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About of the possibility of quantum interferential transitions and entanglement in vacancy and divacancy of silicon

L.S. Martseniuk

Institute of Nuclear Researches
Prospect Nauky 47, Kiev 03680, Ukraine
e-mail: prolisok77@yandex.ua

Annotation. Some characteristics of divacancy in silicon as a radiation bistable defect with the Jahn-Neller stabilization are analyzed. It is shown that by external influence, by change of some properties of material, of concentration of the entered defects and of the type of irradiation it is possible to influence purposefully on the parameters of these defect centers, that indicate on possibility of application of silicon with such centers for the creation of devices of the quantum informative systems.

On the basis of carried out analyses the assumption about of existence of interference transitions between quantum states of minima of adiabatic energy at certain conditions is suggested. It is pointed on generality of such approach and on the possibility of expansion of approach, used for the description of such transitions, on some other bistable defects.

Keywords: silicon, divacancy of silicon, the entangled states, the interference transitions, the superposition states.

Проаналізовані деякі характеристики дивакансії кремнію як радіаційного бістабільного дефекту з ян-теллеровською стабілізацією. Показано, що шляхом зовнішнього впливу, зміни деяких властивостей матеріалу та концентрації введених дефектів, а також виду опромінення можна цілеспрямовано впливати на параметри цих дефектних центрів, що вказує на можливість використання кремнію з такими центрами як матеріалу для створення приладів квантових інформаційних систем.

На підставі проведеного аналізу висловлюється припущення про існування за певних умов інтерференційних переходів між квантовими станами мінімумів адіабатичної енергії дивакансії. Вказується на загальність такого підходу і можливість поширення підходу, застосованого для опису таких переходів в дивакансії , на деякі інші бістабільні дефекти.

Ключові слова: кремній, дивакансія кремнію, заплутані стани, інтерференційні переходи, суперпозиційні стани.

Проанализированы некоторые характеристики дивакансии кремния как радиационного бистабильного дефекта с ян-теллеровской стабилизацией. Показано, что путем внешнего воздействия, изменения некоторых свойств материала и концентрации введенных дефектов, а также вида облучения можно целенаправленно влиять на параметры этих дефектных центров, что указывает на возможность применения кремния с такими центрами для создания приборов квантовых информационных систем.

На основании проведенного анализа высказывается предположение о существовании при определенных условиях интерференционных переходов между квантовыми состояниями минимумов адиабатической энергии дивакансии. Указывается на общность такого подхода и возможность распространения подхода, примененного для описания таких переходов в дивакансии, на некоторые другие бистабильные дефекты.

Ключевые слова: кремний, дивакансия кремния, запутанные состояния, интерференционные переходы, суперпозиционные состояния.

Introduction

The central material in the semiconductor industry is silicon. Despite of the fact that the radiating technologies for modification of properties of this material are used for a long time and are advanced enough, the occurrence of new tasks of a modern science and a instrument making opens new problems, one of which is the decision of a question about possibility the use of silicon as material for creation of quantum computers. The use of the bistable defect centers, which appeared in silicon at the irradiation as a memory cells with two stable states at room temperatures, can appear perspective. The divacancy V_2, and even a vacancy (last is the bistable at low temperatures), and also the certain defects with participation of the atoms impurity, which arise at an irradiation [1], can be such centers.

The divacancy is, apparently, the most acceptable as the active center at creation of devices for information technologies on the basis of silicon. Really, a strong distortion of a crystal lattice of the basic material is take place in the field of formation of divacancy. Therefore the area of divacancy is to some extent shielded from the destroying influences of external environment and can steadily preserve the parameters at an high enough temperatures that specifies the perspectives of use of materials with such centers in modern quantum technologies.

The literature dates about of experimental researchers of properties of vacancies and divacansies in silicon were analyzed in presented work. For the first time it is shown that for these defects may be existed some quantum effects, including quantum interference transitions between the states of minimums of adiabatic energy.

It indicated on perspective of using of silicon materials with artificially entered in them the radiation defects of type of vacancies and divacancies in the devices of quantum information technology

Divacancies in silicon – the literary data

Radiation defects in silicon arise at an irradiation of a material by particles of various energies. Such irradiation is carried out with the purpose of controlled change of properties, for example, for making the materials with the increased radiation resistance. Usually apply technologies of ionic implantation, transmutation doping, of irradiations by the charged particles. Depending on required tasks the silicon material is irradiate with protons, electrons, ions, neutral particles (neutrons, $\gamma -$quantums) with the subsequent annealing of a material. Each of these methods has the advantages and the features of introduction of radiation defects in a material.

The development of technology of introduction of defects and studying of their properties has led to detection of some interesting features of radiation defects. For separate radiating defects as divacancy and some other such qualities as bistability are inherent, for them the display of Jahn-Teller effect is typical.

Bistable are the defects having two or more minimums of adiabatic surface. Besides they should possess the following features, to be found out. Firstly, the power barrier between minima should be big enough: $\Delta E_{\text{bar.}} \geq kT$ and, secondly, it is necessary, that the power location of minima differed on some size δ.

It means that the system will mainly be in one of states which names as the basic. If $\delta \geq kT$, for transition from one state to another the external influence is necessary.

In [2], where numerous the examples of bistable defects are made, it is underlined, that the defects, for which the Jahn-Teller effect is revealed, can possess by properties of bistabilityc. For the last is possible the situations, when the defect with multi-well potential do not display as the bistable defect. So, in [1] is pointed that for defect with the orientation lower than cubic is possible the orientation degeneration and even at presence of transitions between states such defect do not emerge as bistable.

The divacancy in silicon is the radiation defect and is forming at irradiation by the particles of different type, for example, by neutrons, by electrons with energy in range of 1.5 - 4.5 MeV , or at ionic implantations; it is the deep muli-charged center.

In according with [3] the levels between the states, which define the energy of divacancy, correspond to the next position in forbidden zone:

$$E(2\text{-}/\text{-}) = E_c - 0.23 \text{ eV}$$
$$E(\text{-}/0) = E_c - (0.43 - 0.41) \text{ eV}$$
$$E(0/+) = E_v + (0.23 - 0.25) \text{ eV}.$$

In the charge states V_2^+, V_2^- the divacancy has spin ½.

Both the charge states of divacancy is appeared as paramagnetic that is caused by the presence of not coupled electron in the open shell, therefore at addition of the electron non paramagnetic states V_2^0 and V_2^- are generated. To paramagnetic states V_2^+, V_2^-, as pointed in [4], the levels E_v+0.25 eV, E_c–0.4 eV correspond. Thus, the divacancy, in according with [4], brings the three levels, corresponding to four charged states V_2^+, V_2^0 V_2^- и V_2^{2-} (fig. 1).

At forming of divacancy a certain center with the ragged connections, being in full symmetric atomic

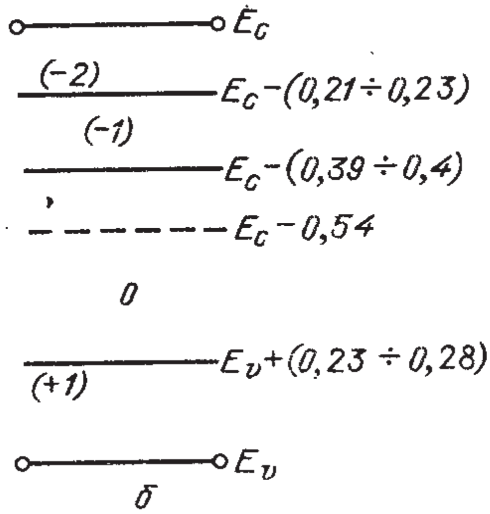

Fig. 1. The energy levels, which correspond to the different charge states of divacancy in silicon

configuration D_{3d}, appears in the beginning, the after ragged connections are filled by electrons. The opened shell here is formed by orbital e_g, and there is a removal of the degeneration of levels of the opened shell at the small distortion $D_{3d} \rightarrow C_{2h}$ (it is answered the component of distortion E_g). In accordance with [3] at lowering of the symmetry corresponding to the process of completion of formation of divacancy, the two modes of distortion E_g - resonant (r) and coupling (p) are appear.

As have shown the direct calculations which have been carried out in [3] for neutral and for two charge states,

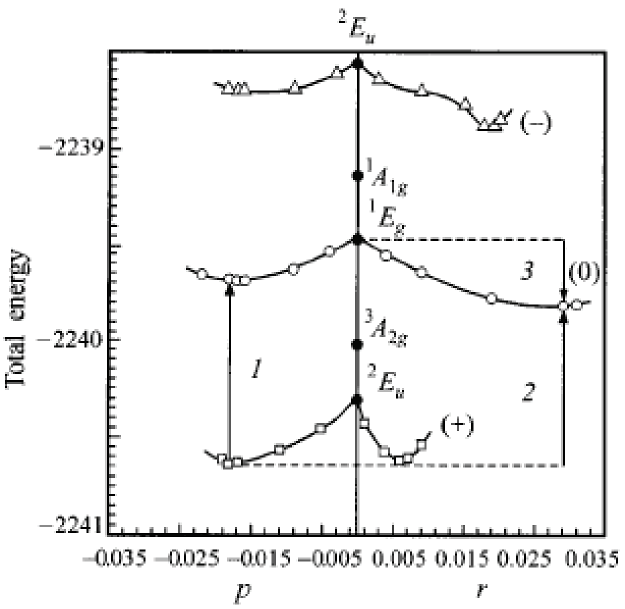

Fig.2. Multiplexed structure of the charged states of divacancy depending on two-mode distortion of Jahn-Teller [3].

the divacancy is the double-well center for all charge states investigated by the author.

According to carried out in [3] calculations, energy of Yahn–Teller stabilization for a neutral state is equal 0.34 eV; the energy differences between absolute and metastable minima of energies is 0.6 eV for V_2^- (r - mode of distortion for the basic state), 0.07 eV for V_2^0 (r - mode) and 0,03 эV for V_2^+ (p -mode), fig. 2).

About of the possible interference transitions in divacancy of silicon

As follows from [3], the adiabatic potential of divacancy in silicon has two minimums, shared by high enough potential barrier (more than kT), that provides stability of this defect at a room temperature. In addition, high enough value of energy of Jahn-Teller stabilizing testifies to presence of strong vibrancy connection. In [2] the criterion of strong vibrancy connection is entered, according to which this type of connection is carried out in the event that energy of Jahn-Teller stabilizing far more energy of zero fluctuations. In such case there are always the local vibrancy states in minimums of adiabatic energy. In a limit, at the high enough barriers, these states become quasi-stationary.

In case when a potential barrier appears transparent enough, the system can make the pulsating fluctuations, caused by tunnel transitions between configurations of equivalent minimums of adiabatic potential. In [2] specified that: «tunnel effects in the Jahn-Teller systems meet much more frequent, than it can appear on the face of it».

In [2] is underlined, that: « tunnel effects in in the systems meet much more often, than it can seem at first sight ».

Mathematically this process can be described as follows [5-7].

We will suppose, that there are two some stationary states Ψ_1 and Ψ_2 with close energy w_1 and w_2, corresponding to operator W. Between these states the transitions are possible and the systems Ψ , described such transition, is non-stationary.

$$\Psi = \alpha_1 \Psi_1 e^{i\omega_1 t} + \alpha_2 \Psi_2 e^{i\omega_2 t} \quad (1)$$

where α_1, α_2 - complex numbers: $a_1 = |a_1| e^{i\delta_1}$, $a_2 = |a_2| e^{i\delta_2}$, satisfying a condition $|\alpha_1|^2 + |\alpha_2|^2 = 1$.

For a defect which has two minimums of surface of potential energy, at transparent barrier the position of system in one of two minima Ψ_1 or Ψ_2 will correspond to stationary states. In case, if the barrier is appeared the transparent for tunneling, the system pass to superposition state, described by equation (1). As pointed in [7], instead of "not coherent mix of two stationary states we deal here with their superposition, adequate to some non-stationary state".

If apart from wave's functions Ψ_1 and Ψ_2 the ortonormal functions φ_1 and φ_2 to enter as follows:

$$\varphi_1 = \frac{\Psi_1 + \Psi_2}{\sqrt{2}}, \quad \varphi_2 = \frac{\Psi_1 - \Psi_2}{\sqrt{2}}, \quad (2)$$

that φ_1, φ_2 will describe too the superposition state of our system also. Really:

$$\Psi = \frac{\alpha_1 e^{i\omega_1 t} + \alpha_2 e^{i\omega_2 t}}{\sqrt{2}} \varphi_1 + \frac{\alpha_1 e^{i\omega_1 t} - \alpha_2 e^{i\omega_2 t}}{\sqrt{2}} \varphi_2 . \quad (3)$$

Here the functions φ_1, φ_2 are correspond to some other operator E having the eigen values $\varepsilon_{1,}$ $\varepsilon_{2,}$.

In such case the probabilities of that the system accepts the values w_1 and w_2 will be estimated by the coefficient α_1, α_2 ; the values $\varepsilon_{1,}$ $\varepsilon_{2,}$ will be estimated by magnitudes $p_{1,} p_2$.

$$p_1 = \frac{1}{2}\{ |a_1|^2 + |a_2|^2 + 2|a_1||a_2| \cos(\Omega t + \delta)$$

$$p_2 = \frac{1}{2}\{ |a_1|^2 + |a_2|^2 - 2|a_1||a_2| \cos(\Omega t + \delta) \quad (4)$$

where: $\Omega = \omega_1 - \omega_2$, $\delta = \delta_1 - \delta_2$.

Thus, if the probabilityes of being in one of the states Ψ_1 or Ψ_2 are defined by coefficients α_1, α_2 and do not depend from time, such dependences is take place for $p_{1,} p_2$ and are defined by equations (4). For $|\alpha_1| = |\alpha_2| =$

1/2 the transitions will be most brightly expressed. To such case correspond (for two well's defect) the absence of the energy's gap δ between the minima on a potential surface.

In common case the state of system with two minima is describe [5 - 7] by equation:

$$\Phi = \beta_1(t)\chi_1 + \beta_2(t)\chi_2 \qquad (5)$$

We will suppose that the functions χ_1 и χ_2, which not depend from time, correspond to orthonormal states of systems from two states, i.e. it its own basal states. The change in time of function $\beta_{1,}$ β_2 is described [7] by system of equations.

$$i\hbar\frac{d\beta_1}{dt} = H_{11}\beta_1 + H_{12}\beta_2$$

$$i\hbar\frac{d\beta_2}{dt} = H_{21}\beta_1 + H_{22}\beta_2 \qquad (6)$$

$$H_{k,l} = \int \Psi_k^* H \Psi_l dV ,$$

where H - operator of disturbance, V - volume.

Coefficients $H_{12,}H_{21}$ are arisen in connection with not zero probability of transitions from state χ_1 in χ_2 and back. We will accept its equal: -A (A – the positive number).

The H_{11}, H_{22} - correspond to energy of the not disturbance state. At the equivalent potential wells, H_{11}, H_{22} accept an identical value of energy, we shall designate this value as E.

For the system of equations (6) in case of absence of decay $H_{1,2} = H^*_{2,1}$, and in case of absence of tunneling (interaction with subsystem) $H_{1,2}$=0 [7].

Let's write out the decisions of the system of equations (5), [7]:

$$\Phi_1 = \frac{}{\sqrt{1\ |\ \ |}}(\quad \chi_1 + \chi_2)$$

$$\Phi_2 = \frac{1}{\sqrt{1+|R|^2}}(\chi_1 - R\chi_2) \qquad (7)$$

$$R = \frac{H_{12}}{\frac{H_1 + H_2}{2} \pm \sqrt{\frac{(H_1 - H_2)^2}{4} + |H_2|^2}}$$

For energies, proper to states χ_1, χ_2, we have:

$$E_{1,2} = \frac{H_{11} + H_{22}}{2} \pm \sqrt{\frac{(H_{11} - H_{22})^2}{4} + |H_{12}|^2} \qquad (8)$$

The inclusion of the mechanism of interaction between subsystems means, that the level with energy of E, corresponds to the states χ_1 and χ_2, under action of some disturbance is slightly splitting. We will designate the size of splitting as ΔE. From (8) we have:

$$\Delta E = E_2 - E_1 = 2H_{12} \qquad (9)$$

According to [5-7], the splitting of a levels means that the states χ_1 and χ_2 are not the stationary and in system are arise the beating with frequency $f = 2H_{12}/\hbar$.

For not symmetrical quantum well the values of H_{11} and H_{22} do not coincide, and, consequently, there are the own location of levels for each of minima: $\mathring{A}_1$ and $\mathring{A}_2$.

In this case we have [6] at $H_{12}H_{21} = A^2$ from (8):

$$E_{1,2} = \frac{H_1 + H_2}{2} \pm \frac{H_1 - H_2}{2}\sqrt{1 + \frac{4A^2}{(H_1 - H_2)}} \qquad (10)$$

If: $|H_1 - H_2| > A$,

$$E_1 \cong H_1 + \frac{A^2}{H_1 - H_2}, E_2 \cong H_2 - \frac{A^2}{H_1 - H_2}. \qquad (11)$$

Thus, the accounting of the amplitude A of a passing from one of state to another gives the insignificant change of levels from the position from levels with energy H_{11} and H_{22} [6] (at which the tunneling is, practically, absent).

As follows from the calculation carried out in [3], the positions of minima in divacancy of silicon is not equivalent, therefore the divacancy is in configuration, corresponding to the central minimum. However it is possible to pick up the parameters of an external field at which the configuration of divacancy will be displaced and at the certain characteristics of this field the pulsations, corresponding to periodic transitions from one configuration minimum in another are possible. If to influence by a variable field, it is possible to pick up the resonant frequency and to have an opportunity of an experimental research of the processes caused by tunnel transitions.

However is possible and another method of influence.

It was found that is observed the dependence of the position of Fermi level, and also the concentrations of defects which are revealed as be situated in some one of the minimums, from the type of irradiation and dose of irradiation [8]. In addition, in accordance with experimental dates consider that for $n-Si$ 0.7 % divacancy have a central minimum in the first configuration, and 0.3% in the second configuration. For $p-Si$, vice versa: 0.3% divacancy have such minimum in the first configuration and 0.7 % in the second.

On the basis of the above mentioned equations, it is possible to postulate that such ratio indicate on the presence of superposed transitions between minima of divacancy. It means that instead of asserting that the certain percent of divacancies has as the central the one minimum and the rest of divacancies has as the central the other minimum, we pass to other treatment of observable dependence. We assert that the states of divacancy are not independent, and are in the superposition state, described by equalization (5), where the ratio between $\beta_{1,}$ and β_2 determine the probability of a presence of the system in each of the states. It means, that divacancies in the given material are identical concerning an arrangement of minima, but here minima are not equivalent. The reasons bring to such non equivalence are ambiguous and in this article are not discussed, however is clear that by introduction of certain radiation defects it is possible to influence on the configuration parameters of divacancy.

Certainly, experimental researches are necessary for detection of pulsing fluctuations of divacancy in silicon at external influence. The defective centers which are used for researches should be in close energy states. It is desirable to investigate simultaneously some such centers, taking into account that in devices of quantum information technologies the usual number of the required active centers no more than several tens.

Let's note that the size of splitting ΔE much less than energy of the possible fluctuations $h\nu$, set by the position of a vibrating level in any from minima of potential adiabatic energy. Usually, as follows from [2], the frequency of pulsations (beatings) f is in the range of micro-waves or ultrasound [2].

Some types of clustered defects can be convenient object for studying of possible collective effects for divacancies, close located between itself. It is known that clusters formed in silicon at an irradiation, mainly consist from divacancies [9], which can be between itself in entangled state. For the decision of multi-aspect tasks on creation of devices of quantum information technology with application as elements of devices of divacancies the additional researches are needed.

It is very important to develop the technologies allowing to create a few active centers, which could be used as qubits being in the entangled state. Thus, the time of decoherency for such centers must be more than the time of execution of various quantum transformations. But such works are conducted and in some cases of uses of some types of the bistable centers find the successful decision. The divacancies of silicon can be such centers.

The offered approach has the general character and can be distributed and on the others bistable centers in silicon or other compounds. It opens the opportunities for creation of devices of quantum information technologies [9] on the basis of such bistable centers.

Conclusions

The bistable defects can have the superposition states, the transitions between which correspond to resonance frequencies of such systems [2]. The divacancy of silicon, as bistable defect, also can display itself as the system with two states (minimums) between which it is possible the interferential transitions. It opens the perspectives of using of divacancies in technology of quantum information systems.

The analyses of the materials of literature sources about of characteristics of divacancy, presented in this article, has been made with the position of theory of interferential transitions in quantum systems.

In accordance with experimental dates consider that for $n-Si$ 0.7 % divacancy have a central minimum in the first configuration, and 0.3 % in the second configuration. For $p-Si$, vice versa: 0.3% divacancy have such minimum in the first configuration and 0.7 % in the second.

It is possible to postulate, on the basis of the above mentioned equations, that such ratio indicates on the presence of superposition transitions between configurations (by minimums) of divacancy. It means that the states, proper to positions of the system in one or another minimum are not independent. In such system there are beatings, proper to the transition of divacancy from one configuration state to other.

In superposition state, the system does not have the stationary position, and the configuration state of the system is determined by probabilistic correlations which are fixing experimentally, but not correctly interpreting as percentage of divacancies, which have a central minimum in the first or in the second configuration.

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