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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.

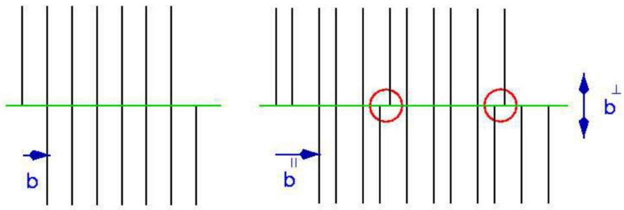

Fig. 1. Displacement along a slip plane in a crystal (left) and a quasicrystal (right).

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 $\tilde{v}$ 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 (v):

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

The reverse transformations (1) which are accompanied by the formation of regular point defects require a significant energy (E_v 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):

$$\frac{\partial C^i_{ph}}{\partial t} = -j_v C^i_{ph} + j_i C^v_{ph}, \tag{2}$$

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

$$j_v \sim D_v \left.\frac{\partial C_v}{\partial r}\right|_{\tilde{i}};\ j_i \sim D_i \left.\frac{\partial C_i}{\partial r}\right|_{\tilde{v}}, \tag{4}$$

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

The equilibrium concentrations of phasons can be derived:

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

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

where $E_{\tilde{v}}$, $E_{\tilde{i}}$ 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):

$$C^i_{ph} = \frac{j_i}{j_v} C^v_{ph}. \tag{7}$$

In this approximation the $\tilde{i}$ -type ($\tilde{v}$ -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].

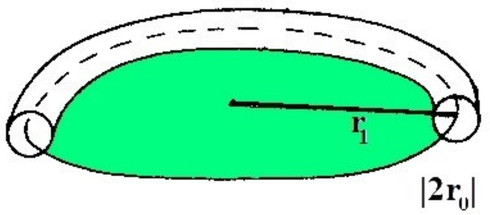

Fig. 2. Dislocation loop with the phason trail inside.

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,

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

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

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

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

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

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

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

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 $r_{0i} = 3b$.

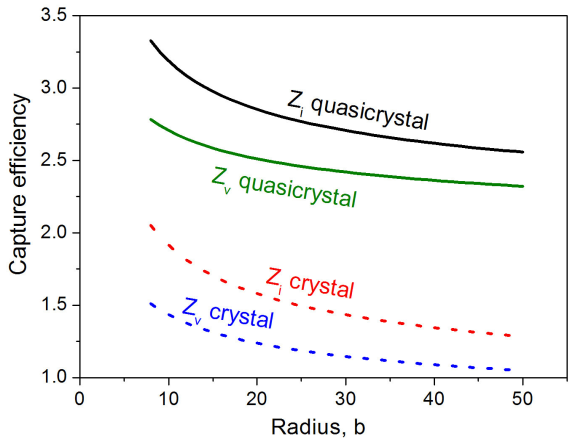

Fig. 3. Capture efficiencies of the dislocation loop for vacancies and SIAs as functions of loop radius.

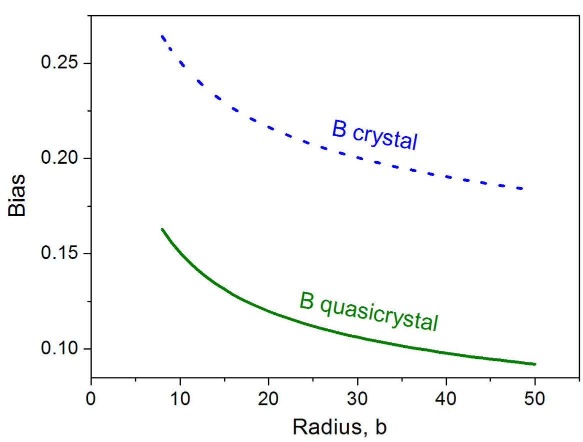

Fig. 4. Dislocation loop bias as a function of loop radius.

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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