeding zone. Note also that Figs. 4e and 4f show that the initial profile of the ignition zone, in fact, imitates roughly the form of NBW front. It is interesting that, for the moment t_8, the ^{239}Pu and ^{238}U distributions in the wave front coincide with those for the moment t_9 in the steady regime, but the level of the neutron flux at t_8 is slightly lower, which corresponds to the initial slowdown of the burning wave mentioned above.

CONCLUSION

The results of studies of establishing the stage of self-sustained NBW regime in the prospective FR under consideration show that an excessive increase of neutron flux and power production, that is mainly due to a lack of adequate amount of fission products at the ignition stage, as compared with the steady state of the NBW regime, can be prevented by using a special smooth start-up method proposed in this paper. This method is based on the selection of the ignition zone composition featured by the fuel component distribution and neutron flux profile roughly similar to the corresponding characteristics inherent to the steady state regime of the NBW propagation in FR. The absence of fission products at the initial stage of the reactor start-up compensate with adding a certain amount of the metallic tantalum, which is a good neutron absorber. The composition and spatial distribution of the fuel components (uranium and plutonium) and absorber (tantalum) in the ignition zone are selected in a way that provides a significant displacement of the neutron flux in the initial assembly of FR to the border between ignition and breeding zones.

The problem is studied by means of the numerical simulation of initiation and evolution of the NBW in a cylindrical FR with metallic U-Pu fuel in the framework of the deterministic approach based on solving the non-stationary diffusion equation of neutron transport together with a set of burn-up equations for fuel components and equations of nuclear kinetics for precursor nuclei of delayed neutrons with making use of the effective multigroup approximation and radial buckling concept.

Basing on this calculation scheme, we have also considered a gradual initial bringing of the neutron flux to an optimum level by using an additional tantalum regulator in order to ensure a relatively short time period of forming the self-sustained NBW regime. This scenario also provides a reduction of the intensity and duration of the external neutron flux used for initiating the NBW regime. The features of the initial stage of operation of the NBW reactor with improved ignition zone are studied in detail. It is shown that using the proposed start-up method makes it possible to suppress the initial increase of neutron flux almost by a factor of ten in comparison with the simplified start-up scheme and to get its value very close to the neutron flux value at the steady NBW regime (Figs. 4a,d). The residual variation of the neutron flux which takes place at the start-up of FR is very slow and has a small enough amplitude and, therefore, can be easily removed in a real reactor by means of control rods or a corresponding change in the efficiency of the radial reflector.

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MAGNETOSTATIC WAVES IN STRUCTURE WITH TWO ANISOTROPIC LAYERS WITH NONCOLLINEAR ORIENTATION OF MAGNETIZATIONS

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In this paper we present a theoretical investigation of the magnetostatic volume wave propagation in bilayer structure consisted of two ferromagnetic layers. The magnetic anisotropy field is assumed to be different in the two layers, and hence the magnetization in one layer can be aligned at an angle with respect to the magnetization direction in the other layer. The case of cubic and indused uniaxial anisotropy have been considered. Numerical calculations for YIG (yttrium-iron-garnet) ferrites show anisotropic propagation of the volume magnetostatic wave in that structure. Dispersion curves for YIG bilayer structure are shown to illustrate the effects of angle between the magnetization vectors in the magnetic layers and propagation direction on the properties of magnetostatic waves.
KEY WORDS: magnetostatic waves, bilayer structure, noncollinear orientation, anisotropy, dispersion relationship.

МАГНИТОСТАТИЧЕСКИЕ ВОЛНЫ В СТРУКТУРЕ С ДВУМЯ АНИЗОТРОПНЫМИ СЛОЯМИ С НЕКОЛЛИНЕАРНОЙ ОРИЕНТАЦИЕЙ НАМАГНИЧЕННОСТЕЙ

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В этой статье представлено теоретическое исследование распространения магнитостатических объемных волн в двухслойной структуре, состоящей из двух ферромагнитных слоев. Предполагается, что поле магнитной анизотропии в этих слоях различно и следовательно намагниченность в одном слое может быть неколлинеарна намагниченности в другом слое. Рассмотрен случай кубической и индуцированной одноосной анизотропии. Численный расчет для ЖИГ (железо-иттриевый гранат) показал, что распространение магнитостатических объемных волн в данной структуре является анизотропным. Для иллюстрации влияния угла между векторами намагниченности магнитных слоев и направления распространения на свойства магнитостатических волн приведены дисперсионные кривые для двухслойной ЖИГ структуры.
КЛЮЧЕВЫЕ СЛОВА: магнитостатические волны, двухслойная структура, неколлинеарная ориентация, анизотропия, дисперсионное соотношение.

МАГНИТОСТАТИЧНІ ХВИЛІ У СТРУКТУРІ З ДВОМА АНІЗОТРОПНИМИ ШАРАМИ З НЕКОЛІНЕАРНОЮ ОРІЄНТАЦІЄЮ НАМАГНІЧЕНОСТЕЙ

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У цій статті представлено теоретичне дослідження поширення магнітостатичних об′ємних хвиль в двошаровій структурі, що складається з двох феромагнітних шарів. Передбачається, що поле магнітної анізотропії в цих шарах різне і отже намагніченість в одному шарі може бути неколінеарна намагніченості в іншому шарі. Розглянутий випадок кубічної та індукованої одновісної анізотропії. Чисельний розрахунок для ЗІГ(залізо-ітрієвий гранат) показав, що поширення магнітостатичних об′ємних хвиль в даній структурі є анізотропним. Для ілюстрації впливу кута між векторами намагніченості магнітних шарів і напряму поширення на властивості магнітостатичних хвиль приведені дисперсійні криві для двошарової ЗІГ структури.
КЛЮЧОВІ СЛОВА: магнитостатичні хвилі, двохшарова структура, неколінеарна орієнтація, анізотропія, дисперсійне співвідношення.

Over the last years the magnetostatic waves have attracted extensive attention on both theoretical and experimental aspects. Their phase velocity is small compared to the speed of light and so in describing magnetostatic waves we can use the equations of magnetostatics. If we take wave vectors in the region 30 $cm^{-1} < |k| < 10^5$ cm^{-1} the dispersion relationship can be derived without taking exchange interactions and electromagnetic retardation into consideration.

Magnetostatic waves have been studied at first by Damon and Eshbach [1]. These waves are separated into three categories: magnetostatic surface waves (MSSW's) and magnetostatic backward-volume waves (MSBVW's) for the in-plane-magnetized film case and magnetostatic forward-volume waves (MSFVW's) for the perpendicularly magnetized film case. It should be pointed out that the exchange effects are not very important for backward-volume waves.

Increased interest in multilayer structures with noncollinear orientation of magnetization vectors associated with the fact that the external magnetic field applied in the plane of a film allows characteristics of the system to be easily changed by varying the angle between the magnetization vectors in the layers [2]. From the application point of view, having a bilayer with noncollinear orientation of magnetization vectors instead of a single film offers more degrees of

freedom for tailoring special properties. Moderately simple and proficient control of properties magnetostatic modes in that structure by means of applying an external magnetic field open up fresh opportunities for their practical implementations.

A deficiency of magnetic or nonmagnetic ions in YIG can give rise to anisotropic terms different from cubic symmetry. The authors [3] found for YIG disks that can be uniaxial in-plane induced magnetic anisotropy as a result of the lattice mismatch. Also, the Bi-doped YIG film have strong induced magnetic anisotropy. For Bi-doped YIG, by controlling the factors affecting the induced magnetic anisotropy one can make the easy axis be either perpendicular or parallel to the structure.

Various authors have considered the influence of anisotropy on magnetostatic waves [4-7]. A substantial amount of work has been devoted to the analysis of magnetostatic waves in multilayers composed of ferromagnetic materials and dielectrics [8-12]. In [7] the theory is developed for dispersion characteristics of spin waves in ferromagnetic films taking into account both dipole-dipole and exchange interactions, crystallographic anisotropy and mixed exchange boundary conditions on the film surfaces.

So far as we know for the investigation of the magnetostatic waves such geometry of structure was employed only by Sun K and Vittoria S. [6]. In [6] the spectrum of MSSW has been studied for structure with noncollinear orientation of magnetizations ($M_1 \neq M_2$) but no consideration has been given to volume magnetostatic waves.

We now consider this problem for the volume magnetostatic waves. The purpose of this paper is to investigate the effect of anisotropy on magnetostatic wave propagation in the layered structures with noncollinear orientation of magnetization vectors. As will be seen, these effect is of more interest in the case of the noncollinear magnetizations as compared to the parallel one. Our investigation have been restricted to the case of magnetization in the plane of the slab.

MODEL AND METHOD

Let us consider the magnetic structure consisting of two ferromagnetic films separated by a nonmagnetic interlayer (Fig.1), where equilibrium orientation of the magnetization vectors in the magnetic layers is supposed to be in the film plane and make a certain angle γ between each other. The film is assumed to be magnetically anisotropic. An external static magnetic field **H** is applied in the film plane at an angle Θ relative to the **X** -axis so that the total internal magnetic fields also lie in the planes of the layers. For simplicity assume that thicknesses of the ferromagnetic layers $d_1 = d_2$. Fig. 1 shows a bilayer structure placed in **X-Y-Z** coordinate system so that the plane of the film coincides with the **X-Y** plane. The vector **k** and angle φ designate the in-plane wave vector and propagation angle, respectively.

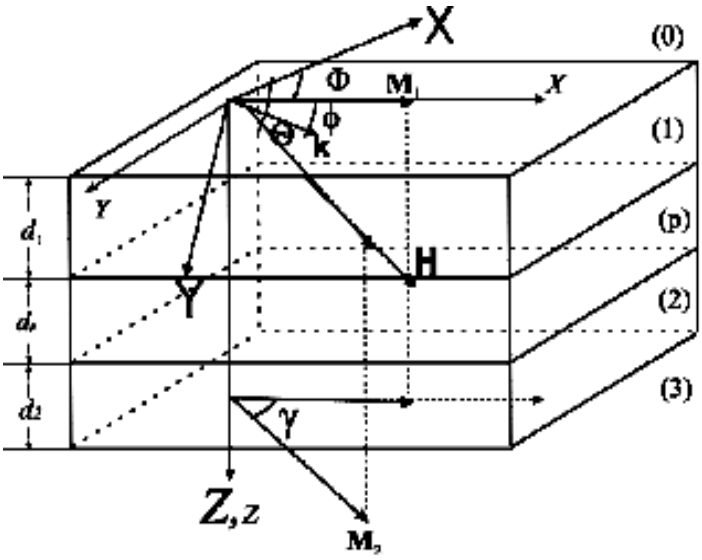


Fig.1. Film, field and magnetizations geometry.

For YIG the **X-,Y,Z-** axes represent the crystallographic directions for the cubic single crystal.

We make the simplifying assumptions that the film is infinite in the **X**- and **Y**-directions and has a thickness *d* in the **Z**-direction. An additional *x-y-z* coordinate system is also shown (the *x*-axis is along the $\mathbf{M}_1$ vector).

The saturation magnetization vector $\mathbf{M}_2$ coincides with vector **H** and the saturation magnetization vector $\mathbf{M}_1$ is at some angle Φ relative to the **X**-axis. The internal fields $H_o^{(1)}$ and $H_o^{(2)}$ also lie in the plane **X-Y**. The quantities $H_o^{(1)}$ and $H_o^{(2)}$ can be expressed in terms of the external field H, the static cubic anisotropy field components $H_A^{(1)}$ and $H_A^{(2)}$, and the static-induced in-plane anisotropy field component $H_U^{(1)}$, where the superscripts (l) and (2) denote the layers corresponding to $\mathbf{M}_1$ and $\mathbf{M}_2$.

We use the macroscopic phenomenological theory: Maxwell's equations, considering the boundary conditions of the structure and the Landau-Lifshitz equation of motion for the magnetization. The macroscopic approach treats the total energy in terms of the magnetization. The magnetostatic dispersion relationship may be expressed in terms of permeability tensor elements for each rnagnetic layer.

The Landau-Lifshitz equation of motion for the magnetization of film *i* (*i*=1,2) is written as

$$\frac{d}{dt}\mathbf{M}_{(i)}=\gamma\left[\mathbf{M}^{(i)}\times\mathbf{H}_o^{(i)}\right] \quad (i=1,2),$$
$$\mathbf{H}_o^{(i)}=-\left(e_x\frac{\partial F}{\partial \mathrm{M}_x^{(i)}}+e_y\frac{\partial F}{\partial \mathrm{M}_y^{(i)}}+e_z\frac{\partial F}{\partial \mathrm{M}_z^{(i)}}\right) \tag{1}$$
$$F=F_A-\mathbf{M}\left(\mathbf{H}+\mathbf{h}\right)$$

where F_A - magnetocrystalline anisotropy free energy density, $\mathbf{H_o}$ – total internal field, **H** - external static magnetic field.

An magnetocrystalline anisotropy free energy density is written as

$$F_A=K_U\left(1-\mathbf{M}_X^2/\mathbf{M}_Y^2\right)+K_1\left(\mathbf{M}_X^2\mathbf{M}_Y^2+\mathbf{M}_Y^2\mathbf{M}_Z^2+\mathbf{M}_Z^2\mathbf{M}_X^2\right) \tag{2}$$

where K_U denotes a uniaxial anisotropy energy density parameter, K_1 denotes a first order cubic anisotropy energy density parameter.

The internal $\mathbf{H}_o^{(i)}$ consists of the static effective field $\mathbf{H_s}$ and dynamic effective field **h** components, that contain anisotropy terms in the dynamic response for magnetostatic waves. Also, the magnetization is written as the sum of a static part **M** and a fluctuating part **m**. For layer (1), in the small signal limit in which $\mathrm{lm(r,t)l} << \mathrm{M_s}$ $\left(\mathrm{M_s}-\text{saturation magnetization}\right)$ is satisfied, m has only transverse components m_y and $\mathrm{m_Z}$.

In order to obtain the magnetostatic dispersion relations, one has to find the permeability tensor elements for each layer.

By linearizing the Landau-Lifshitz equation (1), after some algebraic manipulations, the dynamic permeability tensors are obtained. For layer (1), where the lowest order terms in a small amplitude dynamic response involve only the *y*- and *z*- components of the total magnetization vector $\mathbf{M}^{(1)}$, it is given by

$$\begin{pmatrix} b_y \\ b_z \end{pmatrix}=\hat{\boldsymbol{\mu}}\begin{pmatrix} h_y \\ h_z \end{pmatrix}=\begin{pmatrix} 1+k_\alpha & -i\nu \\ i\nu & 1+k_\beta \end{pmatrix}\begin{pmatrix} h_y \\ h_z \end{pmatrix}$$

$$k_\alpha=\frac{\Omega_\alpha}{\Omega_\alpha\Omega_\beta-\Omega^2},\quad k_\beta=\frac{\Omega_\beta}{\Omega_\alpha\Omega_\beta-\Omega^2},\quad \nu=\frac{\Omega}{\Omega_\alpha\Omega_\beta-\Omega^2} \tag{3}$$

$$\Omega=\frac{\omega/\gamma}{4\pi M_s},\quad \Omega_{\alpha,\beta}=\frac{H_{\alpha,\beta}}{4\pi M_s}$$

where

$$H_\alpha=H\cos\left(\Theta-\Phi\right)+H_U\cos^2\left(\Phi\right)+H_A\left[1-\frac{\sin^2\left(2\Phi\right)}{2}\right]$$
$$H_\beta=H\cos\left(\Theta-\Phi\right)+H_U\cos\left(2\Phi\right)+H_A\cos\left(4\Phi\right) \tag{4}$$

For layer 2 it is given by:

$$\begin{pmatrix} b_x \\ b_y \\ b_z \end{pmatrix}=\hat{\boldsymbol{\mu}}\begin{pmatrix} h_x \\ h_y \\ h_z \end{pmatrix}=\begin{pmatrix} 1+k_\alpha^{(2)}\sin^2(\gamma) & -k_\alpha^{(2)}\cos(\gamma)\sin(\gamma) & i\nu\sin(\gamma) \\ -k_\alpha^{(2)}\cos(\gamma)\sin(\gamma) & 1+k_\alpha^{(2)}\cos^2(\gamma) & -i\nu\cos(\gamma) \\ -i\nu\sin(\gamma) & i\nu\cos(\gamma) & 1+k_\beta^{(2)} \end{pmatrix}\begin{pmatrix} h_x \\ h_y \\ h_z \end{pmatrix}$$

$$k_\alpha=\frac{\Omega_\alpha}{\Omega_\alpha\Omega_\beta-\Omega^2},\quad k_\beta=\frac{\Omega_\beta}{\Omega_\alpha\Omega_\beta-\Omega^2},\quad \nu=\frac{\Omega}{\Omega_\alpha\Omega_\beta-\Omega^2} \tag{5}$$

$$\Omega=\frac{\omega/\gamma}{4\pi M_s},\quad \Omega_{\alpha,\beta}=\frac{H_{\alpha,\beta}}{4\pi M_s},$$

where

$$H_\alpha=H+H_A\left[1-\frac{\sin^2\left(2\Theta\right)}{2}\right]$$
$$H_\beta=H+H_A\cos\left(4\Theta\right). \tag{6}$$

The fluctuating part of the dipole field **h** and the magnetization **m** must satisfy the magnetostatic form of Maxwell's equations

$$\mathrm{div}\left[\mathbf{h}+4\pi\mathbf{m}\right]=0,\quad \mathrm{rot}\mathbf{h}=0. \tag{7}$$

Under the magnetostatic approximation $\mathbf{h}=\mathrm{grad}\left[\psi\exp(-i\omega t)\right]$, where ψ is a magnetic scalar potential. The problem is now reduced to finding the propagating normal mode solutions for the scalar potential ψ which satisfy the condition (7), that gives simple equation:

$$\mu_{11}^{(i)}\frac{\partial^2\psi}{\partial x^2}+\mu_{22}^{(i)}\frac{\partial^2\psi}{\partial y^2}+\mu_{33}^{(i)}\frac{\partial^2\psi}{\partial z^2}+2\mu_{12}^{(i)}\frac{\partial^2\psi}{\partial x\partial y}=0 \tag{8}$$

where

$$\mu_{11}^{(1)}=1;\mu_{22}^{(1)}=1+k_{\alpha}^{(1)};\mu_{33}^{(1)}=1+k_{\beta}^{(1)};\ \mu_{12}^{(1)}=0$$
$$\mu_{11}^{(2)}=1+k_{\alpha}^{(2)}\sin^2(\gamma);\mu_{22}^{(2)}=1+k_{\alpha}^{(2)}\cos^2(\gamma);\mu_{33}^{(2)}=1+k_{\beta}^{(2)};\ \mu_{12}^{(2)}=-k_{\alpha}^{(2)}\cos(\gamma)\sin(\gamma);$$

The scalar potential functions $\psi^{(1,2)}$ are taken in the form:

$$\psi^{(1,2)}=\left(a^{(1,2)}\exp\left(k_z^{(1,2)}z\right)+b^{(1,2)}\exp\left(k_z^{(1,2)}z\right)\right)\exp\left(i\kappa_x^{(1,2)}x\right)\exp\left(i\kappa_y^{(1,2)}y\right) \tag{9}$$

$k_z^{(1,2)}$ parameters are related to the propagation wave number $\kappa=\sqrt{\kappa_x^{(1)2}+\kappa_y^{(1)2}}=\sqrt{\kappa_x^{(2)2}+\kappa_y^{(2)2}}$ through Eq.(8):

$$k_z^{(1)}=i\kappa\sqrt{-\left(1+k_{\alpha}^{(1)}\sin^2(\varphi)\right)/\left(1+k_{\beta}^{(1)}\right)},\quad k_z^{(2)}=i\kappa\sqrt{-\left(1+k_{\alpha}^{(2)}\sin^2(\gamma-\varphi)\right)/\left(1+k_{\beta}^{(2)}\right)} \tag{10}$$

Under the magnetostatic approximation, by imposing the usual electromagnetic boundary conditions, a set of homogeneous equations is generated. The condition for the existence of a nontrivial solution yields the dispersion relation.

$$F_1(\Omega,\kappa d)F_2(\Omega,\kappa d)-e^{-2\kappa d_p}P_1(\Omega,\kappa d)P_2(\Omega,\kappa d)=0 \tag{11}$$

where

$$F_1(\Omega,\kappa)=\kappa+i\kappa_y\mu_{32}^{(1)}+k_z^{(1)}\mu_{33}^{(1)}\left[(B\exp(2k_z^{(1)}d_1)-1)/(B\exp(2k_z^{(1)}d_1)+1)\right]$$
$$F_2(\Omega,\kappa)=\kappa-i\kappa_x\mu_{31}^{(2)}-i\kappa_y\mu_{32}^{(2)}-k_z^{(2)}\mu_{33}^{(2)}\left[(V\exp(2k_z^{(2)}(d_1+d_p))-1)/(V\exp(2k_z^{(2)}(d_1+d_p))+1)\right]$$
$$P_1(\Omega,\kappa)=\kappa-i\kappa_y\mu_{32}^{(1)}-k_z^{(1)}\mu_{33}^{(1)}\left[(B\exp(2k_z^{(1)}d_1)-1)/(B\exp(2k_z^{(1)}d_1)+1)\right]$$
$$P_2(\Omega,\kappa)=\kappa+i\kappa_x\mu_{31}^{(2)}+i\kappa_y\mu_{32}^{(2)}+k_z^{(2)}\mu_{33}^{(2)}\left[(V\exp(2k_z^{(2)}(d_1+d_p))-1)/(V\exp(2k_z^{(2)}(d_1+d_p))+1)\right]$$
$$B=\frac{\kappa-i\kappa_y\mu_{32}^{(1)}+k_z^{(1)}\mu_{33}^{(1)}}{i\kappa_y\mu_{32}^{(1)}+k_z^{(1)}\mu_{33}^{(1)}-\kappa},V=\frac{k_z^{(2)}\mu_{33}^{(2)}-\kappa-i\kappa_y\mu_{32}^{(2)}-i\kappa_x\mu_{31}^{(2)}}{k_z^{(2)}\mu_{33}^{(2)}+\kappa+i\kappa_y\mu_{32}^{(2)}+i\kappa_x\mu_{31}^{(2)}}\exp(-2k_z^{(2)}(2d_1+d_p)),\Omega=\frac{\omega/\gamma}{4\pi M_s}.$$

The dipersion relation includes two parts. One is the product of the individual dispersion of each layer. The other is the coupling term due to the interaction between the two ferromagnetic layers. As the separation between the ferromagnetic layers goes to infinity, than one can obtain the individual dispersion relation for each layer.

NUMERICAL RESULTS

Numerical calculations have been performed to investigate the magnetostatic volume wave properties. The following thicknesses of layers are used: d_1=1 μm, d_2=1 μm, d_p=20 nm. Specifically, the case of YIG ferrites have been considered ($H=800$ Oe, $H_A^{(1)}=-90$ Oe, $H_A^{(2)}=-86$ Oe, $\Theta=57^o$, $H_U^{(1)}=200$ Oe) [5]. For Fig. 2 and Fig.3, which show the dispersion curves, $M_1=M_2=1750$ G. Fig.4 shows other example of the effects of anisotropy for ferromagnetic layers with different static magnetizations $M_1=1750$ G, $M_2=1256$ G [6].

We can see from Fig. 2-4 the two set of dispersion curves corresponding to layer 1 and layer 2 with different volume mode band limits (Fig. 5). Each set and volume mode band corresponds to the individual magnetic layer. It is important to realize at this point that there is an infinite manifold of volume mod dispersion curves. For the range of kd values, the dispersion curves cover the entire volume mode band for each set. All curves correspond to the roots of transcendental equation (11). In the case of one layer (Fig. 3a), only one set of curves exist.

For YIG materials the volume mode band similar for the band for the isotropic film, except for a surviving band width even at in-plane propogation angle $\varphi=90^o$ (as can be expected, in the limit $\varphi\to 90°$ the volume mod band has reduced but has a nonzero width).

As seen from Fig. 2, the propeties of volume magnetostatic modes in that structure are substantially determined by the angle between magnetization vectors in the magnetic layers and the rotation of the direction of propagation in the plane of the film. We can see that splitting between the dispersion curves for layer (1) and layer (2) will rise with a rise in-plane propagation angle φ.

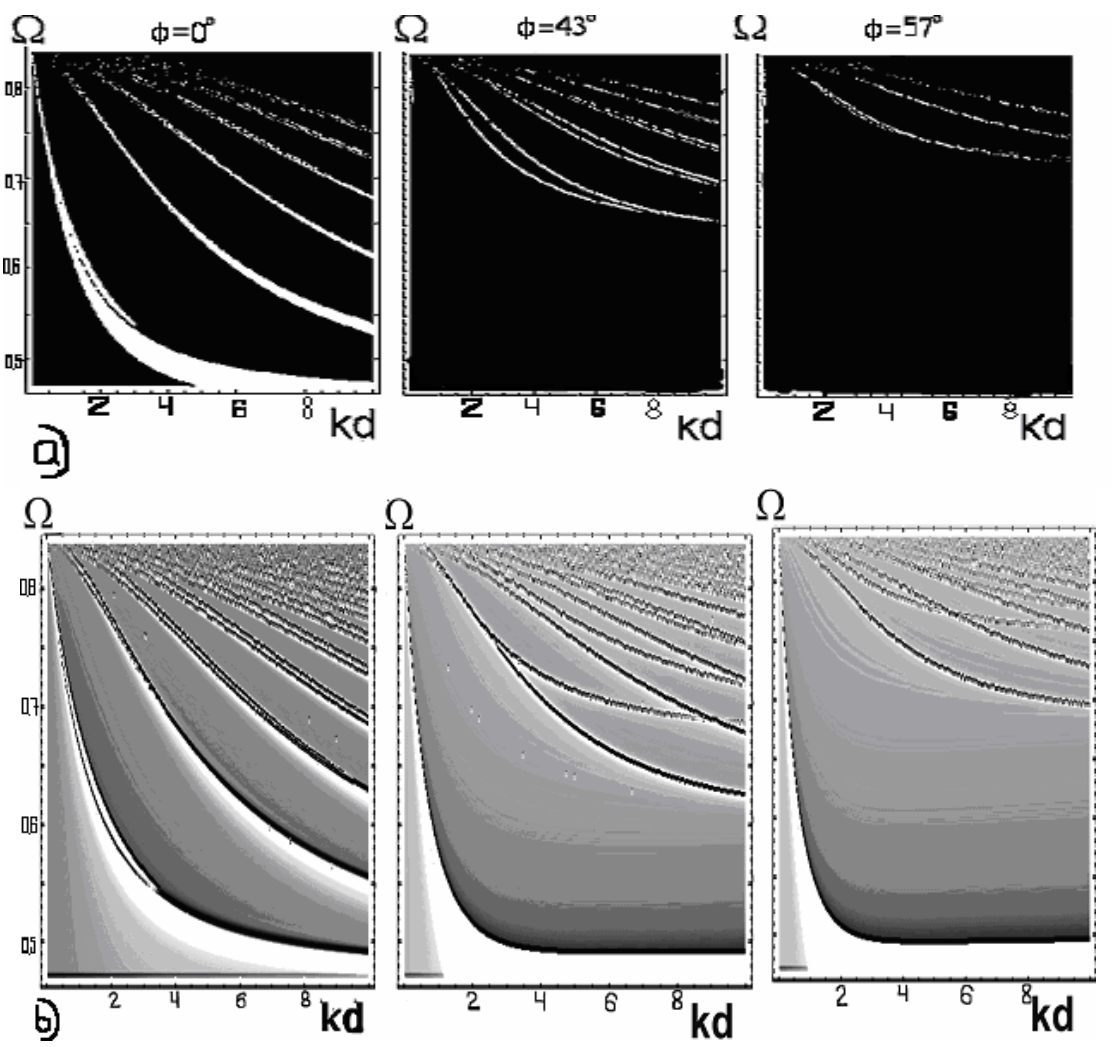


Fig. 2.Dispersion curves of reduced frequency Ω vs. reduced wave number kd for three values of the propagation angle φ.
a)for angle γ=0; b)for angle γ=13° (γ – angle between magnetization vectors in the magnetic layers)

In Fig. 3(b) (for $M_1 = M_2 = 1750$ G) we can see that the dependence of wave number κ from in-plane propogation angle φ for layer (1) differs from that of layer (2).

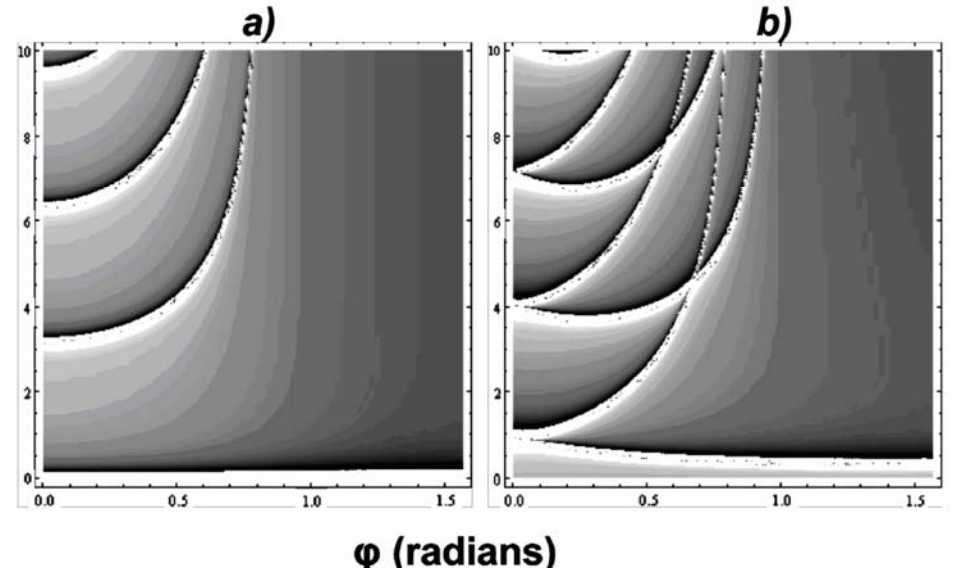


Fig. 3.The reduced wave number kd as a function of in-plane propagation angle φ (reduced frequency Ω=0.8)
a) for one layer, b) for bilayer

Numerical calculations demonstrate that for ferromagnetic layers with different static magnetizations $M_1 = 1750$ G, $M_2 = 1256$ G the dependence of wave number κ from in-plane propogation angle φ can have qualitatively another character than for case ferromagnetic layers with equal static magnetizations.

Similar to Fig. 2, in Fig. 4, for a different propagation direction, the dispersion curves are different.

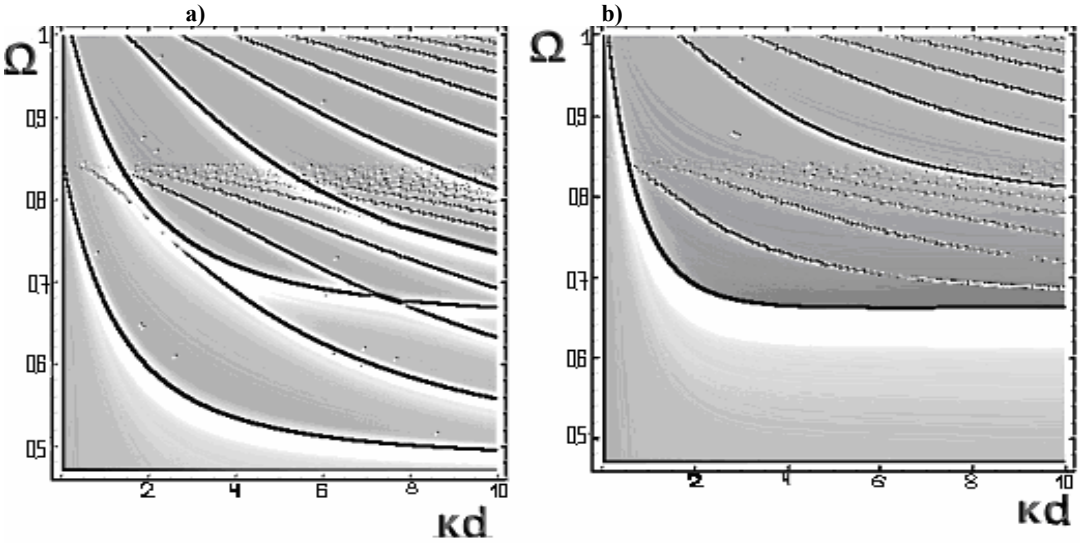
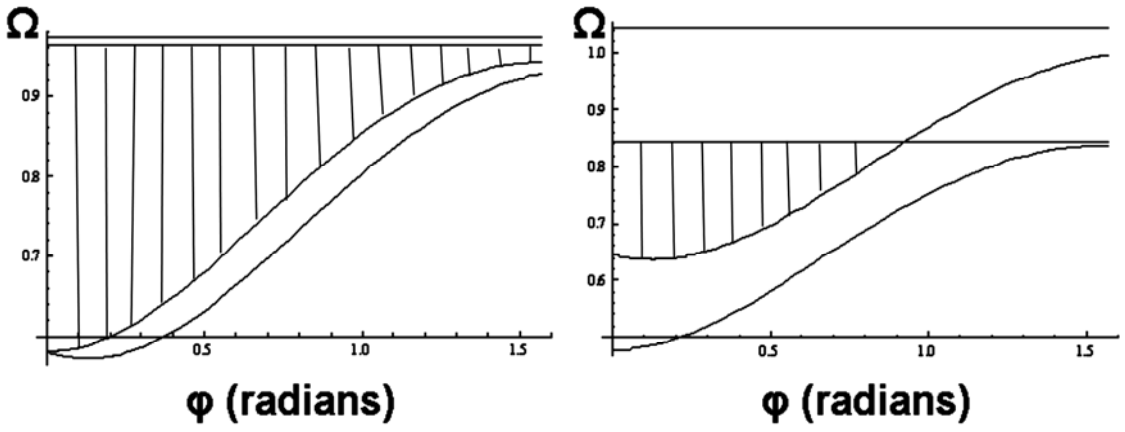


Fig. 4.Dispersion curves of reduced frequency Ω vs. reduced wave number kd .
a) for in-plane propagation angle φ=0; b)for in-plane propagation angle φ=43°

The volume mode bands as a function of in-plane propagation angle φ are shown in Fig.5. It should be pointed out, that contrary article [13], (where the propagation characteristics for backward volume waves were described only for propagation direction parallel to the bias field) in Fig.4 and Fig.5 one can see the overlapping of the volume mode bands for the ferromagnetic layers without any discontinuous. Because of the different static magnetizations in the ferromagnetic layers (Fig.4, Fig.5b), the volume mode band limits for magnetostatic wave excitation for layer (1) strongly differs from that of layer (2).

In the case of the different static magnetizations in the ferromagnetic layers (Fig. 5b), overlapping of the volume mode bands is substantially reduced as compared to Fig. 5a. Also, at that case, as seen from Fig.4 and Fig.5b, the overlapping of the volume mode bands will fall with a rise in-plane propagation angle φ.



a) b)

Fig. 5.The volume mode bands as a function of in-plane propagation angle φ
a) for $M_1 = 1750$ G, $M_2 = 1750$ G , b) for $M_1 = 1750$ G, $M_2 = 1256$ G

CONCLUSION

This work deals with volume magnetostatic modes of bilayer structure with noncollinear in-plane orientation of magnetization vectors. This is caused by the anisotropy field difference in the layers. The essential dependence of the properties of volume magnetostatic modes is demonstrated on an angle between the magnetization vectors in the layers.

In the case of the different static magnetizations and induced in-plane anisotropy fields in the two different layers the dependence of wave number κ from in-plane propogation angle φ for layer (1) differs from that of layer (2).Also, the difference between static magnetizations reduce overlapping of the magnetostatic waves volume bands.

Since the angle between magnetization vectors in the magnetic layers γ has a strong influence on volume magnetostatic waves propagation the angle between magnetization vectors is a potential control parameter for magnetostatic waves based devices.

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PHASON SINKS OF RADIATION DEFECTS IN QUASICRYSTALS

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Phason sinks of radiation defects in quasicrystals are considered as partial point defects. The kinetics of point defect absorption by single phasons is studied. A model of the dislocation loop with the phason fault under irradiation is developed. The capture efficiency of the dislocation loop for point defects is derived. The dependence of the dislocation loop bias on the loop radius is obtained. It is shown that the phason defects decrease the total bias in a quasicrystal as compared to an ordinary crystal.
KEY WORDS: quasicrystal, irradiation, dislocation loop, phason fault, bias.

ФАЗОННЫЕ СТОКИ РАДИАЦИОННЫХ ДЕФЕКТОВ В КВАЗИКРИСТАЛЛАХ
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Фазонные стоки радиационных дефектов в квазикристаллах рассмотрены в качестве частичных точечных дефектов. Исследуется кинетика поглощения точечных дефектов одиночными фазонами. Описана модель дислокационной петли с фазонным дефектом упаковки под облучением. Найдена эффективность захвата точечных дефектов дислокационной петлей. Получена зависимость преференса дислокационной петли от радиуса петли. Показано, что фазонные дефекты уменьшают суммарный преференс в квазикристалле по сравнению с обычным кристаллом.
КЛЮЧЕВЫЕ СЛОВА: квазикристалл, облучение, дислокационная петля, фазонный дефект, преференс.

ФАЗОННІ СТОКИ РАДІАЦІЙНИХ ДЕФЕКТІВ В КВАЗІКРИСТАЛАХ
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Фазонні стоки радіаційних дефектів в квазікристалах розглянуті в якості часткових точкових дефектів. Досліджується кінетика поглинання точкових дефектів окремими фазонами. Описана модель дислокаційної петлі з фазонним дефектом пакування під опроміненням. Знайдена ефективність захоплювання точкових дефектів дислокаційною петлею. Отримана залежність преференсу дислокаційної петлі від радіусу петлі. Показано, що фазонні дефекти зменшують сумарний преференс в квазікристалі у порівнянні зі звичайним кристалом.
КЛЮЧОВІ СЛОВА: квазікристал, опромінення, дислокаційна петля, фазонний дефект, преференс.

Quasicrystals discovered in 1984 have since then been an object of diverse theoretical and experimental research. These solids have a unique structure possessing non-crystallographic rotational symmetry and lacking long-range translational order [1]. The specific structure induces physical, mechanical, and other properties of quasicrystals to be different from the ones of crystals and amorphous solids [2]. Many features of quasicrystals are investigated, however the studies of quasicrystals under irradiation are scarce. It was shown that icosahedral Al-Cu-Fe can easily be amorphized by low-energy ion irradiation, however swift heavy ion irradiation only leads to the production of defects [3-5]. The stability of icosahedral Zr-Ti-Ni-Cu under irradiation with swift heavy ions was examined in [6]. It was indicated that the irradiation with Kr ions did not lead to any changes in the quasicrystalline microstructure, whereas the phase was completely amorphized by the Au-ions. Irradiation-induced vacancies were detected in icosahedral Mg-Zn-Ho and Al-Pd-Mn after electron irradiation [7]. Phase stability of icosahedral Ti-Zr-Ni under X-ray irradiation was reported in [8]. There it was also shown that the quasicrystalline diffraction pattern changes with increasing irradiation dose. This indicates the accumulation and rearrangement of phason defects and dislocations. The objective of this study was to employ a theoretical approach for describing some peculiarities of radiation damage in quasicrystals.

MODEL OF PHASONS AS PARTIAL DEFECTS

In addition to the defects inherent in crystals, i.e. point defects (vacancies and self-interstitial atoms (SIAs)), dislocations, grain boundaries, quasicrystals have distinct topological structural defects referred to as phasons. They appear as a result of one part of the material shifting relative to the other one (e.g., owing to the movement of dislocations) due to the lack of translational symmetry. The shifts also disrupt the orientational order of structural elements. The phasons that are schematically formed as the non-coincident sites after the shift of aperiodic structural elements are shown in Fig. 1.

The non-coincident site topologically corresponds to the cavity between the regular sites of a quasicrystal lattice and coincident sites in the shift layer. The non-coincident site can be vacant or occupied by an atom. A vacant non-

coincident site is a vacancy-like defect, but it has smaller volume than the vacancy volume. It can be regarded as a free volume associated with surrounding atoms. The non-coincident site occupied by an atom is an interstitial-like defect, since the volume related to the non-coincident site is greater than the volume of regular interstitial cavities but smaller than the volume of a regular vacancy. Non-coincident sites do not form extended chains in the shift layer due to the lack of translational invariance.

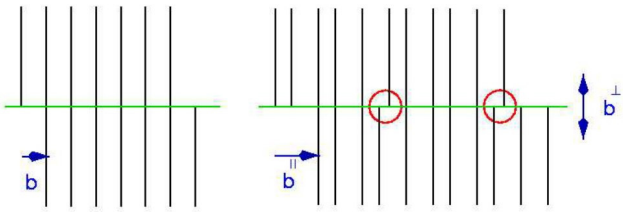

Fig. 1. Displacement along a slip plane in a crystal (left) and a quasicrystal (right).

Similar structural defects exist in amorphous solids and are described in [9] for the case of structures with short-range order. Such structural defects are in a less defined form known as the "free volume" and "antifree volume" in metallic glasses. These defects are similar to p- and n-defects introduced in [10,11] during the analysis of amorphous structures obtained by MD methods.

Partial point defects actively participate in the kinetic processes of regular point defects (PD) [12,13]. Let us denote the phason quasi-vacancy as $\tilde{\nu}$ and phason quasi-interstitial as $\tilde{i}$. Since the movement of these defects requires cooperative rearrangement of their environment, they are almost immobile localized defects. However, they may undergo structural transformations while interacting with regular point defects, i.e. SIAs (i) and vacancies (ν):

$$\begin{aligned} \tilde{i} + \nu &\leftrightarrow \tilde{\nu}; \\ \tilde{\nu} + i &\leftrightarrow \tilde{i}. \end{aligned} \tag{1}$$

The reverse transformations (1) which are accompanied by the formation of regular point defects require a significant energy (E_ν or E_i) increase and are unlikely. The frequency of direct reactions depends on the concentration of freely migrating regular point defects. It increases considerably in the presence of excess point defects formed under irradiation (as Frenkel pairs).

The quantitative description of the kinetics of freely migrating point defects and phasons is given by the following system of equations (in the chemical kinetics approximation):

$$\frac{\partial C^i_{ph}}{\partial t} = -j_\nu C^i_{ph} + j_i C^\nu_{ph}, \tag{2}$$

$$C^i_{ph} + C^\nu_{ph} = 1, \tag{3}$$

$$j_\nu \sim D_\nu \frac{\partial C_\nu}{\partial r}\bigg|_{\tilde{i}}; j_i \sim D_i \frac{\partial C_i}{\partial r}\bigg|_{\tilde{\nu}}, \tag{4}$$

where C^i_{ph}, C^ν_{ph} are the concentrations of phason quasi-interstitials and quasi-vacancies, correspondingly, $j_{i,\nu}$ is the average flux of SIAs (vacancies) on a phason, $D_{\nu,i}$ are the diffusion coefficients of vacancies (SIAs), $C_{i,\nu}$ are the concentrations of regular SIAs (vacancies).

The equilibrium concentrations of phasons can be derived:

$$C^i_{ph} = \frac{\exp\left(-E_{\tilde{\nu}}/k_B T\right)}{\exp\left(-E_{\tilde{\nu}}/k_B T\right) + \exp\left(-E_{\tilde{i}}/k_B T\right)}, \tag{5}$$

$$C^\nu_{ph} = C^i_{ph} \exp\left[\left(E_{\tilde{\nu}} - E_{\tilde{i}}\right)/k_B T\right], \tag{6}$$

where $E_{\tilde{\nu}}$, $E_{\tilde{i}}$ are the energies of phason defects in vacant and occupied states, k_B is the Boltzmann constant, T is the temperature. The reverse transformations (1) are not considered in (2). They should be accounted for while describing the structural relaxation of phasons in the absence of irradiation.

The relation for equilibrium concentrations of phason defects in the irradiated quasicrystal follows from (2):

$$C^i_{ph} = \frac{j_i}{j_\nu} C^\nu_{ph}. \tag{7}$$

In this approximation the $\tilde{i}$ -type ($\tilde{\nu}$ -type) phasons are the sinks for vacancies (SIAs) with the bias equal to 1. Owing to mutual transformations of structural states of phasons, on time average they are nonbiased sinks, which is appropriate for recombination centers of point defects with variable polarity discussed in [14].

BIAS OF THE DISLOCATION LOOP

Dislocations are known to be the sinks of point defects. In a quasicrystal the behavior of dislocations under irradiation is somewhat different from that in a crystal due to phason defects. Experiments have shown that a moving dislocation in a quasicrystal trails a phason fault which exhibits gradual thermally activated "phason dispersion" [15,16]. In view of this, we consider a simplified model of a circular dislocation loop under irradiation containing a phason

"disc" inside. We presume the temperature to be low enough for the phason disc not to disperse in the bulk. A theory of the dislocation loop sink strength in crystals was proposed in [17].

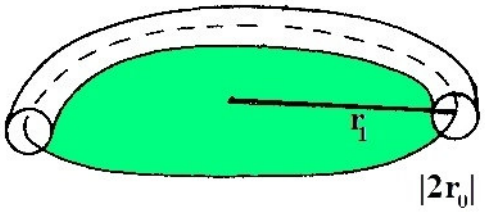

Fig. 2. Dislocation loop with the phason trail inside.

In order to be applicable for quasicrystals this model has to be modified taking into account the phason trail of the dislocation loop.

A dislocation loop of radius r_1 and its local sink-free environment (Fig. 2) is to be placed in the effective medium. We assume that there is a negligible probability that any other sink lies within a spherical volume of radius r_1 containing the loop and the phason disc as one diameter.

If we neglect the point defect (PD), vacancy or SIA, generation as well as other sinks, a simplified diffusion problem for PD concentration *C* near the dislocation loop is

$$\Delta C = 0, \tag{8}$$

subject to conditions

$$C(R) = \overline{C}, \tag{9}$$

$$\left.\frac{\partial C}{\partial n}\right|_{S_s} = \frac{C_1 v_n}{D}, \tag{10}$$

where R is the size of the sample, $C_1 v_n$ is the PD flux density at the loop surface, v_n is the transfer velocity on the toroidal sink surface S_s of the loop and C_1 is the concentration there. This problem has an electrostatic analogue: we can take C as the counterpart of the potential and $\frac{\partial C}{\partial n}$ as the value of the electric field at the surface of a metal torus. Thus, we are given that the 'electric field' is $\frac{C_1 v_n}{D}$, where C_1 is the 'metal potential'. It is also equal to 4π times the 'surface charge':

$$\frac{C_1 v_n}{D} = 4\pi \frac{\overline{C} C_s}{S_s}, \tag{11}$$

where C_s is the sink capacitance.

The sink strength is defined as follows:

$$k^2 = \frac{N_{\text{sinks}}}{V} \frac{J}{D\overline{C}}, \tag{12}$$

where N_{sinks} is the number of sinks in the volume *V*, $J = C_1 v_n S_s$ is the total PD flux on the sink surface. Substituting $C_1 v_n$ from (5.4) in (5.5) we obtain

$$k^2 = \frac{N_{\text{sinks}}}{V} 4\pi C_s. \tag{13}$$

The capacitances of the phason disc and the dislocation loop torus are, respectively,

$$C_{ph} = \frac{2}{\pi} r_1, \; C_d = \frac{\pi r_1}{\ln\left(\frac{8r_1}{r_0}\right)}. \tag{14}$$

Combining (13) and (14) we obtain the sink strengths of the dislocation loop and phason disc:

$$k_d^2 = \rho_d \frac{2\pi}{\ln\left(\frac{8r_1}{r_0}\right)}, \; k_{ph}^2 = \frac{N_{\text{d}}}{V} 8r_1, \tag{15}$$

where ρ_d is the dislocation loop density, r_0 is the PD capture radius.

Another important concept of the theory of point defect reactions in materials undergoing irradiation is the capture efficiency of the sink for point defects, $Z^{v,i}$:

$$Z^{v,i} = \frac{k^2}{\rho_s}, \tag{16}$$

where ρ_s is the density of sinks.

For quasicrystals the diffusion problem can be solved analytically in the approximation of a simple superposition of sinks. Evidently, the interplay of sinks in this approximation is ignored. In this case the capture efficiencies of a

dislocation loop for vacancies and SIAs are

$$Z_{qcr}^{v,i} = \frac{2\pi}{\ln\left(\frac{8r_1}{r_0^{v,i}}\right)} + \frac{4}{\pi}. \tag{17}$$

The bias factor determines the swelling rate of a material under irradiation. The dislocation bias is defined as follows:

$$B_{qcr} = 1 - \frac{Z_{qcr}^{v}}{Z_{qcr}^{i}}. \tag{18}$$

The dependencies of the dislocation loop capture efficiencies and the loop bias on the loop radius (in the units of Burgers vector value, b) for crystals and quasicrystals are calculated using the experimentally obtained parameters for the Al-Pd-Mn quasicrystal (see Fig. 3,4). The capture radius for vacancies is considered to be $r_{0v} = b$, and for the SIAs $r_{0i} = 3b$.

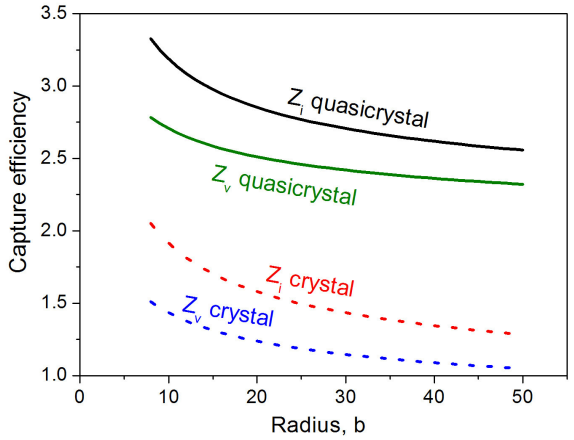

Fig. 3. Capture efficiencies of the dislocation loop for vacancies and SIAs as functions of loop radius.

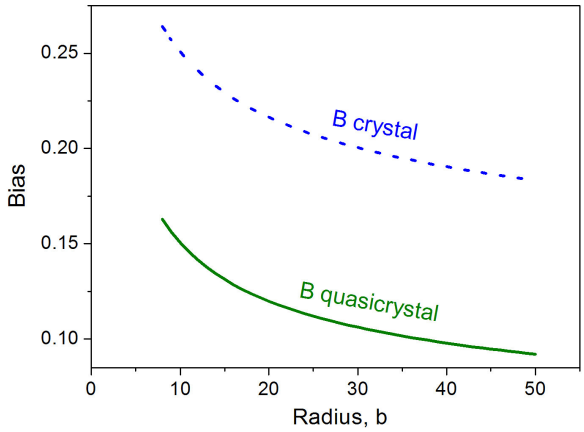

Fig. 4. Dislocation loop bias as a function of loop radius.

As expected, the capture efficiencies for point defects in a quasicrystal are greater than those in a crystal because of the higher concentration of sinks. The bias of dislocation loops towards SIAs, on the other hand, is lower in quasicrystals, and it significantly depends on the loop radius.

CONCLUSIONS

Regarding phasons as partial point defects we have shown that phason quasi-interstitials and quasi-vacancies are the sinks for vacancies and SIAs, correspondingly, with the bias equal to 1. Still on time average they are non-biased sinks due to mutual transformations of structural states of phasons. A simple model of a dislocation loop with non-dispersing phason trail inside under irradiation was also described. We have found that the absorbing capacity of dislocation loops in quasicrystals is several times greater than that in crystals due to the contribution of phason defects. The difference in dislocation loop bias for crystals and quasicrystals increases with the loop radius.

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УДК 533.9

ПОДОБИЕ В ОПИСАНИИ 1D ПАРАМЕТРИЧЕСКОЙ НЕУСТОЙЧИВОСТИ ЛЕГНМЮРОВСКИХ ВОЛН

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Показано, что процессы модуляционной неустойчивости длинноволновых ленгмюровских колебаний как в горячей, так и в холодной плазме имеют ту же симметрию и механизмы возбуждения коротковолнового спектра. При уменьшении амплитуды накачки максимум инкремента в холодной плазме сдвигается в коротковолновую область, а в горячей плазме – уменьшает инкременты во всей области спектра. Максимальный инкремент в холодной плазме при уменьшении амплитуды поля накачки не изменяется, в горячей – уменьшается. Движение энергии в коротковолновую часть спектра обусловлено взаимодействием мод, но в холодной плазме этому также способствует сдвиг максимума линейного инкремента, а в горячей плазме - большие инкременты в коротковолновой части спектра. Если возмущения ионов симметричны в пространстве, то структура поля и электронной плотности будет представлять собой стоячую волну, амплитуда которой растет, а полуширина уменьшается. При отсутствии такой симметрии поле и искажения плотности формируются за счет сложной интерференции возмущений разных масштабов.
КЛЮЧЕВЫЕ СЛОВА: модуляционная неустойчивость, ленгмюровские колебания, горячая и холодная плазма, симметрии пространственных возмущений

SIMILARITY IN 1D DESCRIPTION PARAMETRIC INSTABILITIES OF LANGMUIR WAVES

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It is shown, the modulation instability processes of long-wave Langmuir oscillation in hot and cold plasmas are possessed such a symmetry and mechanism of short-wave oscillation excitation. The maximum of the growth rate of the instability in cold plasma moves in short-wave part of spectrum, in hot plasma the growth rates in all over the spectral region are reduced, if the amplitude of pump wave has decreased. The value of the growth rate maximum in cold plasma in this case not changes, but in hot plasma similar value decreases. The energy motion along the spectrum is due to mode coupling and in cold plasma the drift of the growth rate maximum, in hot plasma – large-scale increments in short-wave part of spectrum. The spatial symmetry of ions perturbation is associated with such symmetry type of field and electrons perturbation. The amplitude of standing wave structure, which is appeared in that case, is increasing and the half-width of it is reducing in initial stage of the instability. When such symmetry is absent, the field and the density deformation are formed at the expense of the interference of different scale perturbation.
KEY WORDS: modulation instability, Langmuir oscillation, hot and cold plasmas, spatial symmetry

ПОДІБНІСТЬ В ОПИСІ 1D ПАРАМЕТРИЧНОЇ НЕСТІЙКОСТІ ЛЕНГМЮРІВСЬКИХ ХВИЛЬ

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Показано, що процеси модуляційної нестійкості довгохвилевих ленгмюрівських коливань, як у гарячій, так і в холодній плазмі мають таку ж симетрію та механізми збудження короткохвилевого спектру. При зменшенні амплітуди накачки максимум інкременту в холодній плазмі прямує до короткохвилевої частини спектру, а у гарячій плазмі це зменшує інкременти всього спектру нестійкості. Максимальний інкремент у холодній плазмі при зменшенні амплітуди поля накачки не змінюється, а максимальний інкремент у гарячій плазмі за тих умов стає меншим. Рух енергії в напрямку короткохвилевої частини спектру, що обумовлено взаємодією мод, у холодній плазмі також підтримується зсувом максимуму інкременту, а в гарячій плазмі пов'язано з тим, що в короткохвилевої частині спектру найбільші інкременти лінійної нестійкості. Коли іонні збудження симетричні в просторі, то структура поля та електронні збудження формують стоячу хвилю, амплітуда якої зростає, а напівширина зменшується на начальної стадії процесу. За відсутності такої симетрії поле та порушення густини формуються за рахунок складної інтерференції збуджень різного масштабу.
КЛЮЧОВІ СЛОВА: модуляційна нестійкість, ленгмюровські коливання, гаряча та холодна плазма, симетрії просторових збуджень

Интерес к параметрической неустойчивости интенсивных ленгмюровских волн, которые легко возбуждаются в плазме различными источниками [1-9], был обусловлен, в частности, открывшимися возможностями нагрева электронов и ионов. Корректный аппарат описания параметрической неустойчивости длинноволновых ленгмюровских колебаний фактически был создан в основополагающих работах В.П. Силина [10] и В.Е. Захарова [11]. Уже в первых численных 1D экспериментах по параметрическому распаду ленгмюровских колебаний [12] были подтверждены теоретические представления [10] (см. также [13,14] и обзор [15]). Однако наибольший интерес у экспериментаторов вызвал обнаруженный В.Е. Захаровым механизм диссипации волновой энергии. Аналитические исследования, аппаратные и численные эксперименты еще на

ранней стадии [16-18].изучения этих явлений подтвердили тот факт, что в некоторых случаях заметная часть энергии поля накачки в результате неустойчивости переходит в энергию коротковолнового ленгмюровского спектра и появляются выбросы быстрых частиц [16-27].

В частности, даже в одномерном численном моделировании процесса на базе обобщенных уравнений Силина [28-30] можно было наблюдать частичный обмен энергией между спектром и интенсивной волной накачки. Ионная каверна «схлопывалась», то есть, переходила в режим пересечения траекторий частиц [31]. Отметим, что динамика процесса совпадала с ранее выполненными численным расчетами [19]. Энергия, которую отбирали ионы, оказалась порядка $(m_e / m_i)^{1/3}$ начальной энергии волны накачки [31] (здесь m_e и m_i - массы электронов и ионов, соответственно). Для электронов переход в режим пересечения траекторий мог сдерживаться существованием ионных каверн, что способно было синхронизовать выброс быстрых электронов и ионов в момент её разрушения. Эксперименты по созданию вблизи плазменного резонанса в неоднородной плазме значительной плотности энергии поля W, превышающей плотность тепловой энергии плазмы $n_{e0}T_e$, с частотой, близкой к ленгмюровской, демонстрировали на фоне нагрева электронов вблизи плазменного резонанса появление коротких импульсов быстрых частиц. Причем, наряду с электронами имел место вынос энергии из области плазменного резонанса ионами [32-33] с достаточно большими энергиями (см., например, обзорную работу [34]). Область источников электронных импульсов соответствовала малым размерам каверн плотности. Соотношение энергии, запасенной как в быстрых ионах, так и в быстрых электронах, после разрушения каверны примерно отвечало приведенным в теории [31] значениям.

Рассмотрение процессов параметрической неустойчивости ленгмюровских волн в условиях применимости уравнений Захарова и уравнений Силина обычно рассматривалось теоретиками раздельно, хотя эксперименты часто не разделяли эти процессы. В данной работе автор сделал попытку на примере одномерного описания согласовать эти близкие по физическому проявлению модели, изучить симметрию возмущений и найти условия перехода от одной модели к другой. Выбор одномерных моделей процессов, как отметил Дж. Даусон, часто сохраняет основные черты процессов, существенно упрощая описание и понимание физических явлений [35]. Обсуждение особенностей подобия и симметрии уравнений, кроме всего прочего, способно прояснить причину достаточно редких случаев наблюдения в экспериментах режимов с обострением, приводящих к аномальному нагреву электронов и тем более ионов.

ВЫСОКОТЕМПЕРАТУРНАЯ ПЛАЗМА, ОДНОМЕРНЫЕ УРАВНЕНИЯ ЗАХАРОВА

Описание поведения электронов плазмы в условиях, когда фазовые скорости ленгмюровских волн превосходят их тепловую скорость может быть гидродинамическим. Ионы можно описывать как гидродинамически, так и кинетически. Для упрощения описания ниже ограничимся одномерным случаем. При этом, для скорости v_e и плотности n_e электронов справедливы следующие уравнения

$$\frac{\partial v_e}{\partial t}+\frac{e}{m_e}E+\frac{1}{m_e n_e}\frac{\partial P_e}{\partial x}=-\{v_e\cdot\frac{\partial}{\partial x}v_e\}, \tag{1}$$

$$\frac{\partial n_e}{\partial t}+n_0\frac{\partial}{\partial x}v_e=-\frac{\partial}{\partial x}(n_e\cdot v_e), \tag{2}$$

$$\frac{\partial}{\partial x}E=4\pi e\cdot(n_i-n_e), \tag{3}$$

где $E=-\partial\phi/\partial x$, ϕ - напряженность и потенциал электрического поля колебаний, $P_e=n_eT_e$ - давление, T_e - температура в энергетических единицах и $v_{Te}=\sqrt{T_e/m_e}$ - тепловая скорость электронов, $c_s=\sqrt{T_e/m_i}$ - скорость звука, n_e и n_i - возмущенные плотности электронов и ионов плазмы, n_0 - невозмущенная плотность как электронов, так и ионов плазмы, $\omega_{pe}=\sqrt{4\pi e^2n_0/m_e}$, $\Omega_i=\sqrt{4\pi e^2n_0/m_i}$ - ленгмюровская электронная и плазменная ионная частоты.

Представим электрическое поле в виде $E=\sum_n E_n\exp\{ik_nx\}=\sum_n E_n\exp\{ink_0x\}$, где величина $k_n=nk_0$ определяет дискретный набор волновых чисел мод спектра. Перепишем уравнения (1) - 2) в виде

$$\frac{\partial v_{en}}{\partial t}-\frac{e}{m_e}E_n+\frac{v_{Te}^2}{n_0}\cdot ik_0n\cdot n_e=-ik_0\sum_m m\cdot v_{en-m}\cdot v_{em}, \tag{4}$$

$$\frac{\partial n_{en}}{\partial t}+n_0\cdot ik_0n\cdot v_{en}=-ik_0\cdot n\cdot\sum_m n_{en-m}\cdot v_{em}, \tag{5}$$

$$ik_0n\cdot E_n=4\pi e(n_{in}-n_{en}). \tag{6}$$

Исключим $E_n = -4\pi ie(n_{in} - n_{en})/k_0 n$ и (4) примет вид

$$\frac{\partial v_{en}}{\partial t} = \frac{4\pi e^2 i}{k_0 n \cdot m_e}(n_{in} - n_{en}) - \frac{v^2_{Te}}{n_0} \cdot ik_0 n \cdot n_e - ik_0 \sum_m m \cdot v_{en-m} \cdot v_{em}. \tag{7}$$

Представим, следуя [36] плотность и скорость электронов в виде

$$-en_{en} = \sum_s u_n^{(s)} \cdot \exp\{is\omega_0 \cdot t\} = u_n^{(0)} + u_n^{(1)} \cdot e^{i\omega_0 t} + u_n^{(-1)} \cdot e^{-i\omega_0 t} + u_n^{(2)} \cdot e^{i2\omega_0 t} + u_n^{(-2)} \cdot e^{-i2\omega_0 t}, \tag{8}$$

$$v_{en} = \sum_s v_n^{(s)} \cdot \exp\{is\omega_0 \cdot t\} = v_n^{(0)} + v_n^{(1)} \cdot e^{i\omega_0 t} + v_n^{(-1)} \cdot e^{-i\omega_0 t} + v_n^{(2)} \cdot e^{i2\omega_0 t} + v_n^{(-2)} \cdot e^{-i2\omega_0 t}, \tag{9}$$

$$E_n = \sum_s E_n^{(s)} \cdot \exp\{is\omega_0 \cdot t\} = \bar{E}_n + \frac{1}{2}(E_n^{(1)} \cdot e^{i\omega_0 t} + E_n^{(-1)} \cdot e^{-i\omega_0 t}) + E_n^{(2)} \cdot e^{i2\omega_0 t} + E_n^{(-2)} \cdot e^{-i2\omega_0 t}. \tag{10}$$

Воспользуемся линейными соотношениями $u^{(\pm 1)}{}_{n-m} = \pm k_0 (n-m) \cdot en_0 \omega_0^{-1} v^{(\pm 1)}{}_{n-m}$ и найдем нерезонансные величины

$$v^{(0)}{}_n = \frac{1}{en_0} \sum_m (u^{(1)}{}_{n-m} \cdot v^{(-1)}{}_m + u^{(-1)}{}_{n-m} \cdot v^{(1)}{}_m) = \frac{1}{i\omega_0}[\frac{\partial v^{(1)}}{\partial x} v^{(-1)} - \frac{\partial v^{(-1)}}{\partial x} v^{(1)}]_n, \tag{11}$$

$$u^{(0)}{}_n + en_{in} = -\frac{m_e}{4\pi e} \frac{\partial^2}{\partial x^2}[v^{(1)} v^{(-1)}]_n, \tag{12}$$

$$v^{(\pm 2)}{}_n = \mp \frac{k_0}{\omega_0} \sum_m m v^{(\pm 1)}{}_{n-m} \cdot v^{(\pm 1)}{}_m = \mp \frac{1}{i\omega_0}[\frac{\partial v^{(\pm 1)}}{\partial x} v^{(\pm 1)}]_n, \tag{13}$$

$$u^{(\pm 2)}{}_n = -\frac{k_0{}^2 n \cdot en_0}{\omega^2_{pe}} \sum_s s v^{(\pm 1)}{}_s \cdot v^{(\pm 1)}{}_{n-s} = +\frac{en_0}{\omega^2_{pe}} \frac{\partial}{\partial x}[\frac{\partial v^{(\pm 1)}}{\partial x} v^{(\pm 1)}]_n. \tag{14}$$

Уравнение для резонансных величин принимает вид

$$\begin{aligned}
&\pm 2i\omega_0 \{\frac{\partial u^{(\pm 1)}{}_n}{\partial t} \mp i \frac{\omega^2_{pe} - \omega_0{}^2 + k^2{}_0 n^2 v^2_{Te}}{2\omega_0} u^{(\pm 1)}{}_n \mp i \frac{\omega_0 n}{2n_0} \sum_m n_{in-m} \frac{u^{(\pm 1)}{}_m}{m}\} = \\
&+k^2{}_0 n \cdot en_0 \sum_m m[v^{(0)}{}_{n-m} \cdot v^{(\pm 1)}{}_m + v^{(\pm 1)}{}_{n-m} \cdot v^{(0)}{}_m] - \\
&-ik_0 \cdot n \cdot (\pm i\omega_0) \sum_m [(u^{(0)}{}_{n-m} + v_{in-m}) \cdot v^{(\pm 1)}{}_m + u^{(\pm 1)}{}_{n-m} \cdot v^{(0)}{}_m] + \\
&+k^2{}_0 n \cdot en_0 \sum_m m v^{(\mp 1)}{}_{n-m} \cdot v^{(\pm 2)}{}_m - ik_0 \cdot n \cdot (\pm i\omega_0) \sum_m [u^{(\pm 2)}{}_{n-m} \cdot v^{(\mp 1)}{}_m.
\end{aligned} \tag{15}$$

Правая часть (15) определяет так называемую электронную нелинейность, которая в одномерном случае обращается в нуль [36,37]. Действительно, правая часть (15) равна $(k_0 n \cdot en_0 / \omega_0) \cdot I$, где для I справедливо тождество

$$\begin{aligned}
I = \{&-\frac{\partial}{\partial x}\{v^{(\pm 1)}[\frac{\partial v^{(1)}}{\partial x} v^{(-1)} - \frac{\partial v^{(-1)}}{\partial x} v^{(1)}] \mp v^{(\pm 1)} \frac{\partial^2}{\partial x^2}[v^{(1)} v^{(-1)}] - \frac{\partial v^{(\pm 1)}}{\partial x}[\frac{\partial v^{(1)}}{\partial x} v^{(-1)} - \frac{\partial v^{(-1)}}{\partial x} v^{(1)}] \pm \\
&\pm v^{(\mp 1)} \frac{\partial}{\partial x}[\frac{\partial v^{(\pm 1)}}{\partial x} v^{(\pm 1)}] \pm v^{(\mp 1)} \frac{\partial}{\partial x}[\frac{\partial v^{(\pm 1)}}{\partial x} v^{(\pm 1)}] = 0.
\end{aligned} \tag{16}$$

Таким образом, для резонансных возмущений плотности справедливо уравнение

$$\frac{\partial u^{(\pm 1)}{}_n}{\partial t} \mp i \frac{\omega^2_{pe} - \omega_0{}^2 + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0} u^{(\pm 1)}{}_n \mp \frac{\omega_0}{2n_0} n \cdot \sum_m \frac{n_{in-m}}{m} u_m{}^{(\pm 1)} = 0, \tag{17}$$

или переходя к напряженности электрического поля

$$E^{(\pm 1)}{}_n = 4\pi ieu^{(\pm 1)}{}_n / 2k_0 n, \tag{18}$$

$$\frac{\partial E^{(\pm 1)}{}_n}{\partial t} \mp i \frac{\omega^2_{pe} - \omega_0{}^2 + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0} E^{(\pm 1)}{}_n \mp i \frac{\omega_0}{2n_0} \cdot \sum_m n_{in-m} E_m{}^{(\pm 1)} = 0. \tag{19}$$

Если ионы описывать крупными частицами, уравнение движения для которых

$$\frac{d^2 x_s}{dt^2} = \frac{e}{m_i} \sum_n \bar{E}_n \cdot \exp\{ik_0 n x_s\}, \tag{20}$$

то плотность ионов определим как

$$n_{in} = n_0 \cdot \frac{k_0}{2\pi} \int_{-\pi/k_0}^{\pi/k_0} \exp[-ink_0 \cdot x_s(x_0, t)] \cdot dx_{s0}. \tag{21}$$

Заметим, что описание ионов крупными частицами, кроме всего прочего, как показано в [31] позволяет увеличить устойчивость расчетной схемы. Компонент медленно меняющегося электрического поля может быть определен следующим образом. Так как для медленных движений справедливо приближение

$$n_e = n_0 \cdot \exp\left\{\frac{e\tilde{\phi} - U}{T}\right\}, \tag{22}$$

то удерживая в уравнении Пуассона первые члены разложения получим

$$\frac{\partial^2}{\partial x^2}\bar{\phi} = 4\pi e \cdot \left(\frac{e\bar{\phi} - U}{T} n_0 - n_i\right), \tag{23}$$

где $\bar{\phi}$ и $\bar{E}_n = -ik_0 n\tilde{\phi}_n$ потенциал и напряженность усредненного по быстрым осцилляциям поля. Для ВЧ потенциала $U = \sum_n U_n \exp\{ik_0 nx\}$, причем $U_n = \frac{e^2}{4m_e\omega_p^{\ 2}} \sum_m E_{n-m}^{(1)} E_m^{(-1)}$.

Очевидно левой частью уравнения (23) можно пренебречь в условиях $k_0^2 n^2 v_{Te}^2 / \omega_{pe}^2 = v_{Te}^2 / v_\Phi^2 << 1$ и тогда напряженность усредненного по быстрым осцилляциям поля

$$\bar{E}_n = -ik_0 n\tilde{\phi}_n = \frac{-ik_0 n n_{in} T}{en_0} + \frac{-ik_0 ne}{4m_e\omega_p^{\ 2}} \sum_m E_{n-m}^{(1)} E_m^{(-1)}. \tag{24}$$

Описывать ионы можно и гидродинамически. Уравнение для медленных возмущений плотности и скорости ионов имеют вид

$$\frac{\partial n_{in}}{\partial t} + v_{in} \cdot ik_0 n \cdot n_0 = -ik_0 \cdot n \cdot \sum_m n_{in-m} \cdot v_{im}, \tag{25}$$

$$\frac{\partial v_{in}}{\partial t} - \frac{e}{m_i}\bar{E} = -ik_0 \cdot \sum_m m v_{in-m} \cdot v_{im} \ . \tag{26}$$

Правыми частями (25) и (26) пренебрежем, полагая их малыми. Тогда для возмущений плотности справедливо уравнение

$$\frac{\partial^2 n_{in}}{\partial t^2} + k_0^2 n^2 c_s^2 n_{in} = -\frac{k_0^2 n^2}{16\pi m_i} \sum_m E_{n-m}^{(1)} E_m^{(-1)} \tag{27}$$

где скорость звука $c_s = \sqrt{T_e / m_i}$. Отметим, что при выполнении условий $k_0^2 n^2 v_{Te}^2 / \omega_{pe}^2 = v_{Te}^2 / v_\Phi^2 << 1$ данное уравнение можно получить, используя соотношение (22) и первые члены разложения (23).

Уравнения (19) и (27) при $\omega_0 = \omega_{pe}$ в виде

$$i\frac{\partial E}{\partial t} + \frac{v^2_{Te}}{2\omega_{pe}}\frac{\partial^2}{\partial x^2}E - \frac{\omega_{pe}}{2n_0} \cdot n_i E = 0, \tag{28}$$

$$\frac{\partial^2 n_i}{\partial t^2} - c_s^2 \frac{\partial^2 n_i}{\partial x^2} = \frac{1}{16\pi m_i}\frac{\partial^2}{\partial x^2} |E|^2 \ , \tag{29}$$

известны как уравнения Захарова [11] в одномерном случае.

Симметрии

Можно убедиться, в том, что комплексно сопряженное уравнение (19) при верхнем знаке принимает вид

$$\frac{\partial (E^{(1)}{}_n)^*}{\partial t} + i\frac{\omega_{pe}^2 - \omega_0^{\ 2} + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0}(E^{(1)}{}_n)^* + i\frac{\omega_0}{2n_0} \cdot \{n^*{}_{in}(E_0^{(1)})^* + \sum_{m\neq 0} n^*{}_{in-m}(E_m^{\ (1)})^*\} = 0 \ , \tag{30}$$

В то же время для отрицательных индексов, это же уравнение может быть записано (при суммировании можно заменить немой индекс $m \to -m$)

$$\frac{\partial E_{-n}^{(-1)}}{\partial t} + i\frac{\omega_{pe}^2 - \omega_0^{\ 2} + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0} E_{-n}^{(-1)} + i\frac{\omega_0}{2n_0} \cdot \{n_{i,-n} E_0^{(-1)} + \sum_{m\neq 0} n_{i,-n+m} E_{-m}^{(-1)}\} = 0. \tag{31}$$

а) Легко видеть, что при $E_{-n}^{(-1)} = (E_n^{(1)})^*$ и $n_{i,-n} = (n_{i,n})^*$ уравнения (30) и (31) идентичны. Точно также можно убедиться, что из подобных преобразований следует $E_n^{(-1)} = (E_{-n}^{(1)})^*$ и $n_{i,-n} = (n_{i,n})^*$. То есть, возмущение плотности ионов обладает симметрией $n_{i,-n} = (n_{i,n})^*$. При этом для корректного описания такой ионной каверны достаточно использовать компоненты ВЧ поля $E_n^{(1)}$, $E_{-n}^{(1)}$ и $E_0^{(1)}$, а также возмущения плотности ионов $n_{i,n}$, так как остальные величины выражаются через них, то есть можно отказаться от использования верхнего индекса.

Система уравнений (18), (27) в этих условиях может быть записана в виде

$$\frac{\partial E_n}{\partial t} - i\frac{\omega_{pe}^2 - \omega_0{}^2 + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0} E_n - i\frac{\omega_0}{2n_0}\cdot\sum_m n_{in-m}E_m = 0, \tag{32}$$

$$\frac{\partial^2 n_{in}}{\partial t^2} + k_0^2 n^2 c_s^2 n_{in} = -\frac{k_0^2 n^2}{16\pi m_i}\sum_m E_{n-m}E^*_{-m} \cdot \tag{33}$$

или при описании ионов частицами, можно воспользоваться уравнениями движения (20) и выражением для ионной плотности (2.21), где напряженность медленно меняющегося электрического поля

$$\bar{E}_n = -ik_0 n\tilde{\phi}_n = \frac{-ik_0 n n_{in} T}{en_0} + \frac{-ik_0 ne}{4m_e\omega_p{}^2}\sum_m E_{n-m}E^*_{-m}. \tag{34}$$

Для поля накачки, которой является длинноволновая ленгмюровская волна большой амплитуды, получим

$$\frac{\partial E_0}{\partial t} - i\frac{\omega_0}{2n_0}\cdot\sum_m n_{i,-m}E_m = 0. \tag{35}$$

Отметим, что величины, отвечающие разному знаку нижнего индекса при этом независимы, что приводит к пространственному искажению интегральных возмущений, не только из-за изменения амплитуды, но и за счет пространственного сдвига возмущений разного масштаба.

б) Кстати, если $n_{i,-n} = n_{i,n} = (n_{i,n})^*$, то есть, возмущения ионной плотности не меняют своего положения в пространстве, то ВЧ электрическое поле также остается симметричным в пространстве $E_n^{(1)} = E_{-n}^{(1)} = (E_n^{(-1)})^* = (E_{-n}^{(-1)})^*$ и для описания процесса достаточно значений $E_n^{(1)}$ и $n_{i,n}$, что обусловлено жесткой связью величин, отвечающих разному знаку нижнего индекса. Структура поля и плотности будет представлять собой неподвижную пространственную структуру, амплитуда которой растет, а полуширина уменьшается, по крайней мере в определенной области.

в) С другой стороны, возмущение ионов вида $n_{i,-n} = -(n_{i,n})^*$ оказывается запрещено электронной дисперсией.

Дозвуковой режим

В условиях, когда $\partial^2 n_{in} / n_{in}\partial t^2 << k_P^2 c_s^2$, где k_P - волновой вектор колебаний, уравнение (33) упрощается

$$n_{in} = -\frac{1}{16\pi m_i c_s^2}\sum_m E_{n-m}^{(1)}E_m^{(-1)}. \tag{36}$$

Подставляя значения n_{in} в уравнение (28), представим его в виде

$$i\frac{\partial E}{\partial t} + \frac{v^2{}_{Te}}{\omega_{pe}}\frac{\partial^2}{\partial x^2}E + \frac{\omega_{pe}}{32m_i c_s^2 n_0}\cdot|E|^2\ E = 0. \tag{37}$$

В другой форме может быть записано в виде

$$\frac{\partial E_n}{\partial t} - i\frac{\omega_{pe}^2 - \omega_0{}^2 + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0}E_n + \frac{i\omega_0}{32\pi m_i n_0 c_s^2}\cdot\sum_m\sum_p E_{n-m-p}E^*_{-p}E_m = 0. \tag{38}$$

Сверхзвуковой режим

При $\partial^2 n_{in} / n_{in}\partial t^2 >> k_P^2 c_s^2$ возможно развитие сверхзвукового режима процесса. В этом случае уравнение (27) для медленных возмущений принимает вид

$$\frac{\partial^2 n_{in}}{\partial t^2} = -\frac{k_0^2 n^2}{16\pi m_i}\sum_{m\neq 0,n} E_{n-m}E^*_{-m}, \tag{39}$$

или

$$\frac{\partial^2 n_i}{\partial t^2} = \frac{1}{16\pi m_i}\frac{\partial^2}{\partial x^2}|E|^2. \tag{40}$$

Для волны большой амплитуды (волны накачки) волновой вектор которой стремится к нулю справедливо уравнение (35), а для коротковолновых возмущений

$$\frac{\partial E_n}{\partial t} - i\frac{\omega_{pe}^2 - \omega_0{}^2 + k^2{}_0 n^2 v^2{}_{Te}}{2\omega_0}E_n - i\frac{\omega_0}{2n_0}\cdot\{n_{in}E_0 + \sum_{m\neq 0} n_{in-m}E_m\} = 0, \tag{41}$$

$$\frac{\partial^2 n_{in}}{\partial t^2} = -\frac{k_0^2 n^2}{16\pi m_i}\{E_n E_0^* + E_0 E^*_{-n} + \sum_{m\neq 0,n} E_{n-m}E^*_{-m}\}\cdot \tag{42}$$

Приведем также значение для медленно меняющейся напряженности поля с учетом волны накачки

$$\bar{E}_n = -ik_0 n\tilde{\phi}_n = \frac{-ik_0 n n_{in} T}{en_0} + \frac{-ik_0 ne}{4m_e \omega_p^{\ 2}}(E_n E_0^* + E_0 E_{-n}^* + \sum_{m\neq 0,n} E_{n-m}E_{-m}^*). \quad (43)$$

ХОЛОДНАЯ ПЛАЗМА, ОДНОМЕРНЫЕ ОБОЩЕННЫЕ УРАВНЕНИЯ СИЛИНА

В случае большой интенсивности внешнего длинноволнового поля для холодной плазмы, следует воспользоваться подходом, изложенным в работах В.П.Силина [38].

$$\frac{\partial v_\alpha}{\partial t} + u_{0\alpha}\frac{\partial}{\partial x}v_\alpha - \frac{e_\alpha}{m_\alpha}E = -\{v_\alpha \cdot \frac{\partial}{\partial x}v_\alpha\}, \quad (44)$$

$$\frac{\partial n_\alpha}{\partial t} + u_{0\alpha}\cdot\frac{\partial}{\partial x}n_\alpha + n_{\alpha 0}\frac{\partial}{\partial x}v_\alpha \cdot = -\{\frac{\partial}{\partial x}(n_\alpha \cdot v_\alpha)\}, \quad (45)$$

$$\frac{\partial}{\partial x}E = 4\pi\sum_\beta e_\beta \cdot n_\beta. \quad (46)$$

Частицы находятся в поле внешней волны, длину которой для упрощений расчетов положим равной бесконечности, осциллируя со скоростью $u_{0\alpha} = -(e_\alpha |\mathrm{E}_0| / m_\alpha \cdot \omega_0)\cdot Cos\Phi$, компоненты напряженности поля внешней волны определяются следующим образом

$$E_0 = -i(|E_0|\exp\{i\omega_0 t + i\phi\} - |E_0|\exp\{-i\omega_0 t - i\phi\})/2. \quad (47)$$

Исключая $E_n = -4\pi ie(n_{in} - n_{en})/k_0 n$, перепишем первое уравнение системы (44)-(46) в следующем виде

$$\frac{\partial v_{\alpha n}}{\partial t} + u_{0\alpha}\cdot ik_0 n\cdot v_{\alpha n} + \frac{4\pi e_\alpha i}{k_0 n\cdot m_\alpha}\sum_\beta e_\beta \cdot n_{\beta m} = -ik_0\sum_m m\cdot v_{\alpha n-m}\cdot v_{\alpha m}. \quad (48)$$

Используем ниже следующие переменные

$$\nu_{\alpha n} = e_\alpha \cdot n_{\alpha n}\cdot\exp\{-ia_{\alpha n}\cdot Sin\Phi\}, \quad (49)$$

$$\theta_{\alpha n} = v_{\alpha n}\cdot\exp\{-ia_{\alpha n}\cdot Sin\Phi\}, \quad (50)$$

где $a_{\alpha n} = ne_\alpha k_0 E_0 / m_\alpha \cdot \omega_0^2$, $\Phi = \omega_0 t + \phi$. (51)

При этом первые два уравнения системы (44)-(46) можно записать в виде

$$\frac{\partial \nu_{\alpha n}}{\partial t} + \theta_{\alpha n}\cdot ik_0 n\cdot e_\alpha n_{\alpha 0} = -ik_0\cdot n\cdot\sum_m \nu_{\alpha n-m}\cdot\theta_{\alpha m}, \quad (52)$$

$$\frac{\partial \theta_{\alpha n}}{\partial t} + \frac{4\pi e_\alpha i}{k_0 n\cdot m_\alpha}\sum_\beta \nu_{\beta n}\cdot\exp\{i(a_{\beta n} - a_{\alpha n})\cdot Sin\Phi\} = -ik_0\cdot\sum_m m\theta_{\alpha n-m}\cdot\theta_{\alpha m}. \quad (53)$$

Очевидно, что $a_{in} - a_{en} = n(ek_0 E_0 / m_i\cdot\omega_0^2) + n(ek_0 E_0 / m_e\cdot\omega_0^2) \approx n(ek_0 E_0 / m_e\cdot\omega_0^2) = a_n$, где величина $k_n = nk_0$, как и прежде, определяет дискретный набор волновых чисел мод спектра. Для электронов уравнения (52)-(53) можно записать как

$$\frac{\partial \nu_{en}}{\partial t} - \theta_{en}\cdot ik_0 n\cdot en_0 = -ik_0\cdot n\cdot\sum_m \nu_{en-m}\cdot\theta_{em}, \quad (54)$$

$$\frac{\partial \theta_{en}}{\partial t} - \frac{4\pi ei}{k_0 n\cdot m_e}(\nu_{en} + \nu_{in}\cdot\exp\{ia_n\cdot Sin\Phi\}) = -ik_0\cdot\sum_m m\theta_{en-m}\cdot\theta_{em}. \quad (55)$$

Используем представление

$$\nu_{en} = \sum_s u_n^{(s)}\cdot\exp\{is\omega_0\cdot t\} = u_n^{(0)} + u_n^{(1)}\cdot e^{i\omega_0 t} + u_n^{(-1)}\cdot e^{-i\omega_0 t} + u_n^{(2)}\cdot e^{i2\omega_0 t} + u_n^{(-2)}\cdot e^{-i2\omega_0 t}, \quad (56)$$

$$\theta_{en} = \sum_s v_n^{(s)}\cdot\exp\{is\omega_0\cdot t\} = v_n^{(0)} + v_n^{(1)}\cdot e^{i\omega_0 t} + v_n^{(-1)}\cdot e^{-i\omega_0 t} + v_n^{(2)}\cdot e^{i2\omega_0 t} + v_n^{(-2)}\cdot e^{-i2\omega_0 t}, , \quad (57)$$

и известное разложение

$$\exp\{ia\cdot Sin\Phi\} = \sum_{m=-\infty}^{\infty} J_m(a)\cdot\exp\{im\Phi\}, \quad (58)$$

где $J_m(x)$ - функция Бесселя, причем $J_0(x) = J_0(-x)$, $J_1(x) = -J_1(-x) = J_{-1}(-x)$, $J_2(x) = J_{-2}(x) = J_2(-x)$ [39], найдем нерезонансные величины возмущений плотности $u_n^{(0)}, u_n^{(2)}, u_n^{(-2)}$ и скорости $v_n^{(0)}, v_n^{(2)}, v_n^{(-2)}$ в осциллирующей системе отсчета:

$$v^{(0)}{}_n = \frac{k_0}{\omega_0}\sum_m (n-m)[v^{(+1)}{}_{n-m}\cdot v^{(-1)}{}_m - v^{(-1)}{}_{n-m}\cdot v^{(1)}{}_m) = \frac{1}{i\omega_0}[\frac{\partial v^{(1)}}{\partial x}v^{(-1)} - \frac{\partial v^{(-1)}}{\partial x}v^{(1)}]_n, \quad (59)$$

$$u^{(0)}{}_n = -\nu_{in}\cdot J_0(a_n) + \frac{k_0^{\ 2}n^2\cdot m_e}{4\pi e}\cdot\sum_m v^{(1)}{}_{n-m}\cdot v^{(-1)}{}_m = -\nu_{in}\cdot J_0(a_n) - \frac{m_e}{4\pi e}\frac{\partial^2}{\partial x^2}[v^{(1)}v^{(-1)}]_n, \quad (60)$$

$$v^{(\pm 2)}{}_n = \pm\frac{2\omega_0}{3k_0 n\cdot en_0}\nu_{in}\cdot J_{\pm 2}(a_n)\exp[\pm 2i\phi]\mp\frac{k_0}{\omega_0}\sum_m m v^{(\pm 1)}{}_{n-m}\cdot v^{(\pm 1)}{}_m =$$
$$=\pm\frac{2\omega_0}{3k_0 n\cdot en_0}\nu_{in}\cdot J_{\pm 2}(a_n)\exp[\pm 2i\phi]\mp\frac{1}{i\omega_0}[\frac{\partial v^{(\pm 1)}}{\partial x}v^{(\pm 1)}]_n, \qquad (61)$$

$$u^{(\pm 2)}{}_n = \frac{1}{3}\nu_{in}\cdot J_{\pm 2}(a_n)\exp[\pm 2i\phi]-\frac{{k_0}^2 n\cdot en_0}{\omega^2{}_{pe}}\sum_s s v^{(\pm 1)}{}_s\cdot v^{(\pm 1)}{}_{n-s} =$$
$$=\frac{1}{3}\nu_{in}\cdot J_{\pm 2}(a_n)\exp[\pm 2i\phi]+\frac{en_0}{\omega^2{}_{pe}}\frac{\partial}{\partial x}[\frac{\partial v^{(\pm 1)}}{\partial x}v^{(\pm 1)}]_n. \qquad (62)$$

Для резонансных величин справедливо уравнение

$$\pm 2i\omega_0\{\frac{\partial u^{(\pm 1)}{}_n}{\partial t}\mp i\frac{\omega_{pe}^2-{\omega_0}^2}{2\omega_0}u^{(\pm 1)}{}_n\mp i\nu_{in}\cdot\frac{\omega_{pe}^2 J_{\pm 1}(a_n)\cdot\exp(\pm i\phi)}{2\omega_0}\}=$$
$$+{k^2}_0 n\cdot en_0\sum_m m[v^{(0)}{}_{n-m}\cdot v^{(\pm 1)}{}_m+v^{(\pm 1)}{}_{n-m}\cdot v^{(0)}{}_m]-$$
$$-ik_0\cdot n\cdot(\pm i\omega_0)\sum_m[u^{(0)}{}_{n-m}\cdot v^{(\pm 1)}{}_m+u^{(\pm 1)}{}_{n-m}\cdot v^{(0)}{}_m]+ \qquad (63)$$
$$+{k^2}_0 n\cdot en_0\sum_m m v^{(\mp 1)}{}_{n-m}\cdot v^{(\pm 2)}{}_m-ik_0\cdot n\cdot(\pm i\omega_0)\sum_m[u^{(\pm 2)}{}_{n-m}\cdot v^{(\mp 1)}{}_m.$$

В работах [28-30] было использовано представление $u^{(\pm 1)}{}_n=\pm k_0 n\cdot en_0 v^{(\pm 1)}{}_n/\omega_0=ik_0 n\cdot E_n^{(\pm 1)}/4\pi$ (где $v_n^{(\pm 1)}=\pm ieE_n^{(\pm 1)}/m_e\omega_0$). В этом случае, выделяя в правую часть (63) слагаемые, ответственные только за электронную нелинейность, перепишем это уравнение для коротковолновых возмущений в виде

$$\pm 2i\omega_0\{\frac{\partial u^{(\pm 1)}{}_n}{\partial t}\mp i\frac{\omega_{pe}^2-{\omega_0}^2}{2\omega_0}u^{(\pm 1)}{}_n\mp i\nu_{in}\cdot\frac{\omega_{pe}^2 J_{\pm 1}(a_n)\cdot\exp(\pm i\phi)}{2\omega_0}\}\cdot e^{\pm i\omega_0 t}+$$
$$+\frac{{\omega^2}_0}{en_0}n\cdot e^{\pm i\omega_0 t}\sum_m\frac{\nu_{in-m}}{m}\cdot[u_m{}^{(\mp 1)}\cdot J_{\pm 2}(a_{n-m})\exp[\pm 2i\phi]+u_m{}^{(\pm 1)}\cdot J_0(a_{n-m})]=(k_0 n\cdot en_0/\omega_0)\cdot I. \qquad (64)$$

Очевидно, и в этом случае правая часть (64) оказывается равной нулю. Перепишем (64) в виде [28]

$$\frac{\partial u^{(\pm 1)}{}_n}{\partial t}\mp i\frac{\omega_{pe}^2-{\omega_0}^2}{2\omega_0}u^{(\pm 1)}{}_n\mp i\nu_{in}\cdot\frac{\omega_{pe}^2 J_{\pm 1}(a_n)\cdot\exp(\pm i\phi)}{2\omega_0}+$$
$$\mp i\frac{\omega_0 n}{2en_0}\sum_m\frac{\nu_{in-m}}{m}\cdot[u_m{}^{(\mp 1)}\cdot J_{\pm 2}(a_{n-m})\exp[\pm 2i\phi]+u_m{}^{(\pm 1)}\cdot J_0(a_{n-m})]=0. \qquad (65)$$

Если использовать представление для поля в виде (2.10) тогда $E_n^{(\pm 1)}\to E_n^{(\pm 1)}/2=-4\pi i u_n^{(\pm 1)}/k_0 n$, и уравнение (65), можно записать иначе

$$\frac{\partial E^{(\pm 1)}{}_n}{\partial t}\mp i\frac{\omega_{pe}^2-{\omega_0}^2}{2\omega_0}E^{(\pm 1)}{}_n\mp\frac{8\pi\omega_{pe}\nu_{in}}{2k_0 n}J_{\pm 1}(a_n)\cdot\exp(\pm i\phi)+$$
$$\mp i\frac{\omega_0}{2en_0}\sum_m\nu_{in-m}\cdot[E_m{}^{(\mp 1)}\cdot J_{\pm 2}(a_{n-m})\exp[\pm 2i\phi]+E_m{}^{(\pm 1)}\cdot J_0(a_{n-m})]=0. \qquad (66)$$

Приведем также уравнение для волны накачки

$$\frac{\partial E_0^{(\pm 1)}}{\partial t}\mp\frac{8\pi\omega_0}{2en_0 k_0}\sum_m\frac{\nu_{i,-m}}{m}\cdot[u_m{}^{(\mp 1)}\cdot J_{\pm 2}(a_{-m})\exp[\pm 2i\phi]+u_m{}^{(\pm 1)}\cdot J_0(a_{-m})]=0. \qquad (67)$$

Из представления волны накачки, соответствующего выбранной скорости осцилляций $u_{0\alpha}=-(e_\alpha E_0/m_\alpha\cdot\omega_0)\cdot Cos\Phi$ (3.4), получим $E_0\to -iE_0$ и $E_0^*\to iE_0^*$ и для E_0 уравнение (67) можно переписать [28]

$$\frac{\partial E_0}{\partial t}=\frac{8\pi i\omega_0}{2en_0 k_0}\sum_m\frac{\nu_{i,-m}}{m}\cdot[u_m^{(-1)}\cdot J_2(a_{-m})\exp[+2i\phi]+u_m^{(+1)}\cdot J_0(a_{-m})], \qquad (68)$$

где $\Delta=(\omega_{pe}^2-{\omega_0}^2)/2\omega_0$, или, выражая возмущения плотности через напряженности электрического поля мод,

$$\frac{\partial E_0}{\partial t}=-\frac{\omega_0}{2en_0}\sum_m\nu_{i,-m}\cdot[E_m{}^{(-1)}\cdot J_2(a_m)\exp[2i\phi]+E_m{}^{(+1)}\cdot J_0(a_m)]. \qquad (69)$$

Медленно изменяющаяся во времени напряженность электрического поля [30]

$$\bar{E}_n = (-\frac{4\pi i}{k_0 n})(\langle\{\nu_{en}\cdot\exp\{-ia_n\cdot Sin\Phi\}\rangle + \nu_{in}) =$$
$$= (-\frac{4\pi i}{k_0 n})\{\nu_{in}[1-J_0^2(a_n)+\frac{2}{3}J_2{}^2(a_n)]+[u_n^{(1)}J_1(a_n)\cdot e^{-i\phi}+u_n^{(-1)}\cdot J_{-1}(a_n)\cdot e^{i\phi}]- \quad (70)$$
$$-\frac{n^2}{en_0}J_0(a_n)\sum_m\frac{u^{(1)}{}_{n-m}\cdot u^{(-1)}{}_m}{(n-m)m}-\frac{n}{en_0}J_2(a_n)\cdot\sum_m\frac{1}{m}[u^{(1)}{}_{n-m}\cdot u^{(1)}{}_m e^{-2i\phi}+u^{(-1)}{}_{n-m}\cdot u^{(-1)}{}_m e^{2i\phi}]\}.$$

может быть представлена иначе

$$\bar{E}_n = (-\frac{4\pi i}{k_0 n})\nu_{in}[1-J_0^2(a_n)+\frac{2}{3}J_2{}^2(a_n)]+\frac{1}{2}[E_n^{(1)}J_1(a_n)\cdot e^{-i\phi}+E_n^{(-1)}\cdot J_{-1}(a_n)\cdot e^{i\phi}]-$$
$$-\frac{ink_0}{16\pi en_0}J_0(a_n)\sum_m E^{(1)}{}_{n-m}\cdot E^{(-1)}{}_m - \quad (71)$$
$$-\frac{ik_0}{16\pi en_0}J_2(a_n)\cdot\sum_m(n-m)[E^{(1)}{}_{n-m}\cdot E^{(1)}{}_m e^{-2i\phi}+E^{(-1)}{}_{n-m}\cdot E^{(-1)}{}_m e^{2i\phi}].$$

что позволяет описывать ионы крупными частицами, уравнения движения для которых приведены выше (2.20) и плотность ионов также определяется выражениями (21). Используя уравнения (52)–(53), в которых правыми частями можно пренебречь вследствие их малости, можно перейти к гидродинамическому описанию ионов. Уравнение для ионной плотности при этом [28]

$$\frac{\partial^2\nu_{in}}{\partial t^2} = -\Omega_i^2\{\nu_{in}[1-J_0^2(a_n)+\frac{2}{3}J_2{}^2(a_n)]+[u_n^{(1)}J_1(a_n)\cdot e^{-i\phi}+u_n^{(-1)}\cdot J_{-1}(a_n)\cdot e^{i\phi}]-$$
$$-\frac{n^2}{en_0}J_0(a_n)\sum_m\frac{u^{(1)}{}_{n-m}\cdot u^{(-1)}{}_m}{(n-m)m}-\frac{n}{en_0}J_2(a_n)\cdot\sum_m\frac{1}{m}[u^{(1)}{}_{n-m}\cdot u^{(1)}{}_m e^{-2i\phi}+u^{(-1)}{}_{n-m}\cdot u^{(-1)}{}_m e^{2i\phi}]\}, \quad (72)$$

или

$$\frac{\partial^2\nu_{in}}{\partial t^2} = -\Omega_i^2\{\nu_{in}[1-J_0^2(a_n)+\frac{2}{3}J_2{}^2(a_n)]+\frac{ik_0 n}{8\pi}[E_n^{(1)}J_1(a_n)\cdot e^{-i\phi}+E_n^{(-1)}\cdot J_{-1}(a_n)\cdot e^{i\phi}]-$$
$$+\frac{in^2k_0^2}{64\pi^2 en_0}\sum_m J_0(a_n)\cdot E^{(1)}{}_{n-m}\cdot E^{(-1)}{}_m + \quad (73)$$
$$+\frac{ink_0^2}{64\pi^2 en_0}\sum_m(n-m)[E^{(1)}{}_{n-m}\cdot E^{(1)}{}_m e^{-2i\phi}+E^{(-1)}{}_{n-m}\cdot E^{(-1)}{}_m e^{2i\phi}]\}.$$

Симметрии

Так как и выше, можно убедиться, в том, что комплексно сопряженное уравнение (67) при нижнем знаке принимает вид (при суммировании можно заменить немой индекс $m\to -m$)

$$\frac{\partial(E^{(-1)}{}_{-n})^*}{\partial t}-i\frac{\omega_{pe}^2-\omega_0^2}{2\omega_0}(E^{(-1)}{}_{-n})^*-\frac{4\pi\omega_{pe}(\nu_{i,-n})^*}{k_0 n}J_1(a_n)\cdot\exp(i\phi)-$$
$$-i\frac{\omega_0}{2en_0}\sum_m(\nu_{i,-n+m})^*\cdot[(E_{-m}{}^{(1)})^*\cdot J_{-2}(a_{-n+m})\exp[2i\phi]+(E_{-m}{}^{(-1)})^*\cdot J_0(a_{-n+m})]=0. \quad (74)$$

В то же время для положительных индексов, это же уравнение может быть записано

$$\frac{\partial E^{(1)}{}_n}{\partial t}-i\frac{\omega_{pe}^2-\omega_0^2}{2\omega_0}E^{(1)}{}_n-\frac{4\pi\omega_{pe}\nu_{in}}{k_0 n}J_{\pm1}(a_n)\cdot\exp(i\phi)-$$
$$-i\frac{\omega_0}{2en_0}\sum_m\nu_{in-m}\cdot[E_m{}^{(-1)}\cdot J_2(a_{n-m})\exp[2i\phi]+E_m{}^{(1)}\cdot J_0(a_{n-m})]=0. \quad (75)$$

а) Легко видеть, что при $E_{-n}^{(-1)}=(E_n^{(1)})^*$ и $\nu_{i,-n}=(\nu_{i,n})^*$ уравнения (72) и (73) идентичны. Точно также можно убедиться, что из подобных преобразований следует $E_n^{(-1)}=(E_{-n}^{(1)})^*$ и $\nu_{i,n}=(\nu_{i,-n})^*$. То есть, возмущения заряда ионов обладают симметрией $n_{i,-n}=(n_{i,n})^*$. При этом для корректного описания процесса неустойчивости достаточно использовать компоненты ВЧ поля $E_n^{(1)}$, $E_{-n}^{(1)}$ и $E_0^{(1)}$, а также возмущения заряда ионов $\nu_{i,n}$ при положительно определенных значениях индекса n. Так как остальные величины выражаются через них, то есть можно отказаться от использования верхнего индекса. Система уравнений (66), (71) в этих условиях может быть записана в виде

$$\frac{\partial E_n}{\partial t} - i\frac{\omega_{pe}^2 - \omega_0^{\,2}}{2\omega_0}E_n - \frac{4\pi\omega_{pe}\nu_{in}}{k_0 n}J_1(a_n)\cdot\exp(i\phi) -$$
$$-i\frac{\omega_0}{2en_0}\sum_m \nu_{in-m}\cdot[E_{-m}{}^*\cdot J_2(a_{n-m})\exp[2i\phi] + E_m\cdot J_0(a_{n-m})] = 0, \qquad (76)$$

$$\frac{\partial^2\nu_{in}}{\partial t^2} = -\Omega_i^2\{\nu_{in}[1 - J_0^2(a_n) + \frac{2}{3}J_2{}^2(a_n)] + \frac{ik_0 n}{8\pi}J_1(a_n)[E_n\cdot e^{-i\phi} - E_{-n}^*\cdot e^{i\phi}] -$$
$$+\frac{in^2k_0^2}{64\pi^2 en_0}\sum_m J_0(a_n)\cdot E_{n-m}\cdot E_{-m}^* + \frac{ink_0^2}{64\pi^2 en_0}\sum_m (n-m)[E_{n-m}\cdot E_m\cdot e^{-2i\phi} + E_{m-n}^*\cdot E_{-m}^*\cdot e^{2i\phi}]\}, \qquad (77)$$

или при описании ионов частицами, можно воспользоваться уравнениями движения (20) и выражением для ионной плотности (21), где напряженность медленно меняющегося электрического поля

$$\bar{E}_n = (-\frac{4\pi i}{k_0 n})\nu_{in}[1 - J_0^2(a_n) + \frac{2}{3}J_2{}^2(a_n)] + \frac{1}{2}J_1(a_n)[E_n\cdot e^{-i\phi} - E_{-n}^*\cdot e^{i\phi}] -$$
$$-\frac{ink_0}{16\pi en_0}J_0(a_n)\sum_m E_{n-m}\cdot E_{-m}^* - \qquad (78)$$
$$-\frac{ik_0}{16\pi en_0}J_2(a_n)\cdot\sum_m (n-m)[E_{n-m}\cdot E_m\cdot e^{-2i\phi} + E_{m-n}^*\cdot E_{-m}^*\cdot e^{2i\phi}].$$

Для E_0 также можно записать уравнение

$$\frac{\partial E_0}{\partial t} = -\frac{\omega_0}{2en_0}\sum_m \nu_{i,-m}\cdot[E_{-m}^*\cdot J_2(a_m)\exp[2i\phi] + E_m\cdot J_0(a_m)]. \qquad (79)$$

Отметим, что величины, отвечающие разному знаку нижнего индекса при этом независимы, что приводит к пространственному искажению интегральных возмущений, не только из-за изменения амплитуды, но и за счет пространственного сдвига отдельных компонент пакета.

б) В случае если $n_{i,-n} = n_{i,n} = (n_{i,n})^*$, то есть, возмущения ионной плотности не меняют своего положения в пространстве, то ВЧ электрическое поле также остается симметричным в пространстве $E_n^{(1)} = E_{-n}^{(1)} = (E_n^{(-1)})^* = (E_{-n}^{(-1)})^*$ и для описания процесса достаточно значений $E_n^{(1)}$ и $n_{i,n}$, что, как отмечено выше, обусловлено жесткой связью величин, отвечающих разному знаку нижнего индекса. Структура поля и плотности как в случае описанном в модели Захарова, будет представлять собой неподвижную пространственную структуру, амплитуда которой растет, а полуширина уменьшается, по крайней мере в определенной области.

в) Растущие во времени возмущения для ионов вида $n_{i,-n} = -(n_{i,n})^*$ не реализуются.

При $a_n << 1$ уравнения (76)-(78) с учетом представления $J_1(a_n) \approx a_n/2$, $J_0(a_n) \approx 1$, $J_2(a_n) \approx a_n^2/8$ совпадает с полученными ранее для высокотемпературного случая (41)-(43), с точностью до величины расстройки и с учетом замен $E_0 \to -iE_0$ и $E_0^* \to iE_0^*$ Точно также совпадают при этих же условиях уравнения для волны накачки (79) и (35).

ЛИНЕЙНАЯ ТЕОРИЯ

Ограничимся ниже рассмотрением наиболее интересного случая длинноволновой накачки. Из уравнений Захарова (32) и (33) в линейном случае, используя представление $\partial E / E\partial t = i\Omega$ можно получить дисперсионное уравнение для высокотемпературного случая в сверхзвуковом пределе $\partial^2 n_{in}/n_{in}\partial t^2 >> k_0^2 c_s^2 n^2$

$$-\Omega^2\{\Omega^2 - \Delta^2\} + \Delta\cdot A = 0, \qquad (80)$$

где расстройка равна $\Delta = v_{Te}^2 n^2 k_0^2/2\omega_p$, $A = \frac{1}{2}\left\{\frac{m_e}{m_i}\frac{k_0^2 n^2 v_{Te}^2}{2\omega_{pe}}\frac{|E_0|^2}{4\pi n_0 T_e}\right\}\omega_{pe}^3$.С другой стороны, линеаризуя уравнения (76) и (77), получим точно такое же дисперсионное уравнение для случая холодной плазмы, где, однако, $\Delta = \Delta_0 = \frac{\omega_{pe}^2 - \omega_0^{\,2}}{2\omega_0}$, а величина $A = J_1^{\,2}(a_n)\omega_{pe}^3\frac{m_e}{m_i}$. Заметим, что дисперсионные уравнения (80) при $a_n << 1$ и с учетом замен $E_0 \to -iE_0$ и $E_0^* \to iE_0^*$ в этих двух случаях совпадают. Положительная определенность расстройки $\Delta = v_{Te}^2 n^2 k_0^2/2\omega_p$ в модели Захарова очевидна, а что касается расстройки $\Delta = (\omega_{pe}^2 - \omega_0^{\,2})/2\omega_0$ в модели Силина, то, в книге [9] показано, что она также положительно определена, по крайней мере, в случае возбуждения длинноволновых ленгмюровских колебаний с частотой $\omega_0 \le \omega_{pe}$ сильноточным релятивистским

пучком электронов.

Для нормированных величин $\delta = \Omega / \omega_{pe}$ и $A \to A / \omega_{pe}^3$ в таблице приведены значения, отвечающие двум моделям описания модуляционной неустойчивости ленгмюровских волн.

Таблица.

Параметры моделей		
Модели	Захаровская модель	Силинская модель
Условия применимости	$\frac{\|E_0\|^2}{4\pi n_0 T_e} \equiv \frac{W}{n_0 T_e} << 1$	$\frac{\|E_0\|^2}{4\pi n_0 T_e} \equiv \frac{W}{n_0 T_e} >> 1$
Квадрат поправки к нормированной частоте	$\delta_1^2 = \frac{\Delta^2}{2} \pm \sqrt{\frac{\Delta^4}{4} + A\Delta}$	$\delta^2 = \frac{\Delta^2}{2} \pm \sqrt{\frac{\Delta^4}{4} + A\Delta}$
Расстройки	$\Delta_n = \frac{\omega_{pe}^2 + v_{Te}^2 k_0^2 n^2 - \omega_0^2}{2\omega_{pe}^2} \approx \frac{v_{Te}^2 k_0^2 n^2}{2\omega_{pe}^2}$	$\Delta = \Delta_0 = \frac{\omega_{pe}^2 - \omega_0^2}{2\omega_{pe}^2}$
Коэффициент А	$A = A(n) = \frac{1}{2}\left\{\frac{m_e}{M}\frac{k_0^2 n^2 v_{Te}^2}{2\omega_{pe}}\frac{\|E_0\|^2}{4\pi n_0 T_e}\right\}$	$A = A(n) = \left(\frac{m_e}{m_i}\right) J_1^2(a_n)$

В модели Захарова, нормированная на ленгмюровскую частоту поправка $\delta = \Omega / \omega_{pe}$, вообще говоря, должна быть записана в виде

$$\delta^2 = \frac{\Delta^2}{2} \pm \sqrt{\frac{\Delta^4}{4} + B\Delta^2}, \tag{81}$$

где

$$B = \frac{1}{2}\{\frac{m_e}{m_i}\frac{|E_0|^2}{4\pi n_0 T_e}\}. \tag{82}$$

Так как $(\Delta^4 + 4B\Delta^2)^{1/2} - \Delta^2$ с ростом Δ монотонно растет, не имея выраженного максимума, то при малых $\Delta^2 << B$, $\Omega^2 \approx -\Delta\sqrt{B}$, при этом $|\Omega^2| < B$, а инкремент неустойчивости равен

$$\mathrm{Im}\,\Omega = |\Omega| \approx \left(\frac{k_0^2 n^2 v_{Te}^2}{2\omega_{pe}^2}\right)^{1/2} \left(\frac{1}{2}\frac{|E_0|^2}{4\pi n_0 T_e}\frac{m_e}{m_i}\right)^{1/4} \omega_{pe}. \tag{83}$$

При больших $\Delta^2 >> B$, $\Omega^2 \approx -B$, при этом инкремент неустойчивости

$$\mathrm{Im}\,\Omega = |\Omega| \approx \left(\frac{1}{2}\frac{|E_0|^2}{4\pi n_0 T_e}\frac{m_e}{m_i}\right)^{1/2}. \tag{84}$$

То есть, инкремент увеличивается с ростом волнового числа возмущений, выходя при больших значениях волнового числа на свое наибольшее значение (84).

В модели Силина при значениях расстройки $\Delta^3 = A/2$ или, что то же самое $\Delta = (\frac{m_e}{2m_i})^{1/3} J_1^{2/3}(a_{n_m})$, относительный инкремент достигает значений

$$\delta = \pm\frac{i}{\sqrt[3]{2}} \cdot A^{1/3} = \pm\frac{i}{\sqrt[3]{2}}(\frac{m_e}{m_i})^{1/3} J_1^{2/3}(a_n). \tag{85}$$

Возмущения с волновым числом $k_m = k_0 n_m$ для которых $a_{n_m} = 1,84$, значение функции Бесселя максимально и величина относительного инкремента для таких возмущений достигает своего наибольшего значения

$$\delta_{\max} = \pm 0.44 i (\frac{m_e}{m_i})^{1/3}. \tag{86}$$

Таким образом, в модели Силина набольшим инкрементом обладают волновые вектора, для которых $a_{n_m} = 1,84$. При развитии неустойчивости амплитуда волны накачки убывает, и максимум инкремента перемещается в коротковолновую область.

Важно отметить, что значения максимальных инкрементов параметрической неустойчивости увеличиваются при уменьшении масштаба возмущений. Причем, если в модели Захарова уменьшение амплитуды поля накачки приводит снижению инкрементов во всей области неустойчивости, то в модели Силина подобный процесс сдвигает максимум инкремента в коротковолновую область, не уменьшая его значения (86). Таким образом, процесс перекачки по спектру в двух моделях в значительной степени обусловлен линейными механизмами роста возмущений.

ВЫВОДЫ

Существует глубокая связь между процессами модуляционной неустойчивости длинноволновых ленгмюровских колебаний как в горячей, так и в холодной плазме. Характер возбуждения имеет ту же симметрию, механизмы возбуждения обширного коротковолнового спектра также подобны. Движение энергии спектру в моделях Захарова и Силина связано не только с перестройкой поля - взаимодействием мод между собой, а в значительной степени есть следствие линейной неустойчивости. Максимальные инкременты для модели Захарова с уменьшением масштаба возмущений увеличиваются. В модели Силина максимальный инкремент при уменьшении амплитуды накачки сдвигается в коротковолновую область [10,38], что подтвердили результаты изучения нелинейной стадии процесса [29]. Важно также, что максимальный инкремент в холодной плазме при уменьшении амплитуды поля накачки не изменяется, а инкременты в горячей плазме при тех же условиях уменьшаются во всей области неустойчивости.

Возбуждаемые сильноточным пучком заряженных частиц ленгмюровские колебания большой амплитуды имеют длину волны не более чем на два порядка большую длин волн возбуждаемого спектра. Возбуждения в плазме в этом случае представляют собой даже при полной синхронизации фаз мод спектра кноидальную волну. Такую синхронизацию мод спектра можно формально моделировать, предполагая, что возмущения ионной плотности не меняют своего положения в пространстве, при этом электрическое поле также остается симметричным в пространстве. Структура поля и плотности будет представлять собой стоячую волну, амплитуда которой растет, а полуширина уменьшается. Подобная симметрия обсуждалась выше (б). Понятно, что каверны плотности в такой симметризованной задаче будут наиболее глубокими [31]. Их можно рассматривать как предельный и, видимо, трудно достижимый случай. В других обсуждаемых выше случаях (а) возмущения одного масштаба, но имеющие разное направление фазовой скорости, остаются независимыми. Медленно меняющееся во времени поле будет представлять собой сложную интерференцию возмущений разных масштабов. Интерференция в этом случае будет вынужденная [40], управляемая внешним полем накачки. Возникновение глубоких каверн, способных захватывать заметную часть ионов, подобно [31,41], в произвольном случае может осложняться интерференционными процессами и будет относительно редким, что, видимо, и наблюдали экспериментаторы.

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VIRTUAL WATER MOLECULE DISSOCIATION IN EXTERNAL ELECTROMAGNETIC FIELDS

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The model is proposed for describing a real water molecule by its two-dimensional analog, namely, the virtual molecule (VM). The proposed VM model provides the condition of coincidence between the fundamental eigenfrequencies of the real molecule and its virtual analog. The other VM parameters (bond length and atomic mass) are renormalized so that the molecule should steadily exist for a long time interval. Linear dynamics of VM atoms in the field of a monochromatic electromagnetic wave has been investigated. It is shown that under the action of an external electromagnetic field on the molecule at a resonance frequency, secular modes of vibrations are observed. The last ones are characterized by a time-linear growth of atomic oscillation amplitudes. The influence of the turn on of an external force at the time of stabilization of eigenfrequencies of the VM on the stability of VM atomic oscillations were made. It is shown that in some cases breaking of one of the VM bonds inevitably leads to the VM dissociation as a whole. As a result of numerical simulation, it has been established that the bond breaking has a threshold character, i.e., dissociation is not observed at the external force, which is below a certain value. In the region of forces exceeding the threshold values, the variation in the external electromagnetic field frequency is insensitive to the resonance effects that are due to the presence of dedicated frequencies of the VM. It is demonstrated that in the region, where the *H–O* bond breaking always takes place, there exist the *H–H* bond stability islands. Optimum parameters of VM dissociation have been determined.
KEY WORDS: virtual water molecule, eigenfrequencies, bond length, atomic mass, external force, dissociation.

ДИССОЦИАЦИЯ ВИРТУАЛЬНОЙ МОЛЕКУЛЫ ВОДЫ ВО ВНЕШНИХ ЭЛЕКТРОМАГНИТНЫХ ПОЛЯХ

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В работе предложена модель описания реальной молекулы воды ее двумерным аналогом – виртуальной молекулой (ВМ). В предложенной модели ВМ обеспечено условие совпадения основных собственных частот молекулы и ее аналога. Остальные параметры ВМ (длина связей и массы атомов) перенормированы таким образом, чтобы молекула устойчиво существовала длительный интервал времени. Исследована линейная динамика атомов ВМ в поле монохроматической электромагнитной волны. Показано, что при воздействии внешнего электромагнитного поля на молекулу на резонансной частоте наблюдаются секулярные режимы колебаний, которые характеризуются линейным во времени ростом амплитуд колебаний атомов. Исследовано влияние включения внешней силы в момент установления собственных колебаний ВМ на устойчивость колебаний ее атомов. Показано, что в некоторых случаях разрыв одной из связей ВМ неизбежно приводит к ее распаду в целом. В результате численного моделирования установлено, что разрыв связей имеет пороговый характер, т.е. диссоциация не наблюдается при внешней силе, меньшей определенного значения. В области сил, превышающих пороговые, варьирование частоты внешнего электромагнитного поля не чувствительно к резонансным эффектам, обусловленным наличием выделенных частот у ВМ. Показано, что в области, где всегда происходит разрыв связи Н–О существуют островки стабильности связи Н–Н. Определены оптимальные параметры диссоциации ВМ.
КЛЮЧЕВЫЕ СЛОВА: виртуальная молекула воды, собственные частоты, длина связи, атомная масса, внешняя сила, диссоциация

ДИСОЦІАЦІЯ ВІРТУАЛЬНОЇ МОЛЕКУЛИ ВОДИ В ЗОВНІШНІХ ЕЛЕКТРОМАГНІТНИХ ПОЛЯХ

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У роботі запропонована модель опису реальної молекули води її двовимірним аналогом - віртуальною молекулою (ВМ). У запропонованої моделі ВМ забезпечена умова збігу основних власних частот молекули і її аналога. Інші параметри ВМ (довжина зв'язків і маси атомів) перенормовані таким чином, щоб молекула стійко існувала тривалий інтервал часу. Досліджено лінійну динаміку атомів ВМ у полімонохроматичної електромагнітної хвилі. Показано, що при впливі зовнішнього електромагнітного поля на молекулу на резонансній частоті спостерігаються секулярні режими коливань, які характеризуються лінійним у часі зростанням амплітуд коливань атомів. Досліджено вплив включення зовнішньої сили в момент установлення власних коливань ВМ на стійкість коливань її атомів. Показано, що в деяких випадках розрив однієї зі

зв'язків ВМ неминуче приводить до її розпаду в цілому. У результаті числового моделювання встановлено, що розрив зв'язків має граничний характер, тобто дисоціація не спостерігається при зовнішній силі, меншої певного значення. В області сил, що перевищують граничні, варіювання частоти зовнішнього електромагнітного поля не відчутно до резонансних ефектів, обумовлених наявністю виділених частот у ВМ. Показано, що в області, де завжди відбувається розрив зв'язку *H–O*, існують острівці стабільності зв'язку *H–H*. Визначено оптимальні параметри дисоціації ВМ.
КЛЮЧОВІ СЛОВА: віртуальна молекула води, власні частоти, довжина зв'язку, атомна маса, зовнішня сила, дисоціація

Today, many economically advanced countries are more closely consider hydrogen not only in the traditional application, but also as a basis for energy tomorrow. Against the background of the catastrophic environmental degradation and depletion of the world hydrocarbon resources, it is tempting to use hydrogen as a fuel is harmless to the means of transport, heating in remote regions, autonomous and stationary sources of secondary energy. Hydrogen is chosen as the most abundant element on the earth and in space, but in nature it almost does not occur in pure form and must be extracted from chemical compounds (H_2O, HCl, HF, etc.)

Triatomic molecules (H_2O, CO_2, NO_2, SO_2, H_2S, etc.) are characterized by the presence of a fine structure of their absorption spectra. A full and exact information on the parameters of these spectra is of basic importance for solving many applied and fundamental problems such as the development of theory and practice of femtochemistry [1]; analysis of the impact of volcanic outbursts, “greenhouse” effect, ozone layer on the ecology and climate variations of the Earth [2]; creation of alternative energy sources based on the controlled molecule dissociation in external electromagnetic fields [3,4].

One of the methods to control the internal dynamics of triatomic molecules is to act upon them through an electromagnetic field, which is oscillating at frequencies close to the frequencies of atomic oscillations in molecules [3,4]. Since the frequencies of atomic oscillations in molecules lie in the infrared spectrum [5], the resonance action on the internal dynamics of the molecule is entirely feasible with the use of lasers that generate electromagnetic radiation of corresponding wave lengths [1].

The other method of water molecule dissociation, different from laser technologies, has been described by Meyerin his patent [6]. Here, to achieve the objective, a sequence of special-shape unipolar voltage pulses was used, with the voltage-time step function for the leading and trailing edges of the pulse and the exponentially increasing function for the pulse peak.

Since the above-described methods of triatomic molecule dissociation by external electromagnetic fields are far from creating of adequate model [3,4] or are based on empirical facts [6], it appears of importance and necessity to continue the research in this direction. The present paper deals with the modeling of the interaction between the real triatomic molecule (H_2O as an example) and the external electromagnetic fields of the virtual molecule (VM).

The aim of this work is a study of the steady state of virtual water molecules, which simulates a real molecule of water, and determination of its dissociation conditions in external electromagnetic fields.

THE MODEL OF WATER MOLECULE

The water molecule presents a triatomic molecule H_2O that consists of one oxygen atom and two hydrogen atoms. Its schematic view is shown in Fig. 1.

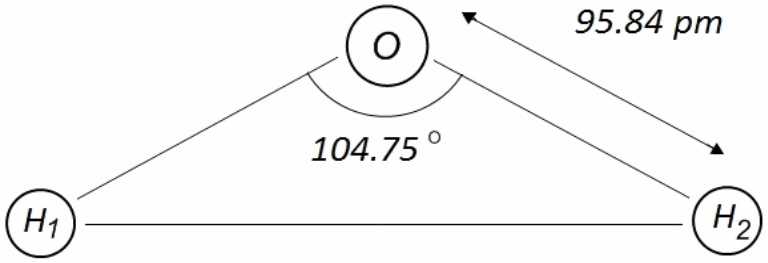

Fig. 1. Scheme of water molecule

The oxygen atoms are linked with the hydrogen atom by covalent chemical bonds, each bond involving two electrons (in the figure, the bonds are shown by lines). The equilibrium length of the *H–O* bond makes 0.9584 A. The valence angle (angle between valence bonds) is equal to 104.75° [4]. The *H–O* bond energy is determined to be 101.3 kcal/mole [7]. This energy is also called the dissociation energy, because its excess leads to bond breaking, and that corresponds to the molecule dissociation.

DETERMINATION OF FICTITIOUS *H–H* BOND COEFFICIENT AND VM PARAMETERS

Similarly to ref. [8], we consider a planar (two-dimensional) model of water molecule. We shall represent the atoms by point masses, denoting the hydrogen atomic mass by m_H , and the oxygen atomic mass by m_O. In the equilibrium state, the hydrogen atoms are situated at the ends of the base of the isosceles triangle, and the oxygen atom is found at the vertex of the angle formed by its lateral sides. We introduce the notation a_{HO} and a_{HH} , which correspond

to the equilibrium distance between the oxygen atom and the hydrogen atom, and between hydrogen atoms, respectively.

In the centre-of-mass system (C.M.S.) the equations of motion for the molecule atoms being in the external electromagnetic field are written as

$$\begin{cases} m_H \dfrac{d^2\vec{R}_{H_1}}{dt^2} = \vec{F}_{H_1} + \vec{F}_{H_1O} + \vec{F}_{H_1H_2}, \\ m_O \dfrac{d^2\vec{R}_O}{dt^2} = \vec{F}_O + \vec{F}_{OH_1} + \vec{F}_{OH_2}, \\ m_H \dfrac{d^2\vec{R}_{H_2}}{dt^2} = \vec{F}_{H_2} + \vec{F}_{H_2O} + \vec{F}_{H_2H_1}. \end{cases} \quad (1)$$

Here $\vec{R}_O = \{X_O, Y_O\}$, $\vec{R}_{H_1} = \{X_{H_1}, Y_{H_1}\}$ и $\vec{R}_{H_2} = \{X_{H_2}, Y_{H_2}\}$ are the radii-vectors of oxygen and hydrogen atoms, drawn from the centre of mass; $\vec{F}_O, \vec{F}_{H_1}, \vec{F}_{H_2}$ are the vectorial forces of electromagnetic field action on oxygen atoms; $\vec{F}_{H_1O}$, $\vec{F}_{OH_1}$, $\vec{F}_{H_2O}$, $\vec{F}_{OH_2}$, $\vec{F}_{H_1H_2}$, $\vec{F}_{H_2H_1}$ are the vectorial action forces of atoms indicated by the first on the atoms indicated by the second.

We suppose that the electromagnetic field can be described by a monochromatic wave propagating in the assigned direction, and take into consideration only the electric field strength. Since the treatment is carried out in the C.M.S., and the molecule is immobile, then the total action of the electric field strength on the molecule equals zero. In this case, the following equalities may be considered as fulfilled for the moduli of external forces:

$$\left|\vec{F}_{H_1}\right| = \left|\vec{F}_{H_2}\right| = -\frac{1}{2}\left|\vec{F}_O\right| \equiv \left|F\right|. \quad (2)$$

The external force direction $\vec{F}$ is given by the unit vector $\vec{e}$: $\vec{F} = \left|\vec{F}\right| \cdot \vec{e}$, and the force value is given by the relation: $\left|\vec{F}\right| \approx d' \cdot E(t)$, where d' - is the derivative of the dipole *H–O* bond moment with respect to the interatomic distance, is the electric field strength amplitude prescribed externally.

For intramolecular forces the relationship $\vec{F}_{AB} = -\vec{F}_{BA}$ is valid.

We now determine the intramolecular force values proceeding from the assumption that the forces are paired and central. The assumption is corresponds to the Morse potential representation of the interaction force field [8]

$$\prod_{AB}(\vec{r}) = D_{AB}(\exp(-2\alpha_{AB}(r - a_{AB})) - 2\exp(\alpha_{AB}(r - a_{AB}))), \quad (3)$$

where $D_{AB} = D_{BA}$ is the binding energy between the atoms *A* and *B*, $\alpha_{AB} = \alpha_{BA}$ is the equlilibrium distance between them, $a_{AB} = a_{BA}$ is the parameter describing the width of potential well.

Using eq. (3) we can determine the value and direction of force between the atoms *A* and *B*:

$$\vec{F}_{AB} = -\frac{d}{dr}\prod_{AB}(\vec{R}_A - \vec{R}_B)\frac{\vec{R}_A - \vec{R}_B}{\left|\vec{R}_A - \vec{R}_B\right|}. \quad (4)$$

The analysis of a linearized set of equations (1) in the absence of the external electromagnetic field and with due regard for eq. (4) leads to the following equations for the eigenfrequencies:

$$\left(2m_O\alpha_{HO}^2 + m_O\alpha_{HH}^2\right)C_{HO} - 2m_H m_O \alpha_{HO}^2 \omega^2 = 0 \quad (5)$$

$$\begin{aligned} &2\alpha_{HO}^2 m_O m_H^2 \omega^4 + \left(m_H^2\alpha_{HH}^2 C_{HO} - 4m_H^2\alpha_{HO}^2 C_{HO} - 4m_O m_H \alpha_{HO}^2 C_{HH} - 2m_O m_H \alpha_{HO}^2 C_{HO}\right)\omega^2 + \\ &+4m_O\alpha_{HO}^2 C_{HO} C_{HH} + 8m_H\alpha_{HO}^2 C_{HO} C_{HH} - m_O\alpha_{HH}^2 C_{HO} C_{HH} - 2m_H\alpha_{HH}^2 C_{HO} C_{HH} = 0, \end{aligned} \quad (6)$$

where $C_{AB} = 2\alpha_{AB}^2 D_{AB}$ are the stiffness factors of molecule bonds.

If in Eqs. (5,6) all the parameters were prescribed, then it would be possible to determine from them the eigenfrequencies of antisymmetric ω_{as} (eq. (5)) and symmetric $\omega_s^{(1)}$, $\omega_s^{(2)}$ (Eq. (6)) molecular oscillations.

However, in our case we have only the experimentally measured eigenfrequencies, molecular dimensions α_{OH}, α_{HH} and the bond energy D_{OH}. Their values are listed in Table 1 [9, 10].

The Tabl. 2 gives the width values of potential wells $\alpha_{AB} \equiv \sqrt{C_{AB}(2D_{AB})^{-1}}$ in the Morse representation. Note that

to calculate the unknown width of the *H–H* bond potential well, we assume the relation $D_{HH} \approx 0{,}2 \cdot D_{HO}$ to be true [4].

Table 1.

Equilibrium parameters of the nitrogen dioxide molecule

Parameter	Notation	Values	
		SI units	Hartree units
Oxygen atomic mass	m_O	$2.657 \cdot 10^{-26}$ kg	29176
Hydrogen atomic mass	m_H	$1.6737 \cdot 10^{-26}$ kg	18373
H – O bond dissociation energy	D_{HO}	101.3 kcal/mole	0.1614
H – O bond equilibrium distance	α_{OH}	0.93 Å	1.81474
H – H bond equilibrium distance	α_{HH}	1.53 Å	2.8922
Antisymmetric vibration frequency	$\omega_0 \equiv \omega_a$	3938.7 cm^{-1}	$17.92 \cdot 10^{-3}$
Symmetric vibration frequency	$\omega_1 \equiv \omega_s^{(1)}$ $\omega_2 \equiv \omega_s^{(2)}$	3835.4 cm^{-1} 1647.6 cm^{-1}	$17.45 \cdot 10^{-3}$ $7.49 \cdot 10^{-3}$

Since the eigenfrequencies have been observed and measured for the real molecule, for the transition from its three-dimensional model to the planar one some parameters must be renormalized, i.e., they should be changed so that eqs. (5), (6) should become jointly. As a result of these manipulations, the parameters of the two-dimensional VM would be determined, with the use of which the processes in the real molecule could be modeled.

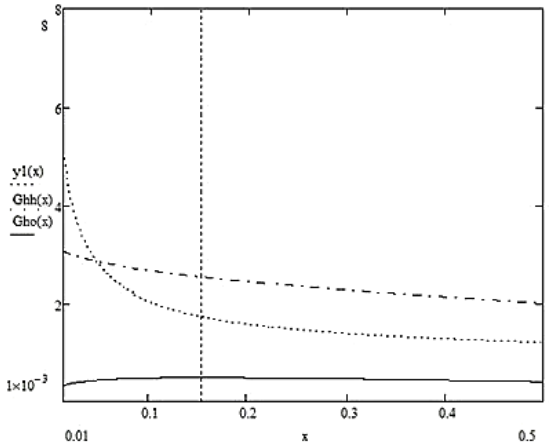

Fig. 2. Solution of eq. (9) for y versus x, and the molecule stiffness factor $Gho \cdot 10^5$ and $Ghh \cdot 10^5$ as a function of the parameter x.

For this purpose we assume the eigenfrequencies ω_i in eqs. (5), (6) be prescribed, and the parameters that have to be determined (i.e., their new values should be found (renormalized)), will be put to be $x = \dfrac{m_H}{m_O}$; $y = \dfrac{1}{2}\left(\dfrac{\alpha_{HH}}{\alpha_{OH}}\right)^2$. In this case, the stiffness factors $C_{HH} \cdot m_H^{-1}$ and $C_{HO} \cdot m_H^{-1}$ are expressed in terms of the eigenfrequencies x, y in the following way:

$$G_{HO} = C_{HO} \cdot m_H^{-1} = \frac{\omega_0^2}{1+xy} \tag{7}$$

$$G_{HH} = C_{HH} \cdot m_H^{-1} = \frac{1}{2}\left(\omega_0^2 + \omega_1^2 + \omega_2^2\right) - \frac{1+x}{1+xy}\omega_0^2 . \tag{8}$$

Transforming eq. (6) with regard for eqs. (7), (8) it is not difficult to derive the required equation, which relates the renormalized parameters x, y (Fig. 2.):

$$Z^2(x,y) - Z(x,y)(1+x)(1+y) + 1 + x(2-y) - \left(\frac{1+xy}{2}\right)^2 \left(\left(\frac{\omega_1}{\omega_0}\right)^2 - \left(\frac{\omega_2}{\omega_0}\right)^2\right)^2 = 0 , \tag{9}$$

where

$$Z(x,y)=\frac{1+xy}{2}\left(1+\left(\frac{\omega_1}{\omega_0}\right)^2+\left(\frac{\omega_2}{\omega_0}\right)^2\right)-x-1\cdot$$

As in [8] were calculated parameters of virtual molecules listed in Table 2.

Table 2.

VM parameters

Parameter	Notation	Hartree units
Oxygen atomic mass (renormalized)	m_O^*	149967
Hydrogen atomic mass	m_H	18373
O–H bond stiffness factor	C_{OH}	4.658
H–H bond stiffness factor	C_{HH}	0.885
Equilibrium length of the *O–H* bond (renormalized)	α_{OH}^*	1.557
Equilibrium length of the *H–H* bond	α_{HH}	2.8922
Width of potential well for the *H–O* bond	α_{HO}	3.798
Width of potential well for the *H–H* bond	α_{HH}	3.703

LINEAR DYNAMICS OF VM ATOMS IN THE FIELD OF MONOCHROMATIC ELECTROMAGNETIC WAVE

We write down the external force created by the electromagnetic wave field, which exerts action on the molecule atoms, as:

$$\left|\vec{F}\right|=d'\cdot E(t)\cdot\vec{e}\equiv d'\cdot E_0e^{-i(\omega t+\theta)}\cdot\vec{e}\,, \tag{10}$$

where E_0,ω,θ are, respectively, the amplitude, frequency and control phase of the electric field strength of the wave.

Let us investigate the linear response of the molecule to the action of the external electromagnetic field. To this end, we derive the equation describing the temporal variation of the bond lengthening $X_{H_1O}\equiv\delta\vec{R}_{H_1}\cdot\vec{e}_{H_1O}$, which characterizes small deviations of the hydrogen atom H_1 from the equilibrium position along the $O-H_1$ bond. In this case it is necessary to use the VM parameters presented in Table 2.

Since in the proposed model the atoms of water molecule are described by the triangle with the corresponding stiffness coefficients, to estimate the dynamic strength of this structure, it will suffice to have information about the lengthening of one of the bonds, e.g., $O-H_1$.

After linearization of the initial set of equations (1), assuming the peak value of force $\left|\vec{F}_d\right|\equiv d'\cdot E_0(t)$ to be the function weakly dependent on time ($\frac{dE_0}{dt}<<\omega E_0$),we obtain the equation that describes the temporal variation of the bond lengthening X_{H_1O} under the action of the external field with the frequency ω_0:

$$\frac{d}{dt}X_{H_1O}=-\frac{F_d}{2}\frac{C_{HO}(1+2\frac{m_H}{m_O^*})}{m_H^2\omega_H^3}\cos\varphi_0\cos\varphi\,, \tag{11}$$

where $\phi_0\approx37.625^o$ is the renormalized angle at the base of the molecule, φ is the angle between the external force direction and the H_1-H_2 direction, is the time in Hartree units, $\theta=-\frac{\pi}{2}$.

It is not hard to show that the lengthening of oxygen bonds with other atoms of the molecule is determined through X_{H_1O} in the following way:

$$\delta\vec{R}_{H_1}\cdot\vec{e}_{H_2O}\gamma^{-1}=\delta\vec{R}_{H_1}\cdot\vec{e}_{H_1H_2}\beta^{-1}=-\delta\vec{R}_{H_2}\cdot\vec{e}_{H_1O}\gamma^{-1}=-\delta\vec{R}_{H_2}\cdot\vec{e}_{H_2O}=\delta\vec{R}_{H_2}\cdot\vec{e}_{H_1H_2}\beta^{-1}=\delta\vec{R}_{H_1}\cdot\vec{e}_{H_1O}\,, \tag{12}$$

where $\beta=\frac{a_{HH}}{2a_{OH}^*}=0.929$, $\gamma=\left(\frac{a_{HH}}{a_{OH}^*}\right)^2=-0.726$.

From eq. (11) it follows that the $O-H_1$ bond length increases linearly with time at the angles of action $\frac{\pi}{2}<\varphi<\frac{3\pi}{2}$. The length of other bonds also changes with time by the linear law in accord with relations.

Thus, the presence of secular regimes in eq. (11), which result from the action of the external electromagnetic field on the molecule at a resonance frequency, points to the adequacy of the proposed model to the physical processes, which are to take place in the real molecule.

Since the linear dynamics of the molecule displays its resonant properties, it appears of interest to retrace the VM behavior at great atomic displacement amplitudes, i.e., to investigate VM nonlinear oscillations up to the bond breaking.

NONLINEAR DYNAMICS AND DISSOCIATIVE MODES OF THE VM IN THE MONOCHROMATIC ELECTROMAGNETIC WAVE FIELD

Nonlinear dynamics of the VM

The investigation on the VM nonlinear dynamics in external fields must be started from the adjustment of nonlinear oscillations of a free molecule, i.e., from initial data fitting in the original equations (1) in the absence of external fields. As a result of this adjustment, the VM oscillation spectrum must comprise eigenfrequencies ω_i. In this case, the initial arrangement of VM atoms must be in accord with the linear theory.

The numerical calculation data on the temporal change of VM atom coordinates as well as their spectral resolution are presented in Fig. 3,4. It follows from these figures that with time the molecular atoms fit into the parameters of the Morse potential, i.e., oxygen atoms oscillate relative to the points with the coordinates $X_O \approx 0.0$; $Y_O \approx 0.057$ and the hydrogen atom oscillates relative to the point with the coordinates $X_{H1,H2} \approx \pm 1.44735$; $Y_{H1,H2} \approx -0.4917$.

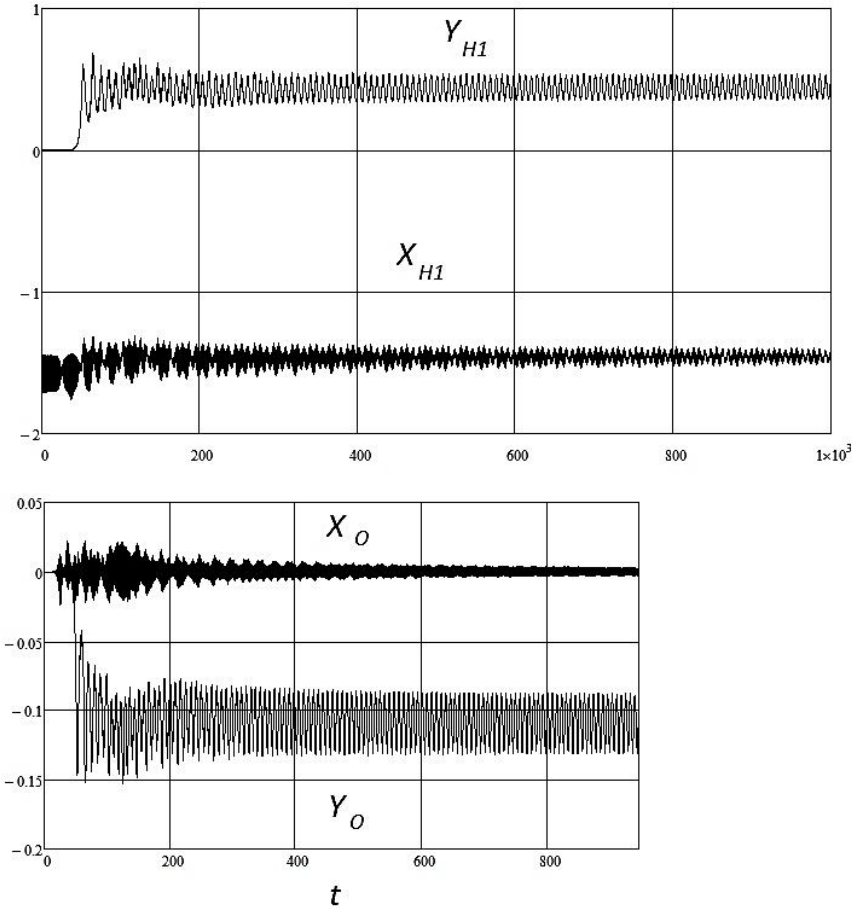

Fig. 3. Coordinates of hydrogen and oxygen atoms in the molecule versus time t.

The VM oscillation spectrum intensity I_Ω was obtained by the use of a fast Fourier transform of atomic displacement projections in the x, y, coordinates, calculation of their arithmetic mean and a subsequent moving average smoothing (Fig. 4). For identification of peaks of the thus obtained spectrum we make use of the fact that the maximum resonance frequency Ω_0 should have the peak intensity (Very Strong), and the lowest frequency Ω_2 should have a lower intensity (Strong).

In view of the above, the spectrum analysis permits us to separate the following resonance frequencies of VM oscillations: $\Omega_0 \approx 0.13916$; $\Omega_1 \approx 0.27588$; $\Omega_2 \approx 0.41016$ which the appropriate choice of a new mass of an oxygen atom m_0' equivalent to the eigenfrequencies ω_2. So, the data given in Fig. 4, show that the proposed model adequately describes nonlinear nitrogen dioxide molecular oscillations: the eigenfrequencies of VM oscillations correspond to the frequencies of symmetrical and antisymmetrical oscillations of real nitrogen dioxide.

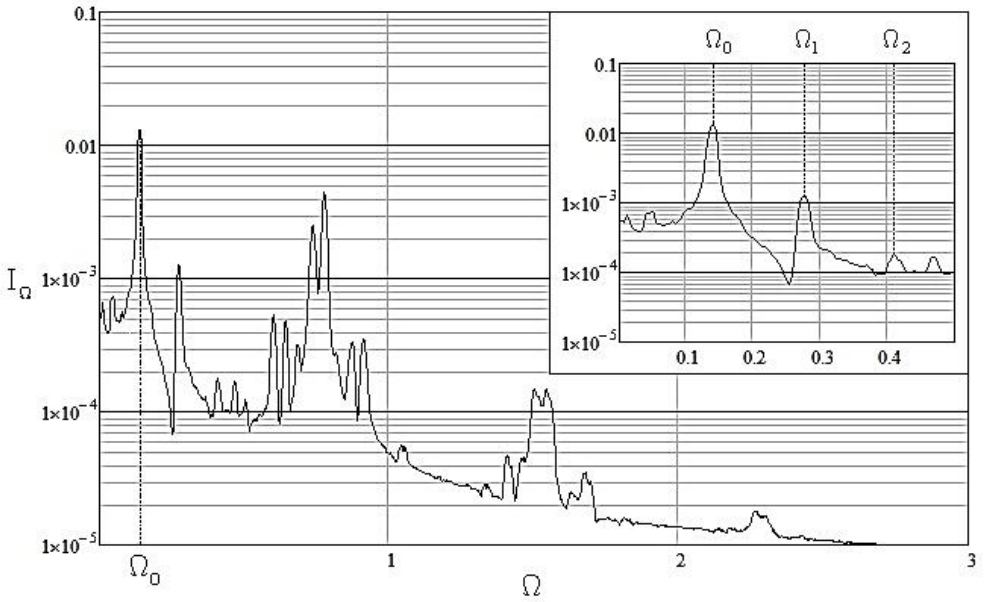

Fig. 4. Averaged and smoothed intensities I_Ω of the oscillation spectrum of water VM atoms. After appropriate transformations, the peaks, marked with dashed lines, coincide with resonant frequencies of the real water molecule ω_i.

VM dissociative modes in the field of a monochromatic electromagnetic wave

Examine dissociative modes VM fields of external electromagnetic radiation. To do this, at the moment the eigenfrequencies of the VM to include the external force. The force value is determined by expression (10), where the control phase may equal zero, and the force direction is prescribed by the unit vector $\vec{e}$.

As it follows from the calculations, at the moment of external force switch on, the molecule atoms oscillate in the neighborhood of vertices of the isosceles triangle with the coordinates $X_{H1,H2} \approx \pm 1.44735$; $Y_{H1,H2} \approx -0.4917$; $X_O \approx 0.0$; $Y_O \approx 0.057$. This state of the VM will be characterized as equilibrium.

In numerical calculations, the harmonic component of the external force is prescribed in the form of $\approx F \cdot \sin(\Omega t)$, where the amplitude F varies in the range $0 \le F \le 3$, and the angle of force action φ ranges within $0 < \varphi < 2\pi$.

In calculations, we shall assume that an increase in the *H–H* or *H–O* bond length by more than two times leads to bond breaking. And if one takes into account that all the calculations are carried out in the C.M.S., then the breaking of one of the bonds gives such a reactive force to the other VM atoms, that it inevitably results in the VM dissociation as a whole. This conclusion is confirmed by numerical simulation, too.

The main question of numerical simulation of VM dynamics in the field of external forces consists only in what bond will be the first to break and at what conditions. The answer to this question is given by numerical simulation of atom dynamics of the triatomic VM in the field of the external electromagnetic wave.

Fig. 5-8 show the numerical simulation results for VM bond dissociation versus the F amplitude and the angle of action of the external force, φ specified by both the electromagnetic wave (Fig. 5-7) and the stationary electric field (Fig. 8). In the figures, the bottom plane specifies the parameters of the *H–H*, bond breaking, and the top plane – *H–O* bond breaking. The areas in the planes, marked by small squares with a side length of 0.1, correspond to these bond breakings.

The data presented in Fig. 5-8 are characterized by the periodicity in the angle of external force action φ.

From Fig. 5-7 it follows that for all resonance frequencies the bond dissociation does not take place at the external force lower than a certain value $F \le 0.5 \div 0.8$, the range of this value being dependent on the angle φ.

At $F \ge 0.8$ the change in the frequency of the external electromagnetic field gives no resonance effects specified by the presence of dedicated frequencies of the molecule.

This may be due to a strong nonlinear link of atoms in the molecule, when linear connections cannot manifest themselves. The observed correlation of minimum forces F, leading to breaking of *H–H* and *H–O* bonds, can also be attributed to a strong nonlinear link of atoms in the molecule.

From Fig. 5-7 it can be seen that at $F > 0.4$ the *H–O* bond breaking always takes place, whereas the *H–H* bond may exhibit the stability islands. This is particularly evident for the resonance frequency Ω_0, which is characterized by the maximum amplitude of oscillations.

Since the VM dissociation occurs at breaking of any bond, it is of interest to find the optimum parameters of dissociation, viz., the minimum force and the corresponding to it angle of action on the molecule.

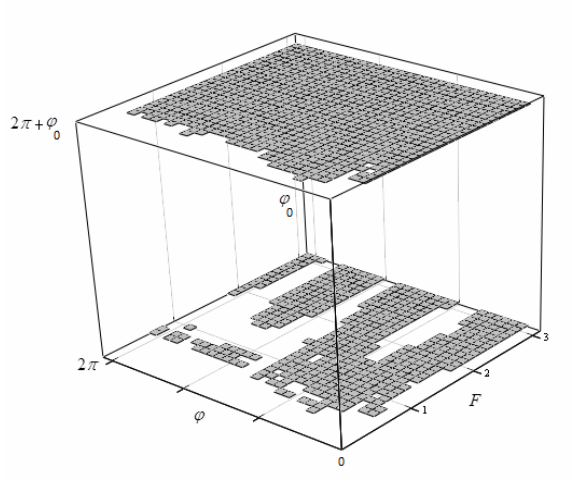

Fig. 5. Electromagnetic field frequency Ω_0.

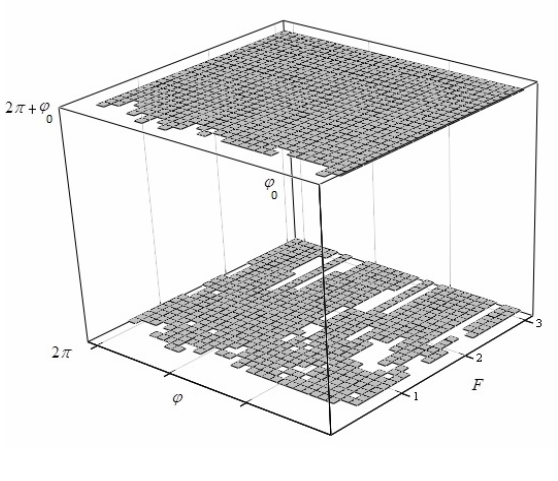

Fig. 6. Electromagnetic field frequency Ω_1.

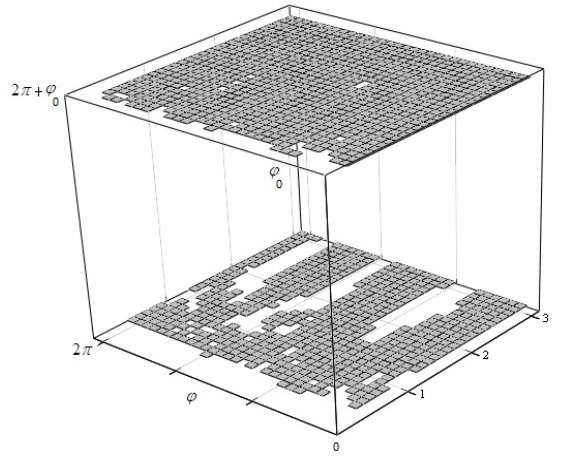

Fig. 7. Electromagnetic field frequency Ω_2.

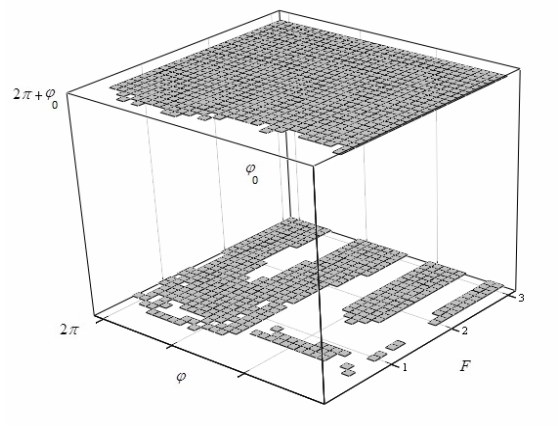

Fig. 8. The electromagnetic field is constant.

The numerical simulation data on the optimum parameters of dissociation are presented in Table 3.

Table 3.

Optimum VM dissociation parameters

Electromagnetic wave field of the frequency, Ω	Force, F	Angle of action, φ
Ω_0	0.4	$\pi(4/15) \le \varphi \le \pi(2/5)$
Ω_1	0.4	$\pi(23/15) \le \varphi \le \pi(49/30)$
Ω_2	0.4	$\pi(16/15) \le \varphi \le \pi(61/30)$ $\pi(26/15) \le \varphi \le \pi(61/30)$
Constant field	0.3	$\pi(46/30) \le \varphi \le \pi(49/30)$

Theoretical studies have shown that the development of the experimental cell needs to apply a constant field with a rectangular pulse of force F = 0.3 in units of Hartree in the Si units F = 2.2 V/cm and at angles of impact of $\pi(46/30) \le \varphi \le \pi(49/30)$.

CONCLUSIONS

Thus, we have proposed the model for description of the real water molecule by its two-dimensional analog, namely, the virtual molecule (VM). In the proposed VM model, the condition of coincidence between the eigenfrequencies of the molecule and its analog is provided. The other VM parameters (bond length and atomic mass) are renormalized so that the molecule should steadily exist for a long time interval.

Linear dynamics of VM atoms in the field of a monochromatic electromagnetic wave has been investigated. It has been shown that under the action of an external electromagnetic field on the molecule at a resonance frequency, secular regimes of oscillations are observed. The last ones are characterized by a time-linear growth of atomic oscillation amplitudes. The increase in the atomic oscillation amplitudes places the molecule in the nonlinear regime. Under these

conditions, the dynamics of VM atoms in the field of the monochromatic electromagnetic wave causing the VM dissociation can be investigated only by the numerical simulation method. To this end, after the VM eigenfrequencies settled, the action of the external force on the molecule dissociation was investigated. It has been demonstrated that in some cases the breaking of one of VM bonds inevitably leads to the VM dissociation as a whole. As a result of numerical simulation, it has been established that the bond breaking has a threshold character, i.e., dissociation is not observed at the external force, which is lower than a certain value of $F \leq 0.3 \div 0.7$. The range of external force variations depends on the angle of external action φ. In the range of forces exceeding the threshold values, $F > 0.7$ the variation in the external electromagnetic field frequency is insensitive to the resonance effects that are due to the presence of dedicated frequencies of the VM. It has been demonstrated that at $F > 0.4$ the *H–O* bond breaking always takes place, whereas the *H–H* bond may exhibit stability islands. Optimum parameters of VM dissociation have been determined and set parameters of the experimental cell.

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ROLE OF ANGULAR MOMENTUMUM IN CAPTURE OF HEAVY NUCLEI

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The influence of angular momentum on the dynamics of the heavy nucleus interaction in the capture process is analyzed on a dynamic-statistical approach. The range of light nuclei and stability region for angular momentum, where capture is possible, are determined on the basis of analysis of the nucleus-nucleus potential for reactions with heavy nuclei $^{238}_{92}$U, $^{244}_{94}$Pu, $^{248}_{96}$Cm and $^{251}_{98}$Cf. The capture cross sections of compound nuclei with $Z_0 = 120$ and 126 are calculated, and the most perspective reactions to obtain the superheavy elements are pointed out.
KEY WORDS: angular momentum, synthesis of superheavy elements, stability region, capture cross section.

РОЛЬ УГЛОВОГО МОМЕНТА В ПРОЦЕССЕ ЗАХВАТА ТЯЖЕЛЫХ ЯДЕР
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На основании динамико-статистического описания рассматривается влияние углового момента на динамику взаимодействия тяжелых ядер в процессе захвата. Диапазон легких ядер и область стабильности углового момента где возможен захват определены при анализе ядро-ядерного потенциала для реакций с тяжелыми ядрами $^{238}_{92}$U, $^{244}_{94}$Pu, $^{248}_{96}$Cm и $^{251}_{98}$Cf. Было рассчитано сечение захвата для составных ядер с $Z_0 = 120$ и 126 и определены наиболее перспективные реакции для получения сверхтяжелых элементов.
КЛЮЧЕВЫЕ СЛОВА: угловой момент, синтез сверхтяжелых элементов, область стабильности, сечение захвата.

РОЛЬ КУТОВОГО МОМЕНТУ В ПРОЦЕСІ ЗАХВАТУ ВАЖКИХ ЯДЕР
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Виходячи з динаміко-статистичного опису розглядається вплив кутового моменту на динаміку взаємодії важких ядер в процесі захвату. Діапазон легких ядер і область стабільності кутового моменту де можливий захват визначені при аналізі ядро-ядерного потенціалу для реакцій з важкими ядрами $^{238}_{92}$U, $^{244}_{94}$Pu, $^{248}_{96}$Cm і $^{251}_{98}$Cf. Було розраховано переріз захвату для складених ядер з $Z_0 = 120$ і 126 та визначено найбільш перспективні реакції для отримання надважких елементів.
КЛЮЧОВІ СЛОВА: кутовий момент, синтез надважких елементів, область стабільності, переріз захвату

"Cold" and "hot" fusion reactions are used in the experimental study of mechanisms of synthesis of new superheavy elements (SHE). Increase of the charge number of the heavy nucleus enables synthesizes of new elements with accelerators. SHE with $Z_0 = 112$ (charge number) and $Z_0 = 113-118$ [1-3] were obtained in the "cold" and "hot" fusion reactions respectively. The improvement of acceleration technology with increase of beam intensity is required in the course of SHE formation for the purpose of further promotion of experimental works on Z_0 scale, since the expected cross section of new SHE does not exceed several femtobarn [3]. In NSC KIPT acceleration structures are developed for the purpose of experimental study of heavy nuclei fusion characteristics [4, 5].

In the description of heavy nuclei fusion with fixed mass A_i and charge Z_i numbers ($i = 1, 2$) SHE formation cross section is calculated [6] as follows:

$$\sigma_{ER} = \sum_{L=0} \sigma_{cap}(E_{cm}, L) \cdot P_{CN}(E_{cm}, L) \cdot W_s(E_{cm}, L), \quad (1)$$

where $\sigma_{cap}(E_{cm}, L)$ – partial capture cross section of the incident nucleus capture by the target nucleus; $P_{CN}(E_{cm}, L)$ – probability of the compound nucleus formation after capture; $W_s(E_{cm}, L)$ – survivability of the compound nucleus with respect to fission, L – angular momentum, E_{cm} – light nucleus kinetic energy.

The aim of this article is to study influence of the angular momentum on the capture probability and cross section for perspective fusion reactions of heavy nuclei with $Z_0 = Z_1 + Z_2$ equal 120 and 126.

INTERACTION POTENTIAL AND DYNAMICS

The main process determining the capture cross section is the dynamics of interacting nuclei from the moment of contact to the minimum of the nucleus-nucleus potential (interaction potential). The kinetic energy of the beam, which is almost completely converted into the excitation energy, decreases during the change of distance between the nuclei centers; in addition, the angular momentum of the interacting nuclei is reduced leading to the change in the nucleus-nucleus potential.

Interaction potential

In describing dynamics of interacting nuclei, an important role is played by the choice of nucleus-nucleus potential, which is determined as follows: $V_{nn}(R,L) = V_{Coul}(R) + V_n(R) + V_{rot}(R,L)$. $V_{Coul}(R)$ – Coulomb potential which is calculated from the partial overlap of the nuclei volumes according to [7]. $V_n(R)$ – nuclear potential of short-range forces (proximity potential) which has almost no fitted parameters [8]. $V_{rot}(R,L)$ – centrifugal potential, where the expression for the solid momentum of inertia of the nuclear system is applied:

$$V_{rot}(R,L) = \frac{\hbar^2 L(L+1)}{2\mu R^2} \qquad (2)$$

where R – distance between the centers of nuclei, $\hbar$ – Planck constant, μ – reduced mass, and L – system angular momentum. Nucleus-nucleus potential allows to determine the following parameters influencing the dynamics: Coulomb barrier B_{Coul}, quasifission barrier B_{qf}^{R}, distance between the centers of nuclei at the touch, at the Coulomb barrier (maximum) and at the minimum of the nucleus-nucleus potential.

In determining capture cross section, according to [6], $B_{qf}^{R} > 0$ is required, i.e. the existence of potential pocket in the nucleus-nucleus potential is necessary, otherwise σ_{cap} will be equal to zero. Fig. 1 shows the dependence of the potential pocket depth ΔV_{nn} on the charge number of light nucleus for different isotopic configurations of light nuclei, with heavy nucleus – $^{248}_{96}Cm$. These calculations are made for heavy fragments $^{238}_{92}U$, $^{244}_{94}Pu$, $^{248}_{96}Cm$ and $^{251}_{98}Cf$, from which it follows that the depth of the potential pocket is deeper for more asymmetric reactions, while the capture cross section is higher [9]. With increasing the quantity of neutrons in the light nucleus, the depth of the potential pocket increases. Therefore, the choice of the target nuclei and the beam can be made in planning of experimental work on the accelerator. However, as the potential pocket depth is reduced, the probability of capture and, consequently, the capture cross section of the interacting nuclei decrease. Therefore, these characteristics are to be correctly calculated.

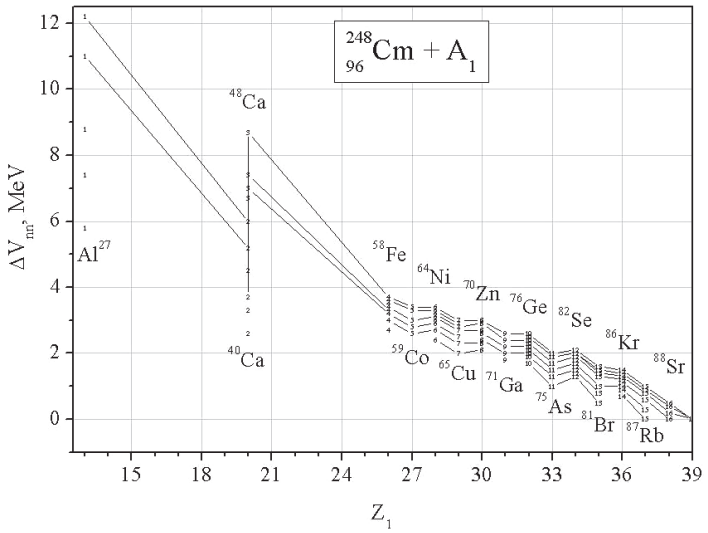

Fig. 1. Dependence of the potential pocket depth in the nucleus-nucleus potential on the charge number of light nucleus with different numbers of neutrons, heavy nucleus – $^{248}_{96}Cm$.

Dependencies of ΔV_{nn} on Z_1 (Fig. 1) are calculated at $L = L_0 = 0$. As a rule, a series of angular momenta, which contribute to the determination of the capture cross section, is involved in fusion reactions. A critical value of the angular momentum L_c exists; if $L > L_c$, then the capture is impossible and $\sigma_{cap}(L > L_c) = 0$. Fig. 2 shows the dependence of the interaction force ($\partial V_{nn} / \partial R = F_{nn}$) on the distance between the centers of nuclei at different values of the angular momentum.

As L increases, the potential pocket depth decreases and convergence of R_{min} and R_{max} (point of minimum and maximum values of V_{nn}) takes place; it corresponds to $F_{nn} = 0$ on the graph. When $L = L_c$, F_{nn} becomes less than

zero. Consequently, the stability region, in which the capture is possible, is determined for each reaction by L_c value (Fig. 3). The capture condition, from which L_c is derived, can be written as follows:

$$\frac{\partial V_{nn}}{\partial R} = \frac{\partial}{\partial R}(V_{Coul} + V_n + V_{rot}) \geq 0 . \quad (3)$$

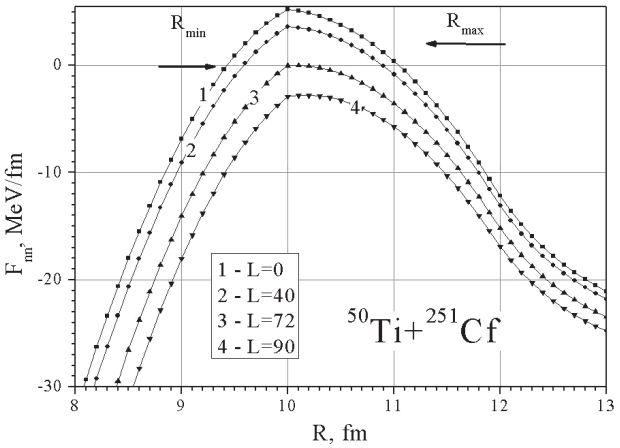

Fig. 2. Dependence of $\partial V_{nn} / \partial R = F_{nn}$ on the distance between the centers of nuclei at different values of the angular momentum.

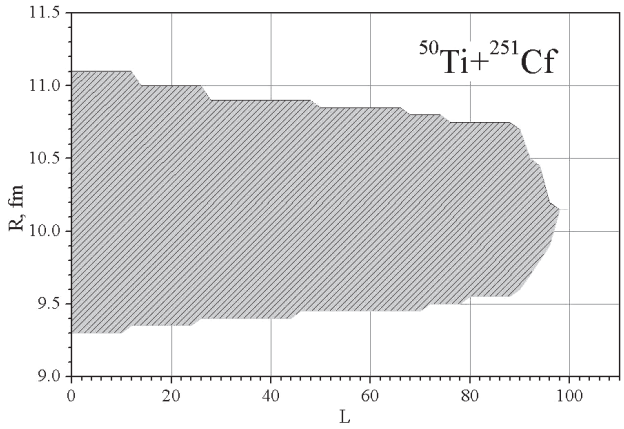

Fig. 3. Stability region depending on the angular momentum.

However, the angular momentum of the system at the point of capture depends on dynamic parameters, the influence of which cannot be disregarded, i.e. $L = L(t)$. For dynamic stability, when the angular momentum depends on the time, system of equations (4) is to be solved. Consequently, nuclei with different initial values of the angular momentum L_{0i} are involved in the fusion reactions; this should be considered within the nucleus-nucleus potential from the contact point to the momentum of capture.

In studies of the dynamics of interacting nuclei at the initial stage of formation of SHE (capture), the dynamics of change in the centrifugal potential and, therefore, of the angular momentum, as it makes a significant contribution to the capture cross section, and, thus, in the cross section of SHE formation, are to be taken into consideration.

Dynamics

For dynamic description of the interacting nuclei the following system of equations [7, 9] is used:

$$\begin{cases} \mu \dfrac{d\dot{R}(t)}{dt} + k_R \left(\dfrac{\partial V_n(R)}{\partial R} \right)^2 \dot{R}(t) = F_{nn}(R, L) \\ \mu \dfrac{dL(t)}{dt} + k_\theta \left(\dfrac{\partial V_n(R)}{\partial R} \right)^2 L(t) = 0 \end{cases}, \quad (4)$$

where $k_R = 1 \cdot 10^{-23}$ s/MeV and $k_\theta = 0.01 \cdot 10^{-23}$ s/MeV are radial and tangential friction coefficients respectively [9]. This system was numerically solved on the range of R from the contact point of interacting nuclei $R_{cont} = 1.28(A_1^{1/3} + A_2^{1/3})$ up to the momentum of capture, where the following condition is met:

$$\sqrt{\Delta E_{cm}} \cdot \Delta R \leq \frac{\hbar}{2 \cdot \sqrt{2\mu}} . \quad (5)$$

This condition is met in the minimum of the potential pocket of the nucleus-nucleus potential, when $E_{cm} \to 0$ (relative kinetic energy of interacting nuclei), and $R \to R_{min}$. In the solution of the system (4), the step was chosen by kinetic energy – 1 MeV, and by angular momentum 1. Fig. 4 shows the dependence of change in the kinetic energy on the distance between the nuclei centers for different initial values of the angular momentum. The figure shows that the system enters the capture channel after overcoming the Coulomb barrier R_{max}, with a sharp decrease of the kinetic energy (curves 1 – 4), for $0 \leq L_0 < 72$.

After overcoming the Coulomb barrier the system oscillates around the interaction potential minimum with decay of the amplitude of E_{cm}, due to dissipative forces, Fig. 4. Then, the condition (5) can be rewritten as follows:

$$\lim_{j\to\infty}\left(\frac{1}{j}\int_{R_2^{min}}^{R_1^{min}}\sqrt{E_{cm}(R)}dR\right)\le\frac{\hbar}{2\cdot\sqrt{2\mu}}, \qquad (6)$$

where j – number of steps in one oscillation. In the solution of system (4) and the evaluation of expression (6) $j\ge 70$; R_1^{min}, R_2^{min} – distance between the centers of interacting nuclei with $E_{cm}\to 0$ (see Fig. 5). The change in oscillation period was determined by the change of sign $\partial E_{cm}/\partial t$ from minus to plus. The integral in expression (6) was numerically calculated for each step according to Δt up to the change in the sign $\partial E_{cm}/\partial t$.

Step by time was chosen $(0.1\div 1)\cdot 10^{-23}$, while the average change in distance between the centers of interacting nuclei after the passage of the Coulomb barrier is equal to $\sim 10^{-4}$ fm, the stopping of calculations was performed under $\Delta E_{cm}\le 0.3\cdot 10^{-13}$ MeV according to the expression (6). Fig. 4 shows the curve 5 for $L_0=80$, the system does not overcome the Coulomb barrier and is disintegrated with the increase in the kinetic energy if $L_0\ge 80$. In this case the solution of system (4) was terminated under conditions where $R\ge R_{max}$. Consequently, the role of change in the angular momentum and thus the centrifugal potential are principal in the determination of the capture cross section.

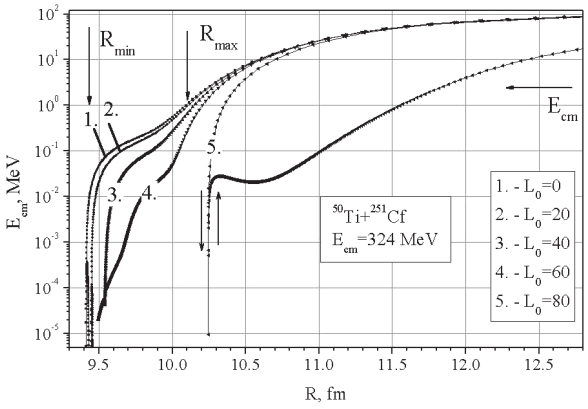

Fig. 4. Dependence of change in the kinetic energy on the distance between the centers of nuclei. Dynamics of the process is shown from right to left. The arrows indicate the regions of R_{max} maximum and R_{min} minimum values of the nucleus-nucleus potential.

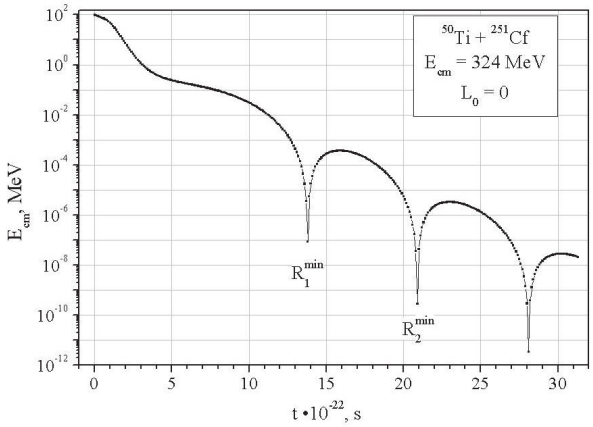

Fig. 5. Dependence of the kinetic energy on the time in the area of minimum of the nucleus-nucleus potential.

Fig. 6 shows the dependence of change in the centrifugal potential on the time required for reaction $^{50}Ti+{}^{251}Cf$ with different values of L_0.

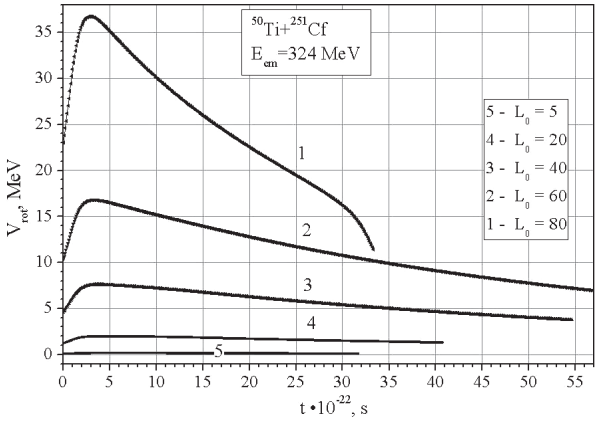

Fig. 6. Dependence of the centrifugal potential on the interaction time for reaction $^{50}Ti+{}^{251}Cf$. 1 – L_0=80, 2 – L_0=60, 3 – L_0=40, 4 – L_0=20, 5 – L_0=5.

The figure shows that at the initial instant the centrifugal potential increases due to the reduction of the distance between centers of nuclei. After overcoming the Coulomb barrier, V_{rot} is reduced due to more strong exponential dependence of the angular momentum on time and reduction of relative velocity of nuclei. This conclusion is supported by the fact that the change of $L(t)$ should be considered in the calculation of the capture cross section, since the change of the Coulomb barrier and the quasifission barrier leads to changes of energy, required for its overcoming, and, consequently, to change in the capture probability.

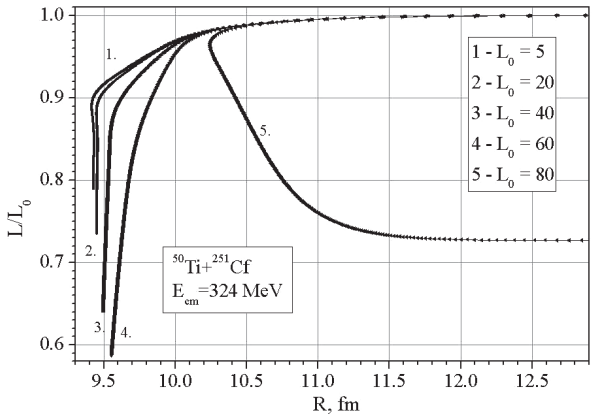

Fig. 7. Dependence of the reduced angular momentum on the relative distance between centers of nuclei.

Fig. 7 shows the dependence of the change in the relative angular momentum for different L_0 on the time when initial kinetic energy $E_{cm} = 324$ MeV.

Curve 5, if $L_0 = 80$, shows the decay of interacting nuclei, which have not overcome the Coulomb barrier; it also demonstrates the need to consider L_c in the calculation of the capture cross sections. Other curves show the entry of the system into the capture channel. With increase of L_0 the velocity of entry $(\partial E_{cm}/\partial R)$ into the capture channel is decreased; it is determined by the rate of the angular momentum change after the Coulomb barrier. This observation illustrates usefulness of condition (6).

It should be borne in mind, that condition (6) limits the dissipation of the kinetic energy into the excitation energy at the capture momentum. Then the system inertial momentum is equal to $\mu R^2 + j_1 + j_2$, where j_1 and j_2 - inertial momenta of light and heavy nuclei.

CAPTURE CROSS SECTION AND PROBABILITY

The expression averaged over all possible angular momenta L_{max} which were involved in the reaction [9] was used in order to calculate the capture cross section σ_{cap} for a fixed isotope configuration of interacting nuclei:

$$\sigma_c(E_{cm}) = \frac{\pi\hbar^2}{2\mu E_{cm}} \cdot \frac{1}{L_{max}(E_{cm})} \sum_{L_{0i}=0}^{L_c(E_{cm},L_{0i})} (2L_{0i}+1) P_i(E_{cm}, L_i), \quad (7)$$

where $P_i(E_{cm}, L_i)$ – capture probability, E_{cm} – kinetic energy, $\mu = m_1 \cdot m_2/(m_1+m_2)$ – reduced mass of nuclei, $L_c(E_{cm}, L_{0i})$ – critical (maximum) value of angular momentum, contributing to the capture cross section, L_{0i} – current value of angular momentum.

Maximum value of the angular momentum L_{max} can be easily obtained from the energy balance at contact points of interacting nuclei: $E_{cm} - V_n^{cont} - V_{Coul}^{cont} - V_{rot}^{cont} = \mu\dot{R}^2/2$, where V_{Coul}^{cont}, V_n^{cont} and V_{rot}^{cont} - Coulomb, nuclear and centrifugal potentials at the contact point. The angular momentum is defined as [7]: $|L| = \mu R \dot{R} \sin\theta$, where $R = R_1 + R_2$, $\dot{R}$ – velocity at the contact point, θ – angle between the axis of the beam and distances between centers of interacting nuclei, which is equal to $\pi/2$ for determination of the maximum value, thus:

$$L_{max} = \frac{\sqrt{2\mu R^2 (E_{cm} - V_{Coul} - V_n)(1-\hbar^2) + 2\hbar^4} - 0.5\hbar^2}{1+\hbar^2},$$

if $\hbar^2 \to 0$:

$$L_{max}(E_{cm}) = (R_1 + R_2) \cdot \sqrt{2\mu(E_{cm} - V_{Coul}^{cont} - V_n^{cont})}. \quad (8)$$

Verification of expression (8) was carried out in the reactions below and confirmed the correctness of the chosen assumption.

At the fixed kinetic energy of the beam and the initial angular momentum the capture probability is determined by [9]:

$$P_i(E_{cm}, L_i) = 1 - \exp\left(-\frac{E_{qf(i)}(L_i) - \Delta E_i^*(E_{cm}, L_i)}{\Theta_i(E_{cm}, L_i)}\right), \quad (9)$$

where $\Theta_i(E_{cm}, L_i) = \sqrt{12E_i^*(E_{cm}, L_i)/A_0}$ - temperature of nuclei after dissipation of the kinetic energy into the excitation energy $E_i^*(L_i)$. $E_{qf(i)}(L_i)$ – energy which is required to overcome the quasifission barrier and is determined from the interaction dynamics. $\Delta E_i^*(E_{cm}, L_i) = \left|E_{1(i)}^*(E_{cm}, L_i) - E_{2(i)}^*(E_{cm}, L_i)\right|$ – difference between the excitation energies of heavy and light nuclei. With regard to the fact that nucleons are not transferred from one nucleus to another and there is no emission of nucleons prior to the momentum of capture, the excitation energy is calculated in proportion to the mass numbers of interacting nuclei. It follows from the above expressions that capture cross section depends on the angular momentum in a complicated fashion.

Fig. 8 shows dependences of the capture probability for $^{50}Ti + ^{251}Cf$ reaction on the angular momentum which were calculated by means of (9) for various initial kinetic energies of the beam. The calculations showed that with the

increase of the kinetic energy, at first, the contribution of values of the angular momentum in the capture reaction is increased, and as E_{cm} is further increased, L value was reduced by the decrease of the energy required to overcome the quasifission barrier E_{qf}. The capture probability is close to 1 with a relatively small E_{cm}, but with energy which is sufficient to overcome the Coulomb barrier. With increase of E_{cm} the excitation energy is increased and E_{qf} is decreased, therefore, the capture probability is decreased. This process limits L_c values in reaction. Changes in the critical angular momentum for $^{46-50}Ti + ^{251}Cf$ reactions from the kinetic energy are shown in Fig. 9.

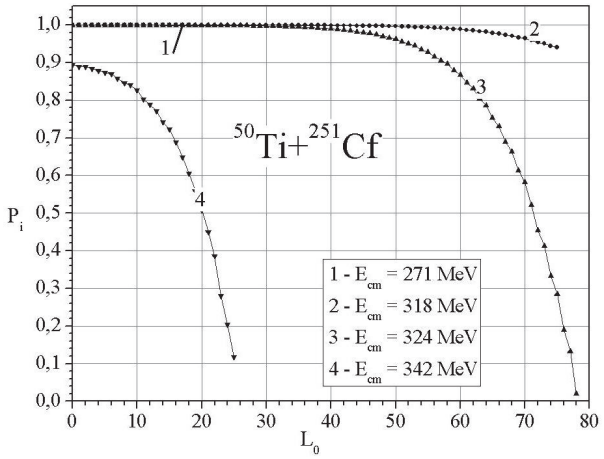

Fig. 8. Dependence of the capture probability on the angular momentum for different kinetic energy of the beam for $^{50}Ti + ^{251}Cf$ reaction.

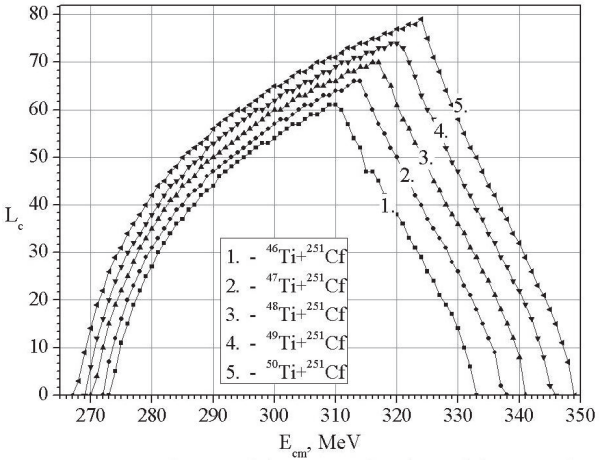

Fig. 9. Dependence of the critical value of the angular momentum on the kinetic energy.

It follows from the graphs that L_c is increased with increase of the kinetic energy due to overcoming the Coulomb barrier by nuclei with higher angular momenta. Maximum L_c is attained after the maximum value of the capture cross section. Then the excitation energy is increased and the capture probability is decreased to zero. While increasing E_{cm} the system temperature rises, but it does not bring significant contribution to the capture cross section. Such dependences were observed in all reactions.

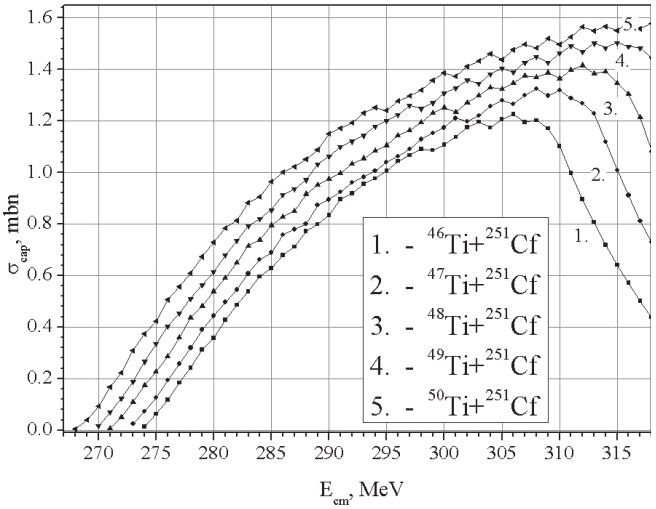

Fig. 10. Dependence of the capture cross section on the kinetic energy.

Since the increase of E_{cm} leads to the increase of the excitation energy which is removed from the compound nucleus by the emission of nucleons and γ-quants, thus reducing the probability of SHE formation, experimental works should be carried out at energies when $0 < \sigma_{cap} \le \sigma_{cap}^{max}$. Therefore, Fig. 10 shows the dependence of capture cross sections on the kinetic energy of the beam in the range of the capture cross section growth. With increase of the neutron number in the light nucleus the kinetic energy range is increased with increase of the capture cross section from zero to a maximum value.

Growth of curves with increase in the kinetic energy (Fig. 10) is due to the inclusion of higher values of the angular momenta which contribute to the reaction. In addition, the excitation energy difference is increased and, consequently, the capture probability is decreased (Fig. 4). Almost upon attainment of the maximum value, the capture probability falls due to the decrease of the quasifission barrier. As the initial angular momentum L_0 is increased, L_c values, contributing to the capture, are decreased and the system passes into the quasifission channel upon disappearance of the quasifission barrier, where σ_{cap} becomes zero.

RESULTS AND DISCUSSIONS

Probabilities (9) and capture cross section (7) have been calculated while solving system (4), from the contact of nuclei to the capture moment which is defined by expression (5). The results of these calculations are shown in Fig. 11, 12 and Table 1.

Calculations showed that the angular momentum has significant effect on the capture process. The increase of the

initial value of the angular momentum leads to the increase of the centrifugal potential and therefore, to the decrease of the quasifission barrier height. For example, for $^{54}Cr+^{248}Cm$ reaction with $L_0 = 0$ $B_{qf} = 4.21$ MeV, and with $L_0 = 70$ $B_{qf} = 0.02$ MeV. Consequently, the capture is impossible for angular momentum that exceeds a critical value.

Table 1.

Results of the calculations

Reaction	E_{cm} / E_{cm}^{avg}, MeV	L_{max}	L_{crit}^{max}	σ_{cap}^{max}, mbn	E^* / E_{avg}^*, MeV
$Z_1 + Z_2 = Z_0 = 120$					
$^{80}Ge+^{222}Rn$	366 – 371 / 368.5	189 – 196	25	0.1	67.75 – 71.98 / 69.87
$^{73}Ge+^{226}Ra$	355 – 362 / 358.5	177 – 185	30	0.14	65.34 – 71.59 / 68.47
$^{74}Ge+^{226}Ra$	354 – 364 / 359	183 – 195	37	0.19	64.5 – 73.58 / 69.04
$^{76}Ge+^{226}Ra$	350 – 366 / 358	179 – 199	48	0.325	61.86 – 76.58 / 69.22
$^{69}Ga+^{227}Ac$	329 – 349 / 339	149 – 174	49	0.425	47.43 – 62.59 / 55.01
$^{71}Ga+^{227}Ac$	329 – 351 / 340	142 – 174	57	0.61	45.44 – 65.48 / 55.46
$^{64}Zn+^{232}Th$	345 – 349 / 347	166 – 173	16	0.025	65.07 – 68.48 / 66.78
$^{66}Zn+^{232}Th$	341 – 350 / 345.5	168 – 177	29	0.15	62.15 – 68.98 / 65.57
$^{67}Zn+^{232}Th$	339 – 351 / 345	171 – 183	36	0.23	60.68 – 69.78 / 65.23
$^{68}Zn+^{232}Th$	338 – 353 / 345.5	166 – 185	44	0.31	60.21 – 73.27 / 66.74
$^{70}Zn+^{232}Th$	335 – 355 / 345	166 – 192	53	0.47	58.21 – 76.27 / 67.24
$^{63}Cu+^{231}Pa$	334 – 347 / 340.5	157 – 172	33	0.22	60.98 – 69.98 / 65.48
$^{65}Cu+^{231}Pa$	332 – 349 / 340.5	159 – 180	45	0.385	58.58 – 73.58 / 66.08
$^{58}Ni+^{238}U$ (1a)	332 – 336 / 334	157 – 162	21	0.09	62.1 – 67.36 / 64.73
$^{60}Ni+^{238}U$ (1b)	329 – 339 / 334	161 – 173	36	0.235	60.23 – 69.5 / 64.87
$^{61}Ni+^{238}U$ (1c)	327 – 339 / 333	159 – 173	41	0.33	59.6 – 69.98 / 64.79
$^{62}Ni+^{238}U$ (1d)	327 – 342 / 334.5	159 – 177	50	0.44	58.19 – 72.42 / 65.31
$^{64}Ni+^{238}U$ (1e)	323 – 343 / 333	160 – 186	57	0.62	53.93 – 74.96 / 64.45
$^{59}Co+^{237}Np$	319 – 336 / 327.5	151 – 173	51	0.529	55.2 – 72.27 / 63.74
$^{54}Fe+^{244}Pu$ (2a)	313 – 324 / 318.5	144 – 158	39	0.405	56.07 – 66.25 / 61.16
$^{56}Fe+^{244}Pu$ (2b)	309 – 328 / 318.5	142 – 166	51	0.624	53.6 – 71.55 / 62.58
$^{57}Fe+^{244}Pu$ (2c)	307 – 324 / 315.5	142 – 163	48	0.71	51.74 – 67.84 / 59.79
$^{58}Fe+^{244}Pu$ (2d)	308 – 331 / 319.5	148 – 177	60	0.82	52.41 – 74.44 / 63.43
$^{55}Mn+^{243}Am$	297 – 326 / 311.5	136 – 173	59	0.892	48.73 – 76.25 / 62.49
$^{50}Cr+^{248}Cm$ (3a)	292 – 315 / 303.5	127 – 156	51	0.797	48.46 – 70.94 / 59.7
$^{52}Cr+^{248}Cm$ (3b)	289 – 319 / 304	130 – 165	62	1.021	46.59 – 76.03 / 61.31
$^{53}Cr+^{248}Cm$ (3c)	288 – 323 / 305.5	130 – 174	65	1.092	45.78 – 79.83 / 62.81
$^{54}Cr+^{248}Cm$ (3d)	286 – 325 / 305.5	128 – 179	69	1.178	44.68 – 82.83 / 63.76
$^{50}V+^{247}Bk$	280 – 318 / 299	122 – 168	65	1.2	44.06 – 81.14 / 62.6
$^{51}V+^{247}Bk$	278 – 320 / 299	121 – 173	69	1.3	42.61 – 84.24 / 63.43
$^{46}Ti+^{251}Cf$ (4a)	274 – 305 / 289.5	116 – 154	58	1.24	43.56 – 74.62 / 59.09
$^{47}Ti+^{251}Cf$ (4b)	273 – 310 / 291.5	120 – 163	64	1.35	42.69 – 79.82 / 61.26
$^{48}Ti+^{251}Cf$ (4c)	271 – 312 / 291.5	120 – 169	68	1.4	41.49 – 82.53 / 62.01
$^{49}Ti+^{251}Cf$ (4d)	270 – 315 / 292.5	121 – 174	72	1.5	40.84 – 85.93 / 63.39
$^{50}Ti+^{251}Cf$ (4e)	268 – 318 / 293	121 – 180	76	1.59	39.6 – 89.62 / 64.61
$^{45}Sc+^{252}Es$	262 – 306 / 284	113 – 161	67	1.583	40.19 – 83.32 / 61.76
$^{48}Ca+^{257}Fm$	245 – 298 / 271.5	111 – 173	82	2.13	33.36 – 86.8 / 60.08
$Z_0 = 126$					
$^{70}Zn+^{247}Cm$	360 – 363 / 361.5	185 – 187	16	0.033	66.5 – 68.56 / 67.53
$^{62}Ni+^{251}Cf$	346 – 350 / 348	166 – 169	17	0.03	65.4 – 68.24 / 66.82
$^{64}Ni+^{251}Cf$	343 – 351 / 347	169 – 179	31	0.17	64.36 – 68.87 / 66.62
$^{59}Co+^{254}Es$	339 – 343 / 341	163 – 166	21	0.08	62.88 – 65.95 / 64.42
$^{56}Fe+^{257}Fm$	328 – 335 / 331.5	153 – 162	26	0.15	58.5 – 65.14 / 61.82
$^{57}Fe+^{257}Fm$	327 – 337 / 332	158 – 171	35	0.245	58.08 – 67.34 / 62.71
$^{58}Fe+^{257}Fm$	326 – 340 / 333	155 – 169	41	0.35	56.24 – 69.24 / 62.74
$^{55}Mn+^{260}Md$	316 – 331 / 323.5	148 – 166	43	0.46	54.37 – 68.43 / 61.4

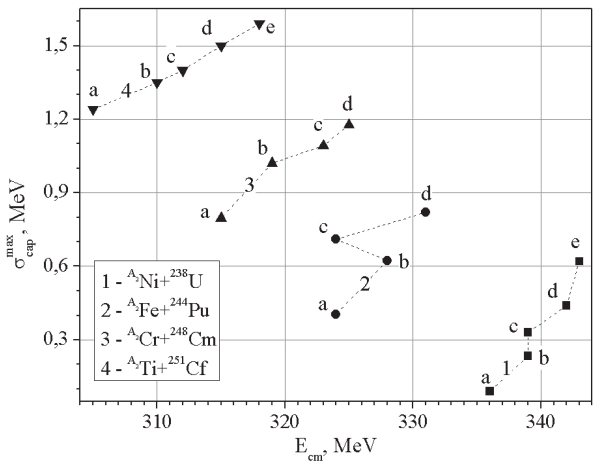

Fig. 11. Dependence of the maximum value of the capture cross section on the initial kinetic energy for perspective reactions of SHE with $Z_0 = 120$. Reactions shown in the graph are specified in the Table 1.

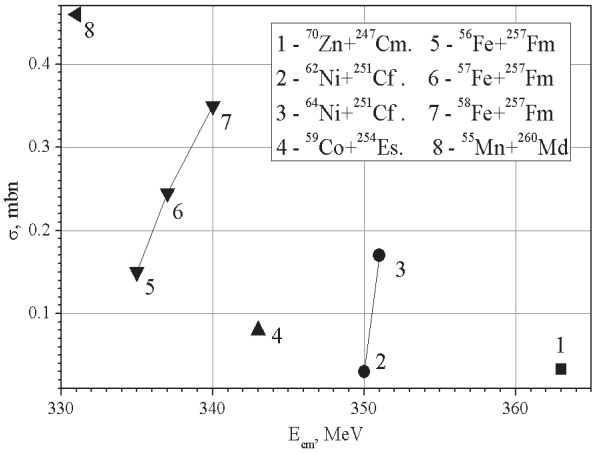

Fig. 12. Dependence of the maximum value of the capture cross section on the initial kinetic energy for some reactions of SHE with $Z_0 = 126$.

Calculations of the dynamics of interacting nuclei showed that the value of the angular momentum is reduced to 30% of the initial value, and therefore there is a potential well in the interaction potential, while it is absent at the momentum of contact. This means that greater number of the angular momenta contributes to the reaction. For example, the critical value for ^{48}Ca+^{257}Fm reaction is 68, but the value amounting to 82 takes part in the reaction.

In case of the isotope configuration it follows from the obtained data that it is appropriate to use elements with high charge asymmetry and neutron-rich light nuclei. The charge asymmetry has an influence due to the fact that the Coulomb potential is reduced with increase of the asymmetry and accordingly the Coulomb barrier is decreased. For example, for ^{80}Ge+^{222}Rn reaction which has $\eta_Z = 0.43$, $L^{max}_{crit} = 25$, $\sigma^{max}_{cap} = 0.1$ mbn and for ^{48}Ca+^{257}Fm reaction – $\eta_Z = 0.67$, $L^{max}_{crit} = 82$, $\sigma^{max}_{cap} = 2.13$ mbn. With decrease of mass asymmetry, where $\eta_Z = Const$, the nuclear potential is increased, and, therefore, the height of quasifission barrier is increased. For example, for ^{47}Ti+^{251}Cf reaction with $\eta_A = 0.68$, $L^{max}_{crit} = 64$, $\sigma^{max}_{cap} = 1.24$ mbn and for ^{50}Ti+^{251}Cf reaction – $\eta_A = 0.67$, $L^{max}_{crit} = 76$, $\sigma^{max}_{cap} = 1.59$ mbn.

Number of the angular momenta due to which light nucleus overcomes the Coulomb barrier is increased with increase of the kinetic energy, as well as the critical value of angular momentum is increased. This leads to increase of the excitation energy and therefore, to the decrease of the capture probability. That is to say that smaller number of angular momenta contributes to the capture process and the capture cross section decreases. Therefore, it is appropriate to carry out experimental works at energies when $0 < \sigma_{cap} < \sigma^{max}_{cap}$.

Increase of the compound nucleus charge reduces the capture cross section and the critical angular momentum, while the kinetic energy and the excitation energy is increased. For example in ^{55}Mn+^{260}Md→^{315}126 reaction these parameters are $\sigma^{max}_{cap} = 0.46$ mbn, $L^{max}_{crit} = 43$, $E^{avg}_{cm} = 323.5$ MeV, $E^{*}_{avg} = 54.37$ MeV. For ^{54}Cr+^{248}Cm→^{302}120 reaction these parameters are $\sigma^{max}_{cap} = 1.178$ mbn, $L^{max}_{crit} = 69$, $E^{avg}_{cm} = 305.5$ MeV, $E^{*}_{min} = 44.68$ MeV. In addition the parameters of mass and charge asymmetry are the same for the above reactions.

CONCLUSIONS

Effect of the angular momentum on the capture cross section and the excitation energy is shown on the basis of the dynamic-statistical description of the capture process in fusion-quasifission reactions of heavy nuclei. Based on this description, it became possible to determine the stability region where the capture and thus the SHE formation are possible. Consequently, effect of the angular momentum on isotope configuration of a target beam and on the collision kinetic energy should be taken into consideration during the planning of experiments.

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BIMONOCRYSTALL MATERIALS – IN SITU REFRACTORY MICROCOMPOSITES

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This article contains observation on the bimonocrystal materials received by using heavy gradient direct crystallization with a high content of the carbide phase. The effects of heat treatment on the microstructural changes and the growth of technological ductility were investigated. The dislocation structure of the phase boundaries, matrix and strengthening phases were studied. High-temperature mechanical testing was performed, mechanism of composition and mechanical microcomposites hardening was observed.
KEY WORDS: solidification, bimonocrystall carbide materials, implementation phase, dislocations, strengths

БИМОНОКРИСТАЛЛИЧЕСКИЕ МАТЕРИАЛЫ – ЕСТЕСТВЕННЫЕ ЖАРОПРОЧНЫЕ МИКРОКОМОЗИТЫ

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Рассматриваются бимонокристаллические материалы, полученные с помощью высокоградиентной направленной кристаллизации с высоким содержанием карбидной фазы. Исследовано влияние термической обработки на микроструктурные изменения и рост технологической пластичности. Изучена дислокационная структура фазовых границ, матричное и фазовое упрочнение. Выполнены высокотемпературные механические испытания, рассмотрен процесс композиционного и механического упрочнения.
КЛЮЧЕВЫЕ СЛОВА: кристаллизация, бимонокристаллические карбидные материалы, фаза внедрения, дислокации, прочность

БІМОНОКРИСТАЛИЧНІ МАТЕРІАЛИ – ПРИРОДНІ ЖАРОМІЦНІ МІКРОКОМПОЗИТИ

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Розглянуті бімонокристалічні матеріали отримані за допомогою високоградієнтної спрямованої кристалізації з високим вмістом карбідної фази. Досліджено вплив термічної обробки на мікроструктурні зміни і зростання технологічної пластичності. Вивчена дислокаційна структура фазових меж, матричне і фазове зміцнення. Виконані високотемпературні механічні випробування, розглянутий процес композиційного та механічного зміцнення.
КЛЮЧОВІ СЛОВА: кристалізація, бімонокристалічні карбідні матеріали, фаза впровадження, дислокації, міцність

One of the greatest challenges nowadays is creating construction materials based on refractory compounds and their alloys which would be capable of working in difficult conditions like high temperature, shock and radiation. There is high perspective in carbide and boride alloys researching, which are an important part of the heat- and wear-resistant materials (cermets in nuclear technology, the blades of gas turbine engines, high-speed steels). Gas temperature in modern aviation turbine is close enough to the melting point of the nickel alloys limiting their use in rockets and space technologiesdeveloped in Ukraine[1-4]. Requirements for high-temperature materials in nuclear reactors are increasing. It is clear that increasing working operating temperature due to the use of the refractory materials as the basis of construction materials is relevant [5, 6]. Most of the known high-temperature alloys (based on refractory metals and strengthened by the introduction phases) are formed by transition metals of IV- V(VI) A groups. The nature of hardening is mostly determined by the amount and structure of reinforce phases and changes depending on the temperature. At temperatures above 1800 K the best solution is carbide hardening due to high stability of the carbide phase in comparison with the oxide and nitride phases. That is explained with the presence of the strong σ-bonds formed by overlapping orbitals of the P6 shells (Fig. 1) [7, 8]. The analysis of the phase diagrams of the Me'-Me''-X indicates that there are eutectics between the bcc refractory metal and refractory phase which is formed by the introduction of elements X and metal Me''. Therefore, these systems can be considered as quasi-binary. The main difficulty we faced using heat-resistant alloys is their low temperature brittleness. This is caused by several features that are typical for cast alloys. They are micro-heterogeneity of the supersaturated solid matrix dissolve, the presence of thermal stress, the release of a large number of eutectic carbides that has a detrimental effect on plastic morphology, embrittle influence of carbon. Intensively developing diffusion processes in these types of alloys define temperature range as 0.6-0.7 $T_{melting}$. A

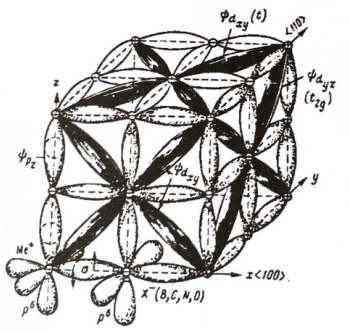


Fig. 1 Formation of strong σ-bonds Me-x in refractory monocarbides and mononitrides due to the overlapping Px, Py, Pz - orbitals split p^6 shells Me^+, C^-, N^- [7].

promising way to increase service characteristics of high-temperature alloys is to create optimal primary structure of the ingot and solidification management. It's clear that directional structure formation technology has high relevance. It allows us to create controlled regular structure in the quasi-eutectic alloy systems. However, available data is limited mainly by low-melting systems. "Practical composites" like NiTaC, CoTaC with exploitation area limited to 1500-1700 K are being developed. The main difficulties of creating high-temperature materials are active components and high melting point of refractory eutectic. Besides, difficult architectonic of the eutectics and their exceptional morphological diversity causes variety of contradictory eutectic structure scheme hypotheses, especially regular ones [5,9].

The main aimes reviewed in this work are the study of structure particulars of Me-Me'X microcomposites (Me – Mo, Nb, Ta; Me'- Zr; X-carbon) with high volume fraction of the reinforcing phase, investigation of bimonocrystal materials obtained with highgradient direct solidification, the effect of various types of heat treatment on the composite microstructure stability and strength properties of materials.

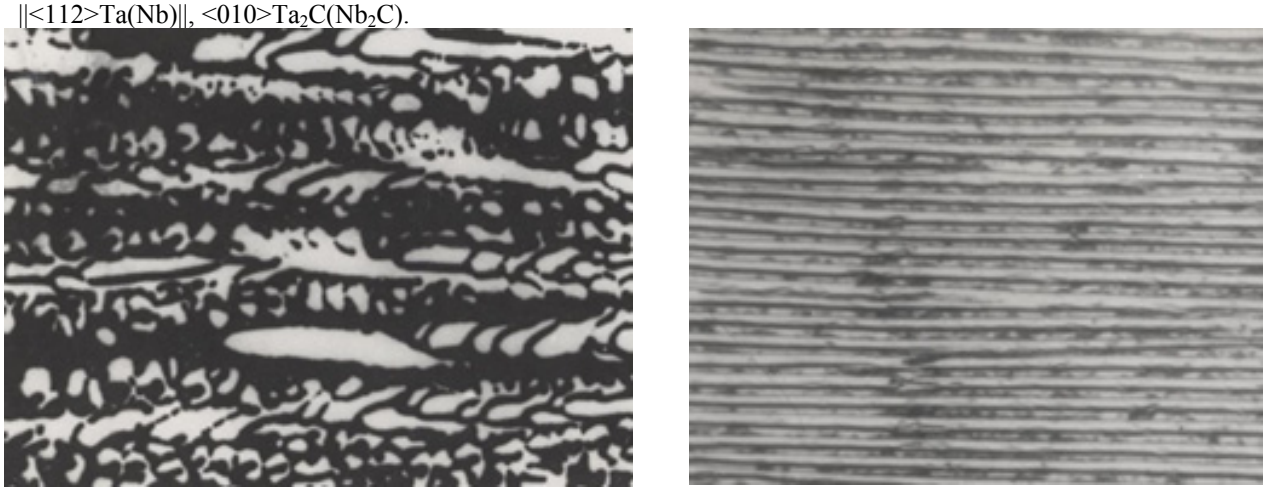
MATERIALS AND METHODS

Starting materials are: Mo - technical purity 99.8 wt%, Zr – 99.97 wt%, Ta, Nb - electron beam melting, C - spectral purity[11]. Volumetric fraction of the carbide phase in quasi-eutectic is: Mo -20-22%ZrC; Ta (Nb)- 28-30%$Ta_2(Nb_2)C$; Mo - 44-46% Mo_2C.

Microcomposites were prepared by the modified method of electron-beam zone recrystallization (vacuum < 10^{-4} Pa). Direct structure formation was produced by electron beam circular sweep. High static gradient G was supported during whole process. Zone refining of refractory metals presented during smelting process allowed the use of source materials of technical purity. Metallographic studies including stereometric analysis were completed on microscope MIM-8M. Drone-4M was used in X-ray diffraction analysis. The last were done in two parts. First part: identification of samples - qualitative analysis. Second part: determination of the relative content of the second phase - quantitative analysis. Dislocation structure was studied on thin foils using transmission microscopy (TEM) microscope JSM-200CK, acceleration voltage-200 kV [10,11]. Bursting test (Instron) performed in temperature range 300-2500K, stretch speed-10^{-2} s^{-1}.

RESULTS AND DISCUSSION

Tested systems of Me-carbide form faced-unfaced phases during solidification with sharply different fusion entropies. Therefore, it's necessary to create high static temperature gradient G on crystallization front during whole process to obtain spatially ordered homogeneous structures. (G = 400-650 K/cm, growth rate R = 10^{-5}…10^{-2} m/sec). It is found that in the process of complete phase growth the increase of temperature gradient G reduces the area of concentration supercooling, crystallization range, basic phase lead distance. This reduces the possibility of its dendrite, undirected branching (Fig. 2a,b). This confirms the referral criteria of structure formation $G/R \geq \Delta T/D$ (ΔT – crystallization range, D – diffusion coefficient). In the process of solidification driven metallic phase decorates leading microrelief of carbide phase. Preferential growth direction (GD) is observed. GD ||<110>ZrC||<110>Mo, ||<112>Ta(Nb)||, <010>$Ta_2C(Nb_2C)$.



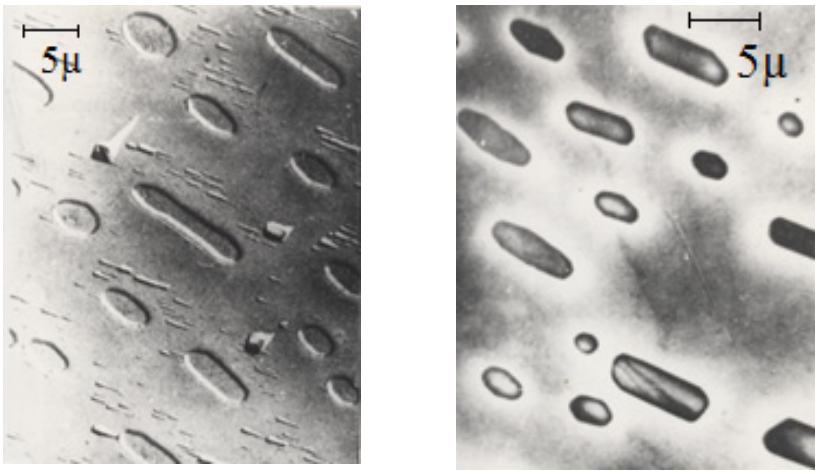
a) b)

Fig. 2 Influence of temperature gradient on microstructure in system Mo - Mo_2C
R=3.5 10^{-4} m/sec, a) dendrite structure G = 350 K/cm b) regular bimonocrystal structure G=550K/cm; longitudinal section; X 650; light areas – carbide phase

The legacy effect of oriented fuse microstructure by growing bi-crystal was discovered. Bimonocrystal materials were obtained after 1 – 2 zone passing. Structure had the appearance of threadlike carbide single crystals embedded in a single-crystal refractory matrix under equilibrium growth conditions. It was found that the dominant morphology of carbides was plate for Mo- Mo_2C, rod for Mo-ZrC, fibrous for Ta(Nb)-C.

Fig.3 Dislocation structure of microcomposite Ta-Ta_2C; R-10^{-4}m/sec; X 15 000

According to TEM researching carbide single crystals with a diameter of 0.6…0, 8 μm contain only stacking faults, other defects weren't detected. Defect concentration decreases during stationary growth. The dislocation density (ρ) of threadlike carbide crystal is $\rho \sim 10^2 cm^{-2}$ while in metal matrix - $\rho \sim 10^8 cm^{-2}$. It was found that in studied systems with condition of equal R and G for minimal phase inconsistency (Δd = 4.3% for Mo-ZrC), the dislocation density of the matrix phase : $\rho < 10^2 cm^{-2}$. In case of Δd = 11.7 % for Mo-Mo_2C, $\rho = 5.9\ 10^8 \ldots\ 10^9 cm^{-2}$. Epitaxial dislocations grid extending to a depth of 25 - 45 nm was observed on a semi-coherent phase boundary surface (Fig. 3). It was determined that bimonocrystal materials had a local cleaning of metal matrix as a result of heat treatment after crystallization (T> 1500 K, τ = 3…5 hours). This is explained by the diffusion carbon transfer to the surface of the crystal base carbide. The latter plays the role of substrate in the decay of a supersaturated solid solution. (Fig. 4a,b). Dislocation density of the matrix phase is $\rho \le 10^7 cm^{-2}$.



a) b)

Fig. 4. Mo-ZrC system microstructure
a) initial composite, b) after annealing T= 1500 K, annealing time -3h.

As a result of after crystallization annealing the system of Mo-ZrC 10^{-4} weight % C was mostly cleaned from carbon. Observed treatment effect complies with the best results of complex refractory metals active crystals refining. That promotes technological ductility of carbide alloys [11].

The overall result established for the case of isothermal annealing of bicrystal materials is coarsening in areas of accelerated diffusion or defect areas. They are priority one phase expansion areas and places of similar plates consolidation where high density of dislocations is $10^9 \ldots 10^{10} cm^{-2}$. Bimonocrystal materials with regular structure are thermally stable up to 0.9 melting temerature. This is due to reduction of migration interphase boundary capability compared to large-general type grain boundaries. The deformation and hardening nature of microcomposite during explosive tests at 300 - 2500K were defined. It was found that the interaction between dislocation (moving in the matrix) and field of interfacial dislocations increase during deformation process. The field length was the same as the distance between the dislocations at phase interfaces 40…80 nm. In case of Mo-ZrC deformation in <110> direction was carried out in (110) plane. New slip plane in the matrix and carbide phases activate at temperatures higher than 0.7 $T_{melting}$. Different carbide crystallographic peculiarities of sliding along the (110) and (100) in <110> direction disappear. Slipping is carried out in one of the close-packed plane according to tension direction. Local stresses were created on carbide surface as a result of dislocation accumulation. These stresses exceed the theoretical shear strength of monocrystalcarbide. Most of the load is carried by extended threadlike carbide single crystals (l /d ~ 1000, where l – length, d- carbide diameter). monocrystalscan withstand multiple fragmentation saving specific strength up to reaching the critical value: l/d critical = $\sigma / 2\tau$ (σ_b -carbide strength,τ- matrix yield strength).

As we can see from Fig. 5 bimonocrystal materials strength is 2 – 4 times higher than the strength of known cast structure alloys within temperature range of 300-2500K[11].

The maximum strength values were observed in Mo-ZrC system and exceeded similar values of the best refractory materials such as W-(Zr,Ti,W)C with isotropic structure[12,13]. Microcomposite technological plasticity increased due to refractory matrix treatment. High strength was caused by typical mechanism of composite reinforcement. Deformation matrix hardening in combination with high recrystallization temperature (over 1800K) of bimonocrystal materials provides additional opportunity to improve the heat resistance of carbide heterophase materials. That kind of materials will surely find new application areas.

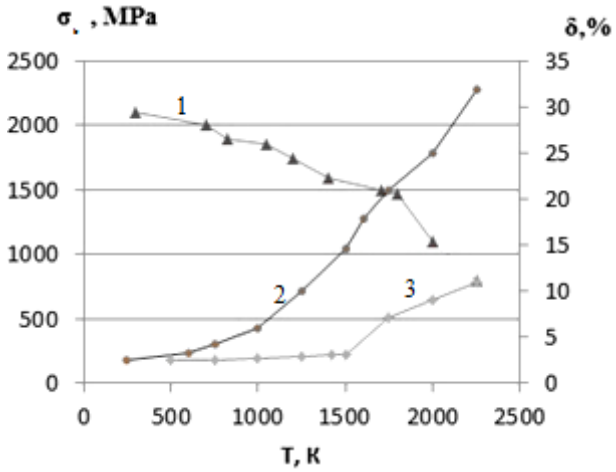


Fig. 5. Temperature dependence: 1 - rupture strength(σ_b); 2 - plasticity (δ) after annealing; 3 - plasticity (δ) before annealing; Mo-ZrC system

CONCLUSIONS

In this work specific type of bimonocrystal material is considered in detail. Structure of this material takes form of threadlike carbide monocrystalswhich are embedded in the refractory metal matrix. Relationship between structural defects of bicrystal materials, dislocation density and structural stability was defined up to 0.9 melting temperature.

It was detected that the dislocation structure of interphase boundaries and the matrix is determined either by crystallization conditions or growth and relaxation processes. It was found that there is structure improvement during the after crystallization period coursed by movement of the phase boundaries into the matrix. Found conditions of material heat treatment leads to the matrix purification from carbon, embrittling carbides and eliminating pockets of local phase hardening.

It was possible to increase carbide materials technological ductility by 10-15%, while maintaining the highest level of specific strength. The behavior of materials with a large content of the carbide phase combined with high recrystallization temperatures was investigated. Such conditions provide additional opportunities to improve heat resistance and technological plasticity of carbide construction materials. Such materials will undoubtedly find new application areas as template stamps for high pressure equipment, wear-resistant coatings or materials for nuclear technology.

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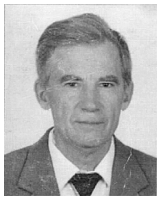

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DEPOSITION OF COATINGS OF TUNGSTEN AND TWO-LAYER COPPER-TUNGSTEN COMPOSITION

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In the work a technology of tungsten films and two-layer copper-tungsten coatings deposition on stainless steel substrates was developed. The coatings were deposited by magnetron and arc sputtering of materials with condensation of them on the testing substrates. The deposition objects were probe of the ICRF antenna on fusion devices and reference samples, on which the properties of obtained coatings were studied. The possibility of tungsten coatings forming on long-length elements of functional blocs was considered.
KEY WORDS: sputtering systems, multilayer coatings, tungsten films, copper films, adhesion

НАНЕСЕНИЕ ПОКРЫТИЙ ВОЛЬФРАМА И ДВУХСЛОЙНОЙ КОМПОЗИЦИИ МЕДЬ-ВОЛЬФРАМ
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В данной работе разработан способ нанесения пленок вольфрама и двухслойных покрытий медь-вольфрам на подложки из нержавеющей стали. Покрытия наносились методами магнетронного и дугового распыления материалов с конденсацией их на тестируемые подложки. В качестве объектов для нанесения выступали пробники ICRF антенны высокочастотного нагрева плазмы в установках управляемого термоядерного синтеза и образцы-свидетели, на которых изучались свойства полученных покрытий. Рассмотрена возможность формирования вольфрамового покрытия на длинномерные элементы функциональных узлов.
КЛЮЧЕВЫЕ СЛОВА: распылительные системы, многослойные покрытия, вольфрамовые пленки, медные пленки, адгезия

НАНЕСЕННЯ ПОКРИТТІВ ВОЛЬФРАМУ І ДВОШАРОВОЇ КОМПОЗИЦІЇ МІДЬ-ВОЛЬФРАМ
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У даній роботі розроблено спосіб нанесення плівок вольфраму і двошарових покриттів мідь-вольфрам на підкладки з нержавіючої сталі. Покриття наносилися методами магнетронного і дугового розпилення матеріалів з конденсацією їх на тестовані підкладки. В якості об'єктів для нанесення виступали пробники ICRF антени високочастотного нагріву плазми в установках керованого термоядерного синтезу та зразки-свідки, на яких вивчалися властивості отриманих покриттів. Розглянуто можливість формування вольфрамового покриття на довгомірні елементи функціональних вузлів.
КЛЮЧОВІ СЛОВА: розпилювальні системи, багатошарові покриття, вольфрамові плівки, мідні плівки, адгезія

The problem of the first wall is the most relevant at the present stage of creating of installations of controlled thermonuclear fusion [1]. In the systems with magnetic plasma confinement surfaces of structural materials facing the plasma will undergo intensive thermal load. According to the experts estimation heat flux on the first wall will be 1 MVt·m^{-2}. It could reach 20 MVt·m^{-2} in the divertor area and limiters. As energetically loaded elements antennas of RF heating of the plasma also may be considered. The first wall materials should withstand such heat flux without degradation. Besides of the high thermal resistance of structural materials, in fusion power devices the requirements to the influx of impurities from the wall into the plasma should be kept. The most important demand is the low level of impurities atoms as they may lose electrons in the plasma filament not in full; that resulting in radiation cooling of plasma [2]. For reducing energy losses due to radiation effects elements with low atomic number Z should be preferably used as the materials of the first wall. Atoms of these elements must be fully ionized in fusion devices plasma and radiation losses by impurity atoms will be minimal. The next important parameter to determine the applicability of a particular material is the retention of the hydrogen isotopes, especially tritium, in a material [3].

As main candidates for construction elements facing plasma carbon composite materials, beryllium and tungsten are consider. Beryllium has the smallest Z among them so it is the most do for the first wall material. At the same time its insufficient thermal resistance does not permit use it for elements [exposed with under powerful thermal fluxes (limiters and divertor plates). Carbon and carbon composite materials seem more attractive as compared with beryllium because after their thermophysical properties they can stand up to powerful thermal load [4]. At this the impurity atoms going into the plasma have acceptable atomic number and do not resulted in intense plasma cooling. But it should be

noted that at all positive properties carbon-base materials suffer from grave shortcomings. Carbon easy forms chemical compounds with hydrogen isotopes, including tritium. In the conditions existing in fusion devices chemical degradation of carbon-base structural materials may be rather high. Besides, carbon-hydrogen compounds spread to vacuum chamber and form films of complicated chemical compositions on construction elements. Such surface contaminations include chemically bounded tritium. That required additional radiation safety precautions for personnel leading in turn to deterioration of operating characteristics of fusion devices. MAGATE recommendation limites tritium amount accumulated in different constructional elements. Therefore the ways to remove carbon-hydrogen contaminations from the surfaces of structural elements of fusion devices are searched.

In spite of high atomic number tungsten has a number of incontestable advantages. These include: high thermal resistivity (the melting temperature is 3380 °C), low sputtering coefficient for hydrogen ions and isotopes, weak hydrogen isotopes retention. High atomic number is a considerable limitation for the material of the fusion devices first wall. For this allowable concentration of tungsten atoms incoming in the plasma must be several orders lower than one of low Z element. In spite of the severe restrictions imposed on the flow of impurity atoms from the wall into the plasma tungsten is considered as a promising material for facing plasma functional assemblies which are exposed to powerful thermal loads in ITER [5]. The studies [6, 7] show validity of this approach.

Tungsten having a number of positive properties that determined its applicability in the fusion devices is a hard and brittle material. Production of irregular shape objects from pure tungsten is technologically complex and expensive task. It is possible to reduce the costs of production of future reactors assemblies, using cheaper and more technologically promising structural materials, protecting the plasma facing surfaces with tungsten-based coatings. In this regard, the development of technology of tungsten and tungsten-based composite coatings on structural elements of experimental facilities of controlled thermonuclear fusion is an important task.

Functional elements of RF heating antennas facing the plasma filament work in hard conditions. Between the antenna and the plasma filament there are powerful high-amplitude high-frequency fields. Functional coatings for antenna elements working in such conditions must have properties characteristic of tungsten. In addition they must be mechanically strong, have good adhesion strength to the substrate, to withstand without breaking repeated cyclic thermal loads. Also, some specific requirements to these coatings exist: they must withstand repeated microbreakdowns without significant coating crippling, have low capacity for arcing. Microbreakdown may be caused on the surface of the coating by local impurities having low electron work function, and by point micro irregularities. Therefore, reducing the surface roughness is an additional technological problem in coatings creating.

In this work the method of deposition of tungsten films and two-layer copper-tungsten coatings on stainless steel objects of irregular shapes was developed. A modifying object was the probe of the ICRF antenna [8]. The aim of this paper is to get the tungsten films of 0.5 μm and 2.2 μm thicknesses on stainless steel (stl.st) and on stl.st with copper sublayer of the thickness at least 3 μm. It was assumed that the copper sublayer reduced the local heat load at the microbreakdown through the redistribution of heat in the volume of material with high thermal conductivity [9]. This resulted in reducing the local temperature and, consequently, to reduce the possibility of arcing. Copper sublayer could also be a damper redistributing the stresses at the locations of microbreakdowns, increasing the mechanical resistance of tungsten coating.

MATERIALS AND METHODS

The list of ways to get the tungsten coating is limited. Metal films can be obtained by electron-beam evaporation, plasma-arc deposition and magnetron sputtering. We chose the latter, as it compares favorably with the previous two. In electron-beam evaporator the source of the coating material is a small region of the melt. In the magnetron one the source of coating material is extended zone of erosion, which is preferable at the coating of objects with irregular shapes. In plasma-arc method material comes on the surface of the modified objects both as an atomic vapor and as clusters. At this there are droplets of molten material of the cathode, and in the case of tungsten even some particulates of the material. These particulates are pulled out from the surface of the cathode by the stresses that arise as a result of strong local overheating of the applying material in the area of the cathode spot. The presence of droplets and particles worse the quality of the surfaces of the coatings; magnetron deposition method is practically free from this imperfection.

The coating deposition was made on the device VUP-5 with the planar magnetron sputtering system of direct target cooling [10] placed on the top of working chamber. The target diameter was 180 mm. It permitted to realize deposition of uniform coating on bulky objects. The targets from pure tungsten, copper and titanium were used.

In addition to carried researches on the creation of multi-layer coatings and check-out of the effectiveness of their use in controlled thermonuclear fusion devices trial experiments on deposition of these coatings on long-length functional units were done. Despite named shortcomings of arc method of application, this method is the most suitable for the modification of large-size products. To realize such a task the coatings deposition on the extended arc sputtering device was tested.

For the coatings deposition by arc discharge in the work modernized in accordance with our requirements extended tube-type arc vapor source of continuous operation was used (Fig. 1) [11-13].

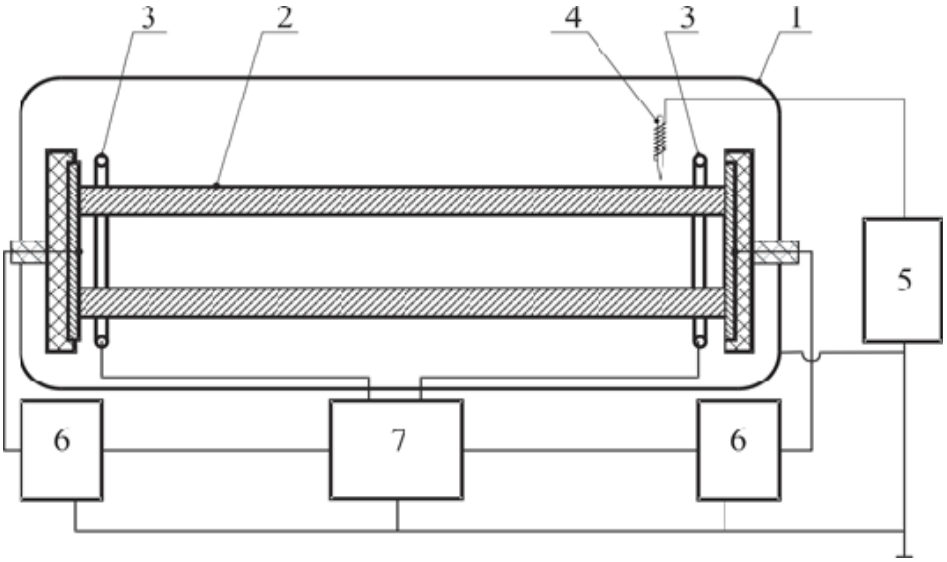

Fig. 1. Extended tube-type arc vapor source
1 – chamber; 2 – tube-type cathode; 3 – arc positional-sensing detector; 4 – ignition unit; 5 – circuit of ignition unit control; 6 – arc power supply unit; 7 – commutation circuit.

Continuous operation mode was provided with two identical power supply units (0-100 V, 0-300 V) [14]. Each modified unit (Fig. 2) was a three-phase thyristor rectifier used three-phase power transformer with a falling current-voltage characteristic and high leakage inductance. Powers from these units were connected to the opposite ends of a tube-type cathode.

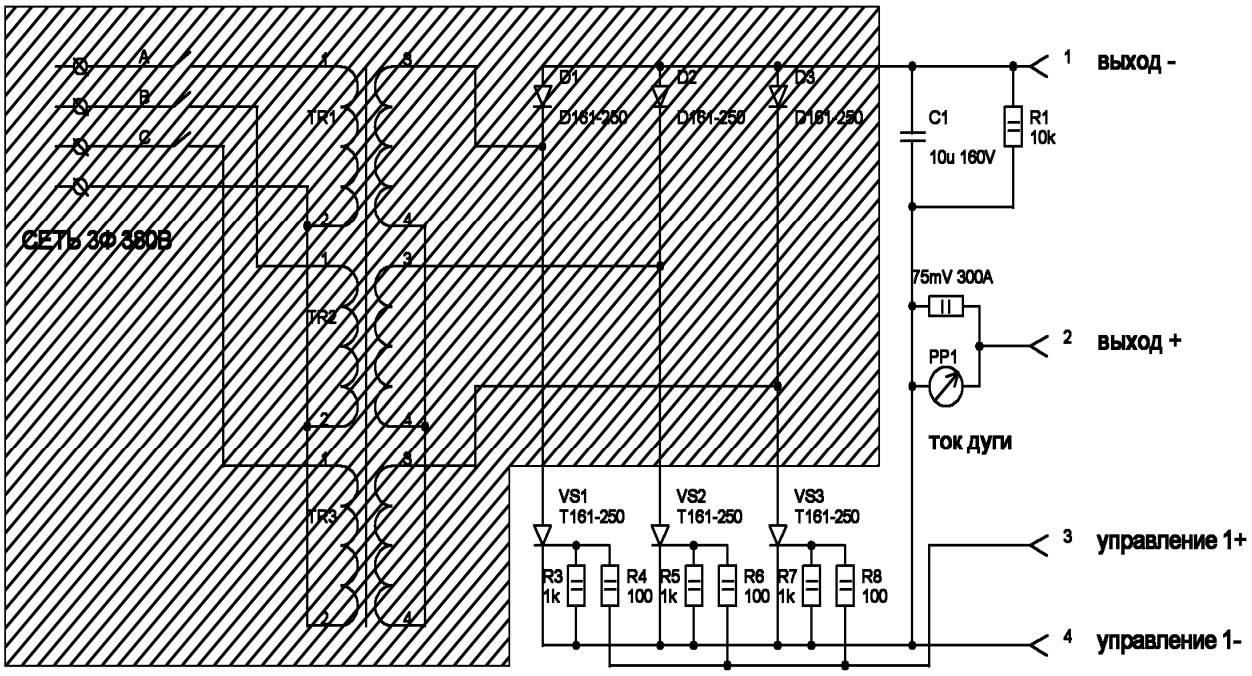

Fig. 2. Arc power supply unit.

Voltage was commuted with a control unit by a signal of arc positional-sensing detector [15]. The modernized circuit (see Fig. 3) was a pulse former converted a signal from the arc positional-sensing detector into an actuating signal for arc power supply thyristors. It permitted to prevent arc extinction in a reconnection moment as the control unit provided short-time simultaneous work of the power supply units before one of them switching-off. Besides, such option of the arc power supply enabled to avoid the commutation of high-current (up to 250 A) circuits.

Arc ignition was done by an electromechanical device powered directly from the cathode. The simplicity of design and small number of operations at continuous duty of arcing provided high reliability of the device and eliminated the relatively complex and often quite uncertain circuits of the high-voltage ignition.

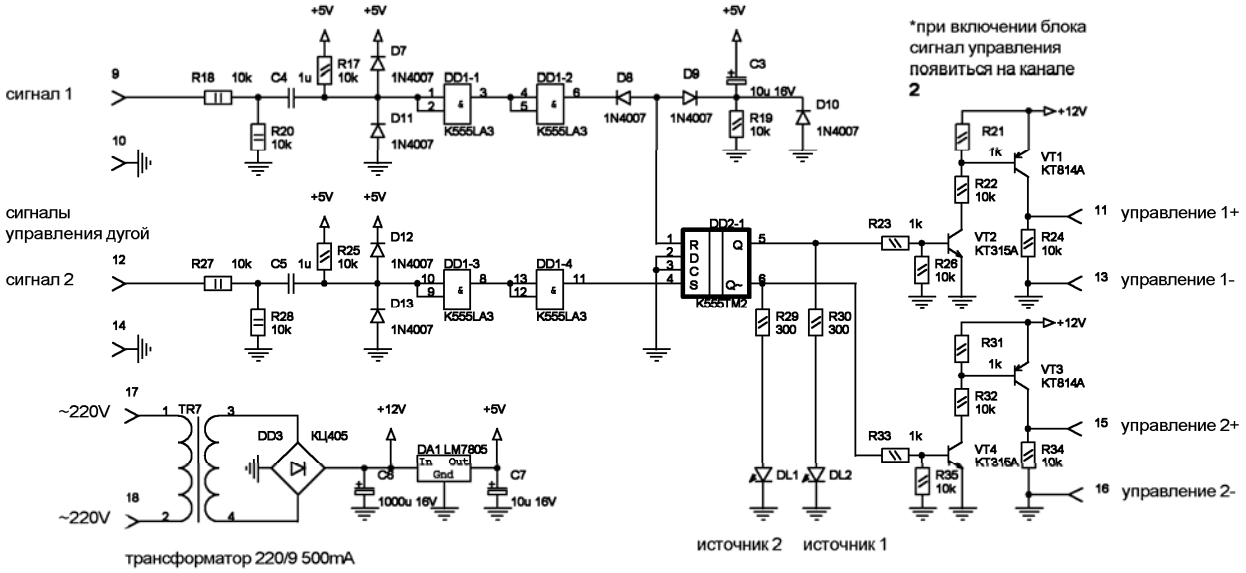

Fig. 3. Diagram of commutation of arc power supply unit

RESULTS AND DISCUSSION

The experiments showed that a tungsten film deposited on a cold substrate had high tensions. They appeared in the process of a tungsten coating forming. Internal stresses were so strong that caused film destruction. In some cases, the destruction of coating as well as the surface layer of the reference samples from a silicon single crystal was observed. We achieved satisfactory results depositing tungsten on the substrate heating up in the temperature range 330-350 °C. The choice of this temperature range was due to the optimum level of adhesion and was consistent with the regime of tungsten-based coatings deposition described in [16].

As our experiments shown coating strength and its adhesion parameters were influenced not only by strains arisen in the film itself but also by intrinsic strains in the substrate and in intermediate layers. The objects for the coating deposition were made from the stainless steel of the next composition: Cr 20 at.%, Fe 70 at.%, Ni 8.5 at.%, Ti 1.5 at.%. Under the requirements to the surface roughness the objects were preliminary polished. Samples were annealed in high vacuum at 800 °C and the residual pressure in the chamber $1 \cdot 10^{-5}$ Torr during 30 min to remove intrinsic strains. Then the samples were cooled in high vacuum down to the room temperature. The surfaces of samples became lustreless after annealing, defects that appeared in the result of preliminary mechanical treatment revealed. The surfaces of annealed in vacuum samples were polished again using a diamond paste of a small grain-size. As pastes were additional contaminant sources the sample surfaces were thoroughly rinsed and degreased in an ultrasonic bath.

In the coatings deposition chamber reference samples were placed on a heated table. RF probe was placed on the specially made heated holder that permitted to rotate the simulator angularly to the flux of the deposited material. The position and rotation velocity of the holder were chosen so as the thickness variations of the coatings did not exceed 15%. The table surface was copper-made to ensure the uniform temperature distribution. The samples temperature was controlled with a thermocouple attached to the copper table. The distance between the table and the target was 150 mm; that ensured the uniform thicknesses of coatings on the samples.

The time of deposition was chosen so as the film thicknesses on the RF probe and on the planar objects were within defined parameters. The chamber was evacuated to a high vacuum by a diffusion pump with a nitrogen trap. The target and substrate were preliminary cleaned in glow discharge. The samples were heated in vacuum up to 330-350 °C. Than the titanium sublayer was deposited on the heated samples with the thickness up to 100 Å. The discharge parameters were the next: discharge current was 2.5 A, discharge voltage was 450 V, the chamber pressure was $1 \cdot 10^{-3}$ Torr, the working gas was argon, the deposition time was 30 s. Titanium covered samples cooled in a high vacuum down to the room temperature. After that nitrogen was inlet in the chamber up to air pressure. This prevented the oxidization of the surface. The copper target was mounted in the magnetron sputtering system. The copper deposition was done at the substrate temperature 300-350 °C. The samples were kept in a high vacuum at this temperature during 15-20 min and after that the discharge in the magnetron sputtering system was light up.

In the first 5÷10 min on all the stage of deposition there was a baffler between the sputtered target and work-in-process items. During this time the target surface was cleaned. Oxides and other contaminations sputtered from the target surface settled on the baffler and did not fall on the object surfaces. That heightened a purity of obtained coatings. Copper was deposited at the next discharge parameters: discharge current was 2.5 A, discharge voltage was 560 V, the chamber pressure was $1 \cdot 10^{-3}$ Torr. The copper film was deposited on reference samples for 30 min, the first 3 minutes of which deposition was done on hot objects, and then the heating was switched off. The reason of the heating switching

was a substantial sample temperature rising due to heat transmission from the magnetron sputtering system and deterioration of coating adhesion and structure in the result. When depositing the copper in the operation condition the objects temperature decreased from 330-350 °C to 180 °C. The obtained in such conditions copper film had tolerable surface roughness. Copper layer was deposited to a thickness of 3 ÷ 4 μm. Samples after the copper deposition cooled down in vacuum to the room temperature.

Fig. 4 shows an electron microscope image of surface of the copper film deposited on the object with the temperature during deposition higher 350 °C. Pores are clearly seen.

The important stage of copper coating deposition was also transient-state conditions from the beginning of the film formation at indirect heating to further the film building-up without this heating. In the experimental conditions of films under study formation if the time of deposition on samples with indirect heating was less than 3 minutes, the substrate cooled down under 150 °C. At this the film was overstressed and had more porous structure than at the deposition on the overheating substrate but consisting from separate columns of significantly smaller cross-section.

At forming the film with transient-state regime at more than 3 minutes there appeared some relief on it and it became lustreless. This is due to the increasing size of the columns that formed up the film.

Studying the structure of the coating in a scanning electron microscope revealed that the film has a densely packed fibrous structure. Fig. 5 shows an electron microscopy image of this copper. Between arrows there is a fracture of the object with a copper coating. It is seen that the lateral dimensions of columns are less than a micron. This is consistent with the results presented in [17]. After that titanium sub-layer was deposited on the copper coating on the technology described above, but without pre-heating of objects.

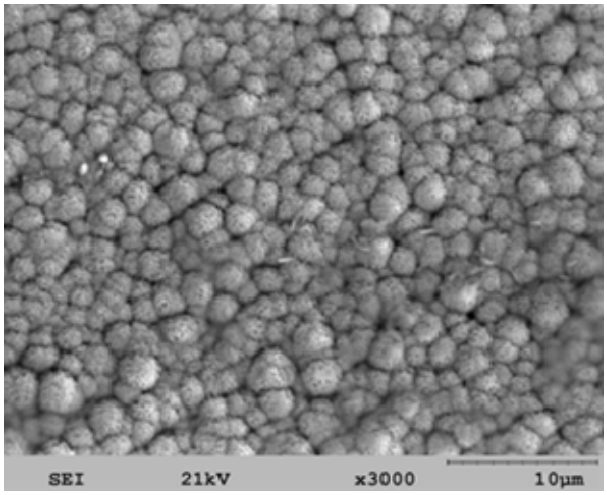

Fig. 4. Copper film on the overheating object.

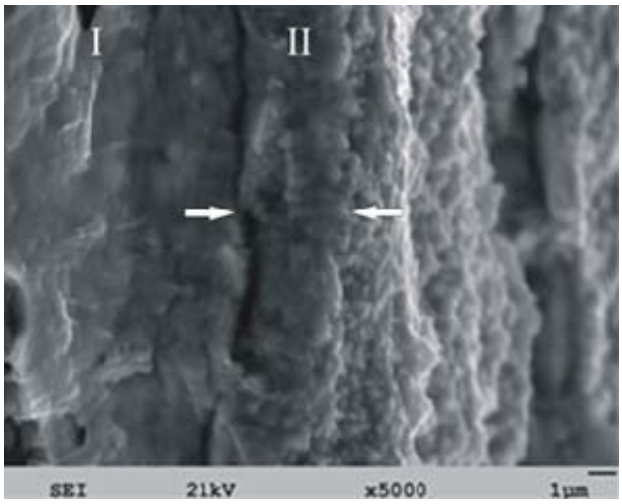

Fig. 5. Fracture of the object with copper coating deposited at the working operating mode

Tungsten was deposited on the hot samples. At that the temperature range 330-350 °C was strictly kept as only at such temperatures good adhesion of tungsten films to the surface of copper or stainless steel was achieved. The discharge parameters at the tungsten deposition were: discharge current was 2.5 A, discharge voltage was 520-560 V and the chamber pressure was $6\text{-}8\cdot10^{-3}$ Torr. Tungsten films of 2.2 μm thickness were created during 1 hour, and of 0.5 μm thickness – in 15 minutes. Samples cooled in a vacuum to the room temperature. The surface morphology of composite structures (stl.st + W) and (stl.st + Cu + W) is shown in Fig. 3. Roughness of the two-layer copper-tungsten coatings apparently was due to the restructuring of the copper sub-layer in the result of copper heating at the deposition of subsequent coating layers.

Along with the deposition of coatings on RF antenna probe for the study of the capture and retention of helium and hydrogen isotopes reference samples of 2 × 10 mm were prepared using the same technology. They were also used for electron microscopic studies. The substrate was stainless steel of 0.5 mm thickness. The samples of two types were created: 1 - stainless steel with Ti sub-layer of thickness up to 10 nm and 0,5 μm or 2.2 μm W layers (stl.st + W (nm, μm)) 2 - stainless steel with Ti sub-layer of thickness up to 10 nm, Cu layer of 3 μm thickness, Ti sub-layer of less than 10 nm thickness, the W layer of 0.5 μm or 2.2 μm thickness (stl.st + Cu + W (nm, μm)).

Tungsten coatings in composite structures (stl.st + Cu + W) had polycrystalline bcc structure with the average grain size near 20 nm in (stl.st + Cu + W (nm)) and 60 nm in (stl.st + Cu + W (μm)) (Fig. 6,7 and Fig. 8,9 respectively).

The tungsten coating was texturing in a little degree ($\Delta\psi > 30^{\circ}$), a texture axis was [110]. The texture axis was inclined towards the normal to the tungsten film to the angle $\Delta\rho \approx 4\text{–}14^{\circ}$. Tungsten coatings had a little tensile macrostress $\sigma = +0.64$ GPa in the composite structure (stl.st + Cu + W (2.2 μm)) and compressive macrostress $\sigma = -8.0$ GPa in the composite structure (stl.st + W (2.2 μm)).

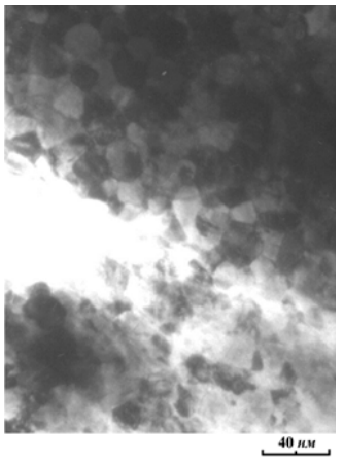

Fig. 6. Electron microscope image of W coating (stl.st + Cu + W (nm)) composition.

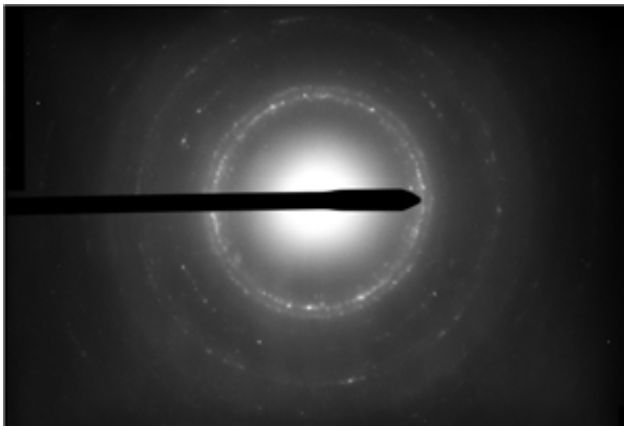

Fig. 7. Microdiffraction pattern of W coating (stl.st + Cu + W (nm)) composition.

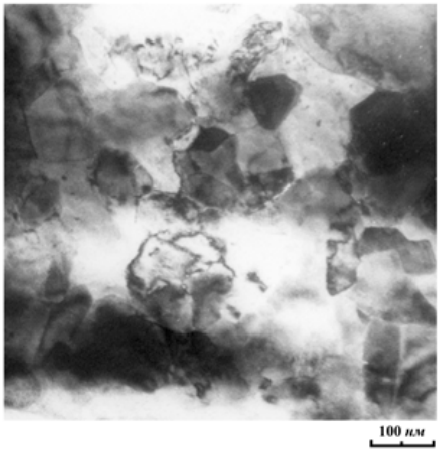

Fig. 8. Electron microscope image of W coating (stl.st + Cu + W (μm)).

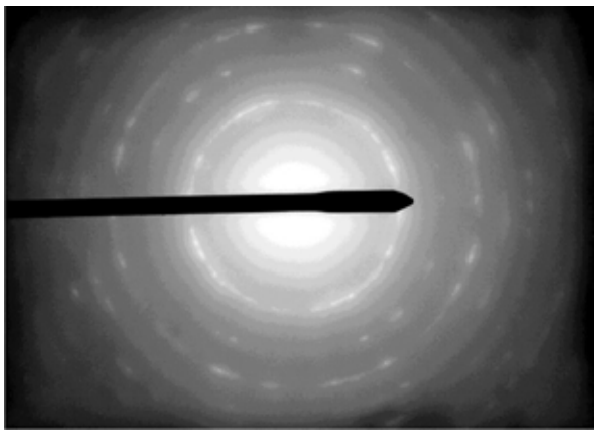

Fig. 9. Microdiffraction pattern of W coating (stl.st + Cu + W (μm)) composition.

The studies of tungsten coatings obtained with the magnetron sputtering system showed that in films there were residual stresses (see the Table). Internal stresses could be both compressive and tensile depending on the thickness of the tungsten film and elemental individuality of the substrate. In any case the presence of the copper sub-layer reduced internal compressive stress

Table.

Values and the type of internal stresses in the coatings

Cu layer thickness, μм	W layer thickness, μм	Internal stresses σ, GPa	The type of internal stresses
-	0.5	- 10.0	compressive
-	2.2	- 8.0	compressive
3	0.5	- 4.5	compressive
3	2.2	+ 0.6	tensile

The coatings in the form of copper sub-layer and working tungsten film coated by the arc sputtering device considerably differed from those formed with magnetron method. After deposition of the copper sub-layer with the thickness of several μm on stainless steel substrate by this technology the strong surface relief turned out so before deposition of the final tungsten layer tumbling of the object surface was needed. After tumbling cold deformation of the copper sub-layer was done. As a result at the following tungsten deposition there appeared high internal stresses that prevented forming final continuous coating. Annealing the object with the deposited copper layer in vacuum at 450°C, the following polish using a diamond paste of a small grain-size and thoroughly surface cleaning in solvents were the necessary operation to get good adhesion of tungsten films to the copper sub-layer.

CONCLUSION

The method of deposition of tungsten and two-layer copper-tungsten coatings on the objects of irregular shapes from stainless steel by magnetron sputtering was developed in the carried studies. It was established that the substrate temperature should be held in the range 330-350 °C to get optimal adhesion and allowable object surface finish class. To get the necessary properties the initial item should be expose to normalizing anneal in vacuum.

It was established that increasing of the coatings thickness leads to the decrease of internal stresses and, if the copper sub-layer is present, to changing of the stress type. The obtained coatings were polycrystalline but with the dominating W [110] plate outcome. Produced with the mentioned above technology coatings on RF probe agreed the requirements to mechanical strength, adhesion and surface roughness. On objects produced by this technology, studies of coatings resistance to the influence of the particle fluxes, the capture and retention of hydrogen isotopes were carried down.

Multilayer copper- and tungsten-based coatings were got with the arc sputtering system. At this the surface roughness was higher than at the magnetron sputtering system using. Functionality of such coatings needed further investigations.

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An author and coauthor are the 47 publications.

ILLYA IVANOVYCH ZALYUBOVSKY

(15.06.1929 - 21.02.2013)

A prominent physicist and organizer of national science, Honored scientist of Ukraine, laureate of the State Prizes of Ukraine, corresponding member of the National Academy of Sciences of Ukraine, professor Illya Ivanovych Zalyubovsky passed away.

His personal contribution to the development of nuclear physics, radiation physics of solids, cosmic ray physics and biophysics significantly influenced the level of research in the experimental physics in general.

Professor I.I. Zalyubovsky was born in 1929 in Poltava region. In 1949 he entered the School of Physics and Mathematics of Krarkiv State University (now V.N. Karazin Kharkiv National University). Since that time the fate of I.I. Zalyubovsky was inseparably linked with the University. Here in 1952, he started his scientific career under the supervision of academician A.K. Walter. He successfully combined his scientific work with training in graduate school, and then - with teaching. In 1963-1965, he headed a group of soviet scientists engaged in scientific research and training of highly qualified specialists in the Nuclear Center of the Arab Republic of Egypt. In 1966, he defended his doctoral thesis, and in 1967 he became a Professor. In 1968, he took part in the research and lectured at Manchester (former Rutherford) laboratory in United Kingdom. Since 1965, he has headed the Department of Experimental Nuclear Physics, and since 1967, he was a Vice-president of the University.

Professor I.I. Zalyubovsky dedicated the first series of his scientific research to studying the interaction of accelerated particles with nuclei. The results of these studies, which were notable by systematic nature and ingenuity, not only stimulated the development of new theoretical models, but also significantly expanded the possibilities of using the nuclear reactions for experimental studies of the nucleus structure. Professor I.I. Zalyubovskiy managed solving the problem of measuring the static electromagnetic momentum of atomic nuclei by methods based on the phenomenon of perturbing the angular correlations. In 1983, this work was awarded the K.D. Sinelnikov prize of Academy of Science of Ukraine, it was applied for the further development on modern accelerators.

After I.I. Zalyubovskiy became a head of the Department of Experimental Nuclear Physics, the range of his research interests expanded significantly. He founded new (for himself and for the department staff) branches of research related to space physics, radiation physics of solids and biophysics.

At the initiative of Professor I.I. Zalyubovsky the development of experimental methods for studying the interaction of cosmic rays with the atmosphere and the Earth's magnetosphere had rapidly started. At the beginning of these studies, due to a series of precise experiments carried out under his leadership, it was discovered a new physical phenomenon - the effect of radio extensive showers of cosmic rays, and then the mechanism of its occurrence was studied in detail. In 1971, this work was awarded the State Prize of the Ukrainian SSR in science and technology.

Under the leadership of I.I. Zalyubovsky a powerful experimental basis for solving the fundamental problems of radiation physics of solids, radiation material science, biophysics and medical physics, radiation tests and technologies, as well as microanalysis of substance was built in V.N. Karazin Kharkiv National University.

During the comprehensive experimental studies, organized by professor, on interaction of radiation of different origin and energy with substances or materials, previously unknown patterns and phenomena associated with radiation effects on physical properties of metals, alloys, semiconductors, polymers, and biological objects were found. In particular, the effect of amplifying the acoustic signal generated by the flow of radiation in metals under the influence of static tensile stresses was discovered. It was found to be a general property of acoustic radiation phenomena in any combination of substances and materials, and the mechanism of sound generation by means of radiation fluxes was found to be universal one. In 1994, I.I. Zalyubovsky was awarded the Yaroslav the Wise Prize for the series of complex studies of nuclei and processes of interaction of particles, nuclei, and radiation of different energy with the matter.

Scientific style of Professor I.I. Zalyubovsky formed at the first stage of his entry into science was characterized not only by the depth and fundamentality of approaches, but also by the close connection with the application prospects. One of the most active periods of scientific activity of I.I. Zalyubovsky was associated with the implementation of scientific achievements in the military defense orders.

Professor I.I. Zalyubovsky was giving special importance to the improvement of organization of scientific research. The structural units, which were organized by him and which are headed by highly qualified specialists trained by him, continue previously initiated research in collaboration with institutions of NAS and National Space Agency of Ukraine, as well as with leading nuclear physics research centers in other countries. In the framework of international cooperation, the structure of exotic nuclei was studied on heavy ion accelerators. The low-background experiments on the neutrino nature and dark matter search with the use of highly sensitive installations designed in collaboration with Baksan neutrino observatory of Institute for Nuclear Research of Russian Academy of Science were carried out. The successful testing of unique telescope of energetic charged particles that was developed by physicists of the University (project "CORONAS-PHOTON") was carried out on the Russian satellite. Professor I.I. Zalyubovsky provided the scientific management of all of these activities.

Among scientific papers published by professor I.I. Zalyubovsky, which in total are more than 400, there are 5 books, the textbooks "Nuclear Physics" and "Nuclear Spectroscopy" for University students. In 1993 the fourth edition of "Nuclear Physics" was awarded the State Prize of Ukraine.

Educating a new generation of scientists for the new branches of physics had always been considered by professor I.I. Zalyubovsky as the most important problem. He was much merit in the organization and further development of the School of Physics and Technology, the first dean of which he was at Kharkiv State University. Department of Experimental Nuclear Physics, which was headed by Professor I.I. Zalyubovsky, constantly searched for new forms of improving the teaching in Nuclear Physics. There are 8 doctors of science and about 40 PhDs among his students.

I.I. Zalyubovsky gave much efforts to the organization of scientific and social work. He was a member of the committee on the State prizes of Ukraine, an authorized representative of the government of Ukraine at the Joint Institute for Nuclear Research and vice-president of the Ukrainian Physical Society.

For many years, he was the chairman of the Council of vice-rectors for research of the Ministry of Education and Science of Ukraine, chairman of the Scientific and Expert Council for the professional branch of "Physics" at Scientific and Methodological Council of the Ministry of Education and Science of Ukraine, chairman of the Professional Council for licensing and accreditation of higher educational institutions of Ukraine on natural sciences, member of the scientific councils of National Academy of Science of Ukraine on nuclear physics and high energy physics, head of the specialized council on defending the doctoral and PhD theses in the field of Nuclear Physics, Elementary Particle Physics, Plasma Physics, chief editor of the journal of Kharkiv University "Nuclei, Particles, Fields", member of the editorial board of the "Ukrainian Journal of Physics."

Professor I.I. Zalyubovsky was a Honored Worker of Science and Technology of Ukraine, the Excellent in Education of Ukraine. He was awarded two Orders of the Red Banner, the Order "For Merit" of all the three degrees, and medals. In 2007, he was awarded the title of "Honorary Citizen of the city of Kharkiv."

Fruitful scientific, pedagogical and scientific-organizational activity, the sincere kindness, the willingness to always come to help earned for Professor I.I Zalyubovsky a deep respect and love of his colleagues and students.

Memory of Professor I.I. Zalyubovsky will live forever in the hearts of his students and friends, of all those who worked with him, and had the happy fortune to communicate with him.

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ПРАВИЛА ДЛЯ АВТОРІВ

“Вісник Харківського національного університету” (серія: фізична «Ядра, частинки, поля») є збірником наукових робіт з фізики елементарних частинок, ядерної фізики, фізики плазми та плазмових технологій, фізики твердого тіла та радіаційної фізики. Журнал публікує наукові статті, короткі повідомлення, оглядові статті та рецензії на книги. До публікації у збірнику приймаються статті, які підготовлені у відповідності до правил для авторів і які отримали дві позитивні рецензії. Рукописи, які не відповідають правилам не розглядаються.

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Об'єм статті, мова, супровідні документи. До редакції подається рукопис об'ємом не менше 3-х сторінок українською, російською або англійською мовами в двох екземплярах з направленням закладу і актом експертизи, а також повний електронний варіант статті у форматі MS Office Word, а також ОКРЕМО електронні варіанти усіх рисунків у форматах "bmp", "tiff" або "jpg". Безпосередня вставка рисунків з інших програм не допускається. Якість рисунків повинна бути достатньою для відтворення тонких ліній, градацій відтінків та кольорів при чорно-білому друці. Редакція залишає за собою право вимагати поліпшення якості малюнків для отримання задовільної якості чорно-білого друку.

Папір, формат, поля. Текст друкується на білих листах формату А4 через один інтервал. Рекомендується використовувати редактор MS Word, шрифт Times New Roman (Cyr), редактор формул MathType версія 5.0 і вище. Поля справа, зліва і знизу по 2 см, зверху - 3 см.

Нумерація сторінок. Сторінки нумеруються послідовно на зворотному боці листа олівцем.

Підписи авторів. Один екземпляр рукопису повинен бути підписаним на зворотному боці листа усіма авторами.

ПОСЛІДОВНІСТЬ РОЗМІЩЕННЯ МАТЕРІАЛУ

Індекс класифікації. На першій сторінці зверху пропускаються два рядка; у третьому рядку у лівому верхньому куті друкується УДК *(курсив*, 9 pt.) і/або PACS і значення індексу.

Назва статті, список авторів статті. Нижче індексу класифікації після пропуску одного рядка розміщується назва статті (прямий напівжирний шрифт, 12 pt., усі букви прописні, вирівнювання по центру). Нижче назви статті після пропуску одного рядка друкуються ініціали і прізвища авторів (прямий напівжирний шрифт, 12 pt., вирівнювання по центру).

Назва і адреса організацій, що представляють автори. Нижче списку авторів у наступному рядку друкуються повні назви і адреси організацій, які представляють автори (шрифт *курсив*, 9 pt., вирівнювання по центру), у наступному рядку - адреса електронної пошти для переписки. Якщо організацій декілька, то для вказівки відповідності авторів і організацій слід застосовувати виноски зірочкою або цифрами.

Дата представлення статті в редакцію. Нижче адреси електронної пошти друкується дата представлення статті в редакцію: число - цифрами, місяць - прописом, рік - цифрами (шрифт прямий, 9 pt., вирівнювання по центру).

Реферати, ключові слова іншими мовами*. Після пропуску одного рядка друкується реферат мовою статті об’ємом не менше ніж 500 знаків без відступів, з коротким викладом постановки задачі, методів, що були використані та основних результатів (шрифт прямий 9 pt., вирівнювання по ширині). Слово "реферат" не друкується. У наступному рядку після слів (мовою статті) "**КЛЮЧОВІ СЛОВА:"** (прописом, шрифт прямий напівжирний, 9 pt., без відступу) мовою статті розміщуються ключові слова (5-8 слів, шрифт прямий 9 pt., вирівнювання по ширині). Далі після пропуску одного рядка двома іншими мовами друкується назва статті (шрифт прямий напівжирний 9 pt., вирівнювання по центру), список авторів (шрифт прямий напівжирний 9 pt., вирівнювання по центру), список організацій, що представляють автори (шрифт курсив 9 pt., вирівнювання по центру), текст реферату та ключові слова.

Основний текст статті, абзацний відступ. Нижче реферату після пропуску одного рядка друкується основний текст статті (шрифт прямий 10 pt.). Абзацний відступ 0,75 см.

Розбиття статті на розділи. Рекомендується розбиття статті на такі розділи: вступ (назва цього розділу не друкується) **МАТЕРІАЛИ І МЕТОДИ** (обов'язково для експериментальних робіт), **РЕЗУЛЬТАТИ І ОБГОВОРЕННЯ, ВИСНОВКИ.**

Для теоретичних робіт допускається більш вільний розподіл матеріалу на розділи, наприклад, замість розділу **МАТЕРІАЛИ І МЕТОДИ** рекомендуються розділи **ПОСТАНОВКА ЗАВДАННЯ, МОДЕЛЬ** і тому подібне. Розділи не нумеруються, в назвах розділів усі букви прописні і виділяються напівжирним шрифтом, вирівнювання по центру. При необхідності розділи діляться на підрозділи. Назви підрозділів друкуються з великої літери і виділяються напівжирним шрифтом, вирівнювання по центру. Після кожного розділу чи підрозділу залишається один пустий рядок.

Фонди, гранти. Наприкінці тексту статті після пропуску одного рядка, якщо потрібно, вказується назва фонду, який фінансував роботу, і номер гранту.

Формули, таблиці, малюнки, підписи, нумерація. Математичні і хімічні символи, рівняння і формули друкуються в тексті статті за допомогою програми Math Type. Рисунки вставляються в текст статті у форматах: «bmp», «tiff» або «jpg». Всі надписи на рисунках і осях друкуються шрифтом не менше 8 pt. Підписи під рисунками друкуються шрифтом 9 pt. Формули, таблиці і рисунки послідовно нумеруються арабськими цифрами, наприклад: (1); Табл. 1; Рис. 1. Назва таблиць і рисунків є обов'язковими.

Посилання і список літератури. Використані у рукопису літературні джерела нумеруються в порядку цитування в тексті, номер посилання друкується в квадратних дужках. Список літератури (шрифт прямий 9 pt.) розміщується відразу за основним текстом статті і виділяється як розділ **СПИСОК ЛІТЕРАТУРИ** (шрифт прямий напівжирний 9 pt.). Не допускаються посилання на неопубліковані роботи.

* For foreign authors is sufficient to provide abstracts in Russian and English.
Для зарубежных авторов достаточно рефератов на русском и английском.

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