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POST-IRRADIATION MODULATION OF DISTRIBUTION OF INTERACTING VACANCIES IN THE ELASTICALLY ANISOTROPIC B.C.C. CRYSTALS

Spinodal mechanism of formation of a modulated structure in a spatial distribution of vacancies within the body-centred cubic (b.c.c.) crystal after irradiation is considered. The criterion of modulated-structure formation for the closed interacting-vacancies subsystem within the elastically anisotropic b.c.c. crystal is estimated. As shown, in case of positive factor of elastic anisotropy ($\xi > 0$ as for Mo, Nb, W crystals), the modulated structures can be formed along the [111] direction, and in case of negative factor of elastic anisotropy ($\xi < 0$ as for Fe crystal), the modulated structure can be formed along the [100] direction. Dependence of the modulated-structure period of b.c.c.-Mo (Fe)-vacancies' solution on temperature is plotted. Period of a modulated structure in a spatial distribution of vacancies, which is formed by means of the spinodal mechanism, increases with temperature and is determined by the entropy factor, '(electro)chemical' interaction of vacancies, and elastic properties of b.c.c. crystal.

Keywords: vacancies, 'strain-induced' interaction, '(electro)chemical' interaction, spinodal decomposition, modulated structure.

Introduction

Vacancies (v) form the important type of defects. Presence of vacancies in a solid plays an essential role in its thermodynamical properties. Appearance of vacancies in a metal crystal leads to change of the ion and electron subsystems of a metal. For instance, a new equilibrium state corresponds to changed conditions. Therefore, atoms around a vacancy are displaced to new equilibrium positions.

Vacancies generally influence bulk properties of a solid, namely, self-diffusion and diffusion by means of the vacancy mechanism that significantly determines process of transfer of substance in a crystal

[1], phase transformations, in particular, affecting the possible mechanism of the martensitic transformation [2], stability of intermetallides (problems of stability of intermetallic phases and areas of their homogeneity at high temperatures are inseparably linked with formation of vacancies and their arrangement) [3]. Presence of the vacancy clusters can influence on optical properties of solids [4]. In References [5–18], participation of vacancies is considerable in phenomenon of formation of nanovoids in crystals under radiation. Therefore, the necessity of the study of the vacancies' subsystem in solids is a direct consequence of need for the investigation of specified phenomena and processes.

In a given article, evolution of pseudo-binary b.c.c.-*Me*-vacancies' solution (*Me* = Mo, Fe, *etc.*), which was formed due to radiation effects, is considered after stopped radiation. (Among the different ways for the fabrication of substitutional *Me*-vacancies' solid solution, there is a rapid quenching from high temperatures, which fixes surplus amount of 'residual' premelting vacancies, too.) As supposed, the average relative concentration \bar{c}_v of post-irradiation vacancies formed because of radiation remains invariable for a long time, and vacancies have a time to reach a surface or to disappear on a sink. Using atomistic consideration of the diffusion-controlled formation of nanovoids, which are a three-dimensional superposition of the spatially ordered one-dimensional concentration waves in distribution of vacancies, let us take into account both the 'direct' (electro)chemical and indirect 'strain-induced' interactions of vacancies. For the first time, Chang [19, 20] noted such an analogy. Nevertheless, in his opinion, vacancies are quasi-particles, which, due to the 'elastic' interaction between them only, array into 'superlattice' of vacancies under radiation. However, interaction between vacancies is similar to interaction between host-crystal atoms, as approved in Ref. [21], and vacancies have the same redistribution kinetics as for host-crystal atoms. The total ('(electro)chemical' + 'strain-induced') interchange energies are used to describe the instability of b.c.c.-*Me*-vacancies' solution during its spinodal decomposition [22]. The vacancies' interactions (consisting of the '(electro)chemical' + 'strain-induced' contributions) are the governing mechanism of formation of the modulated structures in vacancy-containing crystals. Such a problem was already considered in Ref. [23], but for the irradiated face-centred cubic (f.c.c.) crystal.

Calculation of Interaction Parameters for Pseudo-Binary B.C.C.-*Me*-Vacancies' Solid Solution

Our paper is based on the overrunning continuous approximation for the \mathbf{k} -th Fourier components, $\tilde{w}(\mathbf{k})$, of the total 'mixing' energies [22, 23] for the substitutional b.c.c.-*Me*-vacancies' solid solution. Within the small finite region of reciprocal space near $\mathbf{k} = \mathbf{0}$, $\tilde{w}(\mathbf{k})$ may be rep-

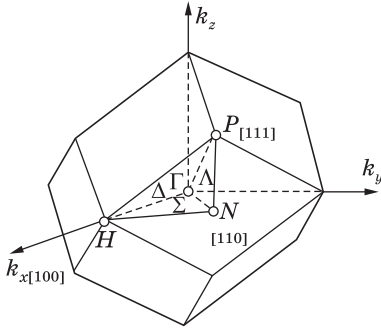


Fig. 1. The 1st BZ of reciprocal space for b.c.c. lattice

resented as follows:

$$w(\mathbf{k}) \approx \tilde{V}^{vv}(\mathbf{k}) + \tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) \cong \\ \cong V_n^{vv} + \tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \beta_{ij}(\mathbf{n})k_i k_j.$$

Here, $\tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) \cong \tilde{\Phi}_{\text{el.chem}}^{\text{MeMe}}(\mathbf{k}) + \tilde{\Phi}_{\text{el.chem}}^{\text{vv}}(\mathbf{k}) - 2\tilde{\Phi}_{\text{el.chem}}^{\text{vMe}}(\mathbf{k})$ is the \mathbf{k} -th Fourier component of the ‘mixing’ energies for the direct ‘(electro)chemical’ interactions of constituents in b.c.c.-*Me*-vacancies’ solution; $\tilde{V}^{vv}(\mathbf{k})$ is the \mathbf{k} -th Fourier component of the ‘strain-induced’ v - v -interaction energies; $\beta_{ij}(\mathbf{n})$ are the expansion coefficients ($\mathbf{n} \equiv \mathbf{k}/|\mathbf{k}|$).

Within the small finite region near $\mathbf{k} = 0$, $\tilde{V}^{vv}(\mathbf{k})$ may be approximated as follows: $\tilde{V}^{vv}(\mathbf{k}) \cong \mathcal{A}^{vv}(\mathbf{n}) + \mathcal{B}^{vv}(\mathbf{n})k^2 + \mathcal{Q}^{vv}$; here, the well-known first term is based on the long-wave-limit approximation [22], the second term is a correction to this approximation [24], and the third term is a gauge, which eliminates ‘strain-induced’ self-action of vacancies [22].

The dispersion curves of $\tilde{V}^{vv}(\mathbf{k})$ for the b.c.c. Mo and Fe crystals along all the high-symmetry directions as well as, in particular, at the high-symmetry points, Γ, H, N, P , in the reciprocal-space Brillouin zone (BZ; Fig. 1) are presented in Fig. 2, *a, b*, respectively, where $\bullet - \tilde{V}^{vv}(\mathbf{0})$ at $T = 298$ K. In this investigation, the estimates are carried out for the following values of parameters for the above-mentioned b.c.c. crystals

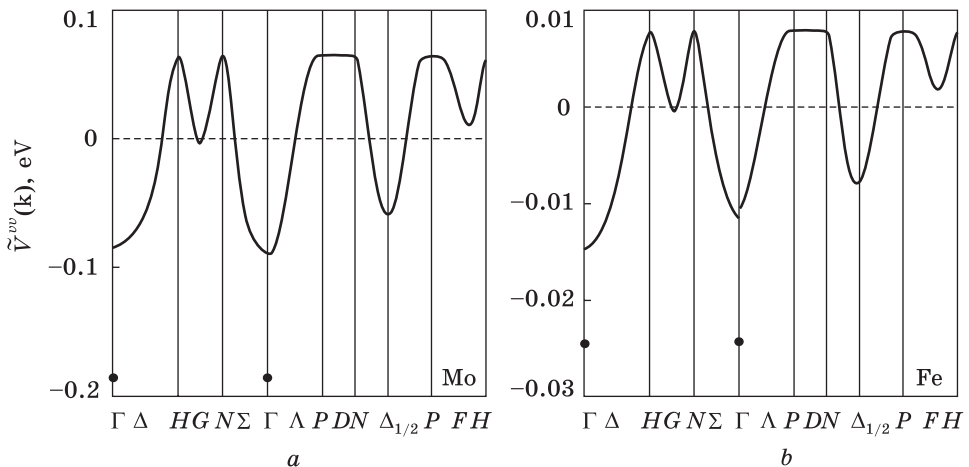


Fig. 2. Dispersion curve for the $\tilde{V}^{vv}(\mathbf{k})$ of ‘strain-induced’ v - v -interaction energies in b.c.c. crystals: (a) molybdenum, (b) iron, $\bullet - \tilde{V}^{vv}(\mathbf{0})$ at $T = 298$ K

with vacancies (at $T = 298$ K): $C_{11} = 440.8$ GPa, $C_{12} = 172.4$ GPa, $C_{44} = 121.7$ GPa (*i.e.*, $\xi > 0$) [25], $a = 3.1475$ Å [26], $L^v = -0.033$ [27] for the b.c.c.-Mo crystal; $C_{11} = 273$ GPa, $C_{12} = 150$ GPa, $C_{44} = 106.73$ GPa (*i.e.*, $\xi < 0$) [28], $a = 2.8663$ Å [29], $L^v = -0.016$ [27] for the b.c.c.-Fe crystal. (Here and then, a is a translation period of a b.c.c. lattice, C_{11} , C_{12} , C_{44} are the elasticity moduli, $\xi \equiv (C_{11} - C_{12} - 2C_{44})/C_{44}$ is an elastic-anisotropy factor, L^v is a concentration coefficient of a b.c.c.-lattice dilatation.)

The $\tilde{V}^{vv}(\mathbf{k})$ function has $\min_{\substack{\mathbf{k} \rightarrow \mathbf{0} \\ \{111\}}} \tilde{V}^{vv}(\mathbf{k}) < 0$ (see Fig. 2, *a*), which is a minimum value within the b.c.c.-crystal BZ (Fig. 1) in case of $\xi > 0$ (for example, for Mo, Nb, and W):

$$\tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_p} \rightarrow \mathbf{0}) \cong -\frac{27K^2 v_0 (L^v)^2 (3 + \xi)^2}{27C_{11} + 9\xi(C_{11} + C_{12}) + (C_{11} + 2C_{12} + C_{44})\xi^2} + \mathcal{B}^{vv}(\mathbf{n}_{\Gamma P})k^2 + \mathcal{Q}^{vv},$$

where, as follows from Ref. [24],

$$\begin{aligned} \mathcal{B}^{vv}(\mathbf{n}_{\Gamma P}) &\cong \\ &\cong a^4(C_{11} + 2C_{12})^2 (L^v)^2 \frac{16a(C_{11} + 4C_{12} + 6C_{44}) + M[8(\omega_{LN}^2 + 2\omega_{T_2N}^2 + \omega_P^2) - \omega_H^2]}{256(C_{11} + 2C_{12} + 4C_{44})^2}, \end{aligned}$$

$K = (C_{11} + 2C_{12})/3$ is a compressibility modulus, $v_0 = a^3/2$ — atomic volume in a b.c.c. crystal lattice, ω_p , ω_H are the temperature-dependent frequencies of degenerate phonon modes at the $P(2\pi(1/2, 1/2, 1/2)/a)$, $H(2\pi(1, 0, 0)/a)$ points, respectively, and ω_{LN} , ω_{T_2N} are the temperature-dependent longitudinal and transversal phonon frequencies at the $N(2\pi(1/2, 1/2, 0)/a)$ point [30] (*e.g.*, for Mo crystal at $T = 298$ K, $\omega_p = 6.49$ THz, $\omega_H = 5.52$ THz, $\omega_{LN} = 8.14$ THz, $\omega_{T_2N} = 4.56$ THz [31]); M is a host atom mass (*e.g.*, for Mo atom, $M \approx 159.31 \cdot 10^{-27}$ kg).

In case of negative elastic-anisotropy factor, $\xi < 0$ (*e.g.*, for the b.c.c.-Fe crystal), the $\tilde{V}^{vv}(\mathbf{k})$ function has $\min_{\substack{\mathbf{k} \rightarrow \mathbf{0} \\ \{100\}}} \tilde{V}^{vv}(\mathbf{k}) < 0$ (see Fig. 2, *b*), which is minimum value within the b.c.c.-crystal BZ (Fig. 1),

$$\tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_H} \rightarrow \mathbf{0}) \cong -\frac{9K^2 v_0 (L^v)^2}{C_{11}} + \mathcal{B}^{vv}(\mathbf{n}_{\Gamma H})k^2 + \mathcal{Q}^{vv},$$

where, as follows from Ref. [24],

$$\begin{aligned} \mathcal{B}^{vv}(\mathbf{n}_{\Gamma H}) &\cong \\ &\cong a^4(C_{11} + 2C_{12})^2 (L^v)^2 \frac{-16a(C_{11} + 2C_{44}) + M[8(\omega_{LN}^2 + \omega_{T_1N}^2 + \omega_{T_2N}^2 - \omega_P^2) - \omega_H^2]}{256C_{11}^2}, \end{aligned}$$

ω_{T_1N} is the temperature-dependent transversal phonon frequency at the $N(2\pi(1/2, 1/2, 0)/a)$ point [32] (for the b.c.c.-Fe crystal at $T = 298$ K, $\omega_p = 7.26$ THz, $\omega_H = 8.56$ THz, $\omega_{LN} = 9.26$ THz, $\omega_{T_1N} = 4.53$ THz, $\omega_{T_2N} = 6.45$ THz [31]; for Fe atom, $M \approx 92.73 \cdot 10^{-27}$ kg).

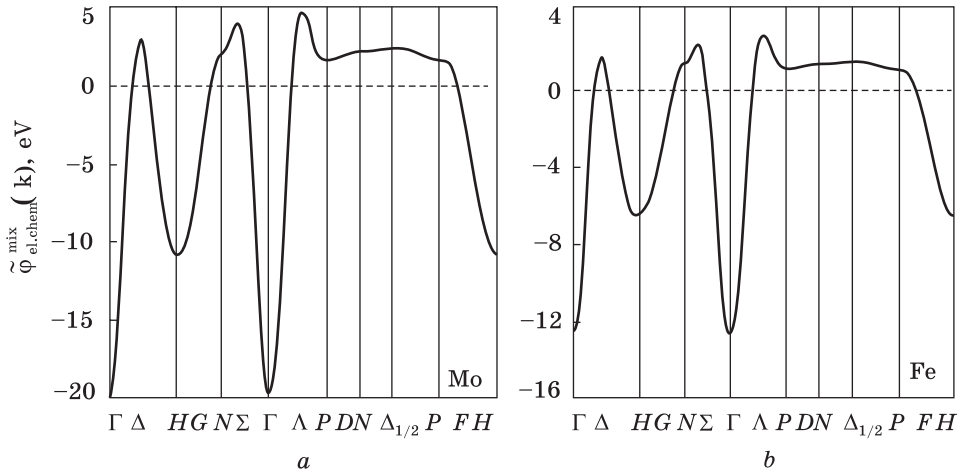


Fig. 3. Dispersion curve for the $\tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k})$ of ‘mixing’ energies for direct ‘(electro)chemical’ $v-v$ -interactions in b.c.c. crystals: *a* — molybdenum, *b* — iron

The dispersion curves of

$$\begin{aligned} \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) \cong & 4 \left\{ 8\varphi^{vv}(r_I) \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{ak_y}{2}\right) \cos\left(\frac{ak_z}{2}\right) + \right. \\ & + 2\varphi^{vv}(r_{II}) [\cos(ak_x) + \cos(ak_y) + \cos(ak_z)] + \\ & + 4\varphi^{vv}(r_{III}) [\cos(ak_x) \cos(ak_y) + \cos(ak_x) \cos(ak_z) + \cos(ak_y) \cos(ak_z)] + \\ & + 8\varphi^{vv}(r_{IV}) \left[\cos\left(\frac{3ak_x}{2}\right) \cos\left(\frac{ak_y}{2}\right) \cos\left(\frac{ak_z}{2}\right) + \cos\left(\frac{3ak_y}{2}\right) \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{ak_z}{2}\right) + \right. \\ & \left. + \cos\left(\frac{3ak_z}{2}\right) \cos\left(\frac{ak_x}{2}\right) \cos\left(\frac{ak_y}{2}\right) \right] + 8\varphi^{vv}(r_V) \cos(ak_x) \cos(ak_y) \cos(ak_z) \left. \right\} \end{aligned}$$

with \mathbf{k} along all the high-symmetry directions within the b.c.c.-lattice BZ for the b.c.c.- $Me-v$ ($Me = \text{Mo}$ or b.c.c. Fe) are presented in Fig. 3, *a*, *b*, respectively; $\phi^{vv}(r_I)$, $\phi^{vv}(r_{II})$, ..., $\phi^{vv}(r_V)$, ... are the ‘(electro)chemical’ $v-v$ -interaction energies at the first, second, ..., fifth, ... coordination shells. Here, as suggested, the dependence of $\phi^{vv}(r_l)$ on normalized intersite distance $r_l(298 \text{ K})/a(298 \text{ K})$ for a b.c.c. crystal is described by the Machlin potential [33] (with cohesive energies $\varepsilon^0 = -6.83 \text{ eV/atom}$ for the b.c.c.-Mo crystal and $\varepsilon^0 = -4.28 \text{ eV/atom}$ for the b.c.c.-Fe crystal [33, 34, 35]).

Within the long-wavelength approximation, Fourier components of the ‘mixing’ energies for direct ‘(electro)chemical’ interactions in b.c.c.- Me -vacancies solution are defined as follow:

$$\tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) \cong \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \gamma_0 k^2 + \dots,$$

where

$$\tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) = \sum_{\mathbf{r} \in \{\mathbf{r}_I, \mathbf{r}_{II}, \dots\}} \varphi_{\text{el.chem}}(|\mathbf{r}|) \approx 4 \{8\varphi(r_I) + 6\varphi(r_{II}) + 12\varphi(r_{III}) + 24\varphi(r_{IV}) + 8\varphi(r_V) + \dots\},$$

$$\gamma_0 \approx -4a^2 \{\varphi(r_I) + \varphi(r_{II}) + 4\varphi(r_{III}) + 11\varphi(r_{IV}) + 4\varphi(r_V) + \dots\}.$$

As found, at least, at distances of the several first coordination spheres' radii, considerable values of corresponding energies provide domination of the cohesive-nature $\tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k})$ to $\tilde{w}(\mathbf{k})$ (in comparison with contribution of the 'strain-induced' $\tilde{V}^{\text{vv}}(\mathbf{k})$) near the BZ centre of the reciprocal space for a b.c.c. lattice.

Spinodal Decomposition of B.C.C.-Me-Vacancies' Solid Solution: the Closed-System Model

Let us consider a spinodal decomposition of a pseudo-binary solid solution of host-crystal atoms and vacancies, b.c.c.-Me-vacancies ($Me = \text{Mo}$, b.c.c.-Fe, *etc.*), redistributing only over the sites of certain compact lattice, which will be called as the Ising lattice. Configuration-dependent energy of such a solution has the following form [22, 36]:

$$E = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} [W^{\text{vv}}(\mathbf{r}, \mathbf{r}') C_v(\mathbf{r}) C_v(\mathbf{r}') + W^{\text{MeMe}}(\mathbf{r}, \mathbf{r}') C_{Me}(\mathbf{r}) C_{Me}(\mathbf{r}') + 2W^{\text{vMe}}(\mathbf{r}, \mathbf{r}') C_v(\mathbf{r}) C_{Me}(\mathbf{r}')], \quad (1)$$

where $W^{\text{vv}}(\mathbf{r}, \mathbf{r}')$, $W^{\text{vMe}}(\mathbf{r}, \mathbf{r}')$, $W^{\text{MeMe}}(\mathbf{r}, \mathbf{r}')$ are energies of total interaction between two vacancies, between vacancy and matrix atom, and between two matrix atoms, respectively. Summation is carried out over all N sites with vectors \mathbf{r} and \mathbf{r}' in a lattice. $C_v(\mathbf{r})$ and $C_{Me}(\mathbf{r})$ are stochastic functions, which are defined as follow:

$$C_v(\mathbf{r}) = \begin{cases} 1, & \text{if at site } \mathbf{r}, \text{ there is a vacancy,} \\ 0, & \text{otherwise;} \end{cases}$$

$$C_{Me}(\mathbf{r}) = \begin{cases} 1, & \text{if at site } \mathbf{r}, \text{ there is a host-crystal atom,} \\ 0, & \text{otherwise;} \end{cases}$$

Besides, the condition

$$C_v(\mathbf{r}) + C_{Me}(\mathbf{r}) = 1 \quad (2)$$

is satisfied and means that each site in a lattice is occupied by the host-crystal atom or by the vacancy.

Substituting $C_{Me}(\mathbf{r})$ expressed from Eq. (2) into Eq. (1), we obtain [22, 36]:

$$E = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} w(\mathbf{r}, \mathbf{r}') C_v(\mathbf{r}) C_v(\mathbf{r}') + \frac{1}{2} \sum_{\mathbf{r}} (1 - 2C_v(\mathbf{r})) \sum_{\mathbf{r}'} W^{\text{MeMe}}(\mathbf{r}, \mathbf{r}') + \sum_{\mathbf{r}} C_v(\mathbf{r}) \sum_{\mathbf{r}'} W^{\text{vMe}}(\mathbf{r}, \mathbf{r}'), \quad (3)$$

where $w(\mathbf{r}, \mathbf{r}') = W^{vv}(\mathbf{r}, \mathbf{r}') + W^{MeMe}(\mathbf{r}, \mathbf{r}') - 2W^{vMe}(\mathbf{r}, \mathbf{r}') = \varphi_{\text{el.chem}}^{\text{mix}}(\mathbf{r}, \mathbf{r}') + V^{vv}(\mathbf{r}, \mathbf{r}')$ is a total ‘mixing’ energy. All sites of the Bravais-type Ising lattice are crystallographically equivalent; therefore, sums

$$\sum_{\mathbf{r}'} W^{MeMe}(\mathbf{r}, \mathbf{r}') = \tilde{W}^{MeMe}(\mathbf{0}),$$

$$\sum_{\mathbf{r}'} W^{vMe}(\mathbf{r}, \mathbf{r}') = \tilde{W}^{vMe}(\mathbf{0})$$

do not depend on the site vector \mathbf{r} . $\sum_{\mathbf{r}} C_v(\mathbf{r}) = N_v$, if N_v is a total number of vacancies. Then, expression (3) has the following form:

$$E = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} w(\mathbf{r}, \mathbf{r}') C_v(\mathbf{r}) C_v(\mathbf{r}') + \frac{1}{2} (N - 2N_v) \tilde{W}^{MeMe}(\mathbf{0}) + N_v \tilde{W}^{vMe}(\mathbf{0}).$$

Designating an average relative vacancies’ concentration as $\bar{c}_v = N_v/N$, the energy per each site can be presented as follows:

$$\frac{E}{N} = \frac{1}{2N} \sum_{\mathbf{r}, \mathbf{r}'} w(\mathbf{r}, \mathbf{r}') C_v(\mathbf{r}) C_v(\mathbf{r}') + \frac{1}{2} (1 - 2\bar{c}_v) \tilde{W}^{MeMe}(\mathbf{0}) + \bar{c}_v \tilde{W}^{vMe}(\mathbf{0}).$$

Distribution of vacancies in such a pseudo-binary atom–vacancies’ solid solution can be described by a probability function $n(\mathbf{r}) = \langle C_v(\mathbf{r}) \rangle$, which defines the one-particle probability of finding of a vacancy at a site \mathbf{r} of the Bravais lattice ($\langle \dots \rangle$ denotes the Gibbs canonical ensemble averaging). The configuration-dependent part of free energy of a pseudo-binary solid solution ‘Me–vacancies’ has the following form within the self-consistent field approximation:

$$F \approx \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}'} w(\mathbf{r}, \mathbf{r}') n(\mathbf{r}) n(\mathbf{r}') + \frac{N}{2} (1 - 2\bar{c}_v) \tilde{W}^{MeMe}(\mathbf{0}) + N \bar{c}_v \tilde{W}^{vMe}(\mathbf{0}) +$$

$$+ k_B T \sum_{\mathbf{r}} [n(\mathbf{r}) \ln n(\mathbf{r}) + (1 - n(\mathbf{r})) \ln(1 - n(\mathbf{r}))],$$

where k_B is the Boltzmann constant, T is the absolute temperature, and summation is carried out over all lattice sites (see also [22, 36]).

It should be noted that such an approach was used also in Ref. [22] for the description of the phenomenon of atomic ordering in substitutional binary solid solutions, for the estimation of parameters of interactions of defects by means of the data on a self-diffusion [36], and for the analysis of formation of the quasi-periodic macrolattice of precipitations [37].

Within the pairwise-interaction approximation, the total free energy of b.c.c.-Me–vacancies’ solid solution has the following form [22, 37] within the reciprocal-space representation:

$$F \approx \frac{1}{2\Omega} \int_{BZ} \tilde{U}(\mathbf{k}) \left\langle \left| \tilde{C}_v(\mathbf{k}) \right|^2 \right\rangle \frac{dk d\omega}{(2\pi)^3}. \quad (4)$$

Integration in Eq. (4) is carried out over moduli k of the \mathbf{k} vectors and their directions within the BZ volume; Ω is a volume per one lattice site ($d\Omega = k^2 dk d\varphi$, $d\varphi = \sin\theta d\theta d\varphi$ is a solid angle). $\tilde{C}_v(\mathbf{k})$ is the \mathbf{k} -th Fourier component of spatial-distribution function for vacancies, $C_v(\mathbf{r})$ (*i.e.*, static vacancy-concentration-wave amplitude) [22], and, within the long-wave approximation [37],

$$\tilde{U}(\mathbf{k}) \cong \left[\tilde{w}(\mathbf{k}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] k^2 \approx \left[\tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) + \tilde{V}^{\text{vv}}(\mathbf{k}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] k^2,$$

where k^2 originates from integration over the BZ volume in Eq. (4).

The main role in formation of a spatial modulation of vacancies' subsystem is played by the long-wave mode of interactions, which can be characterized with expressions as follow [37]:

$$\tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) \cong \tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \gamma_0 k^2 + \beta_0 k^4, \quad (5)$$

$$\tilde{V}^{\text{vv}}(\mathbf{k}) \cong \mathcal{A}^{\text{vv}}(\mathbf{n}) + \mathcal{B}^{\text{vv}}(\mathbf{n})k^2 + \mathcal{E}^{\text{vv}}(\mathbf{n})k^4 + \mathcal{Q}^{\text{vv}}, \quad (6)$$

$$\tilde{U}(\mathbf{k}) \cong \left[\tilde{w}(\mathbf{k}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] k^2 \cong \left[\tilde{w}_n + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] k^2 + \tilde{\mathcal{B}}(\mathbf{n})k^4 + \tilde{\mathcal{E}}(\mathbf{n})k^6, \quad (7)$$

where $\tilde{w}_n = \tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \mathcal{A}^{\text{vv}}(\mathbf{n}) + \mathcal{Q}^{\text{vv}}$, $\tilde{\mathcal{B}}(\mathbf{n}) = \gamma_0 + \mathcal{B}^{\text{vv}}(\mathbf{n})$, $\tilde{\mathcal{E}}^{\text{vv}}(\mathbf{n}) = \beta_0 + \mathcal{E}^{\text{vv}}(\mathbf{n})$.

From the condition for the $\tilde{\Phi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k})$ function minimum, which does not depend on the direction of \mathbf{k} at small \mathbf{k} , follows that $\gamma_0 > 0$, $\beta_0 > 0$ [37]. $\mathcal{A}^{\text{vv}}(\mathbf{n})$ depends on the \mathbf{n} direction; nevertheless, it is everywhere negative. Only the first two summands in right sides of Eqs. (5)–(7) have dominating influence in statistical thermodynamics of processes of formation of a superlattice of the vacancies' subsystem.

Vacancies form rows, which are clearly oriented along the $\mathcal{A}^{\text{vv}}(\mathbf{n})$ dependence-minimum direction, namely, $\mathbf{n} = [100]$ for b.c.c. Fe or $\mathbf{n} = [111]$ for Mo. In Figure 4, *a*, *b*, there are presented the dispersion curves for the total 'mixing' energy, $\tilde{w}(\mathbf{k})$, corresponding to the isostructural decomposition of b.c.c.-*Me*-vacancies' solid solution. However, because of a kinetic factor, isostructural decomposition (*i.e.*, redistribution of vacancies on the long distances) can be slowed down at not high temperatures. Nevertheless, at the same time, if $\tilde{w}_n < 0$, $\tilde{\mathcal{B}}(\mathbf{n}) > 0$, there is a possibility of realization of spinodal decomposition (into a metastable state), during which there is a redistribution of vacancies, but only between the neighbouring crests of modulation of the vacancy-concentration wave arising in a crystal.

Therefore, from the point of view of a kinetics, in b.c.c.-*Me*-vacancies' solid solution at low temperatures ($T < T_c$), a spinodal decomposition can be take place (as far as $\tilde{w}_n < 0$, $\tilde{\mathcal{B}}(\mathbf{n}) > 0$). A spinodal curve $T_c(\bar{c}_v)$ is

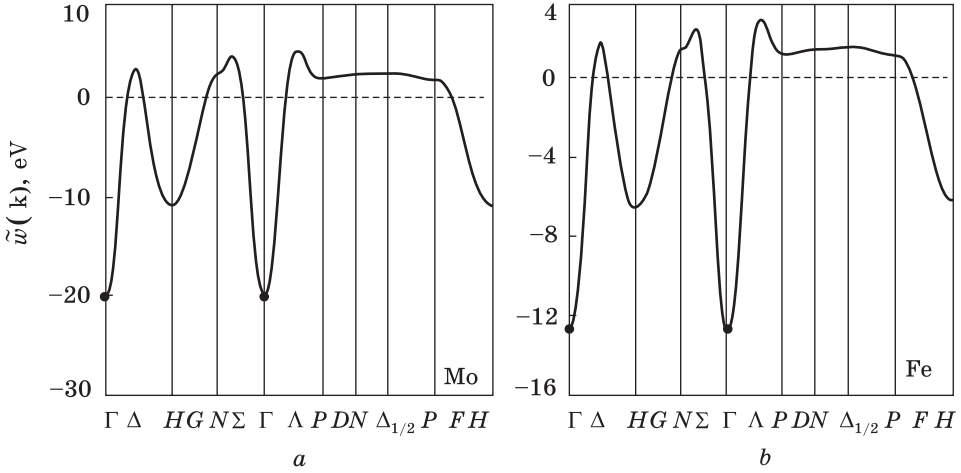


Fig. 4. Dispersion curve for the $\tilde{w}(\mathbf{k})$ of total ‘mixing’ energies $v-v$ -interactions in b.c.c. crystals: *a* — molybdenum, *b* — iron

defined from condition of the loss of stability of the homogeneous b.c.c.-*Me*-vacancies’ solid solution, and, as follows,

$$T_c \approx -\frac{\bar{c}_v(1 - \bar{c}_v)\tilde{w}_n}{k_B}$$

As a result of soft onset of the post-irradiation concentration inhomogeneities, the probability of filling of a lattice site, *r*, with a vacancy has the following form [22]:

$$n(\mathbf{r}) = \bar{c}_v + \delta n(\mathbf{r}),$$

where \bar{c}_v is the average relative concentration \bar{c}_v of ‘residual’ post-irradiation vacancies, $\delta n(\mathbf{r})$ is the probability inhomogeneity. Function $\delta n(\mathbf{r})$ can be presented as superposition of static concentration waves,

$$\delta n(\mathbf{r}) = \frac{1}{2N} \sum_{\mathbf{k}} [\tilde{c}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} + \tilde{c}^*(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}}],$$

where $\tilde{c}(\mathbf{k})$ is the amplitude of a concentration wave with a quasi-wave vector \mathbf{k} .

For the initial stage of spinodal decomposition, phenomenological Onsager equation for the infinitesimal amplitude of a concentration wave has the following form [22, 37]:

$$\frac{d\tilde{c}(\mathbf{k})}{dt} \cong \frac{\tilde{L}(\mathbf{k})\bar{c}_v(1 - \bar{c}_v)}{k_B T} \left[\tilde{w}(\mathbf{k}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] \tilde{c}(\mathbf{k}), \tag{8}$$

where $\tilde{c}(\mathbf{k}) = \sum_{\mathbf{r}} \delta n(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$, $\tilde{L}(\mathbf{k}) = \sum_{\mathbf{r}} L(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}$ is Fourier component of probabilities of jumps of vacancies between sites ($\mathbf{0}$ and \mathbf{r}) per unit time. Within the continual approximation (for small \mathbf{k}), $L(\mathbf{k}) \cong -D_0(\mathbf{n})k^2$,

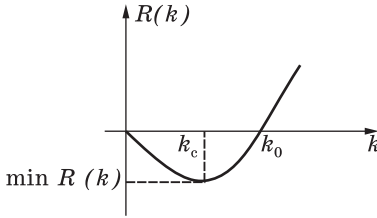


Fig. 5. Dependence of the ‘damping decrement’ on the modulus of the quasi-wave vector, $|\mathbf{k}|$

where D_0 is an expansion coefficient in a Taylor series for the $L(\mathbf{k})$ function, which represents a diffusion coefficient in a regular solid solution of vacancies.

The solution of the equation (8) has the following expression:

$$\tilde{c}(\mathbf{k}, t) = \tilde{c}(\mathbf{k}, 0) e^{-tR(\mathbf{k})}, \quad (9)$$

where $\tilde{c}(\mathbf{k}, 0)$ is the amplitude of \mathbf{k} -th concentration wave in an initial time moment $t = 0$, $R(\mathbf{k}) \cong \frac{D_0 \bar{c}_v (1 - \bar{c}_v) k^2}{k_B T} \left[\tilde{w}_n + \frac{k_B T}{\bar{c}_v (1 - \bar{c}_v)} + \tilde{B}(\mathbf{n}) k^2 \right]$ is the ‘damping decrement’ of such concentration-wave amplitude with a wave vector $\mathbf{k} = k\mathbf{n}$ [22, 38].

As follows from expression (9), at temperatures above the temperature of a spinodal, $T > T_c$, when $\tilde{w}_n + \frac{k_B T}{\bar{c}_v (1 - \bar{c}_v)} > 0$, ‘logarithmic decrement’ $R(\mathbf{k})$ becomes positive magnitude at all \mathbf{k} , and concentration inhomogeneities ‘resolve’ with time as $\tilde{c}(\mathbf{k}, t) \rightarrow 0$ at $t \rightarrow \infty$. In case, if temperature of the homogeneous b.c.c.-*Me*-vacancies’ solid solution is below the temperature of a spinodal ($T < T_c$) and a total interaction energy is such that $\tilde{w}_n + \frac{k_B T}{\bar{c}_v (1 - \bar{c}_v)} < 0$, then ‘logarithmic decrement’ becomes the negative for all the quasi-wave vectors \mathbf{k} , which are inside the sphere with radius k_0 (Fig. 5) that is with $|\mathbf{k}| < k_0$, and according to expression (9), concentration inhomogeneities increase under the exponential law with time. The wave number k_0 at a given \mathbf{n} is defined from the equation [22, 38, 39]:

$$\tilde{w}_n + \frac{k_B T}{\bar{c}_v (1 - \bar{c}_v)} + \tilde{B}(\mathbf{n}) k_0^2 = 0.$$

It is a condition, under which there is a change of the ‘logarithmic decrement’ sign. The schematic diagram [22, 38, 39] for the ‘logarithmic decrement’ $R(\mathbf{k})$ as a function of a wave number in the direction \mathbf{n} is presented in Fig. 5.

Results of Calculations of the Modulated-Structure Period for the Vacancies' Subsystem

The minimum of the $R(\mathbf{k})$ function corresponds to the wave number magnitude obeying the relationship $\partial R(\mathbf{k})/\partial \mathbf{k}|_{\mathbf{k}=\mathbf{k}_c} = \mathbf{0}$, and, as follows,

$$|\mathbf{k}_c| = k_c \approx \min_n \sqrt{-\left[\mathcal{A}^{vv}(\mathbf{n}) + \mathcal{Q}^{vv} + \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] \frac{1}{2[\mathcal{B}^{vv}(\mathbf{n}) + \gamma_0]}} = \frac{2\pi}{d},$$

and, in the minimum, the $R(\mathbf{k})$ function has the negative value of the following form (Fig. 5; see also [22, 38]):

$$\min_n \min_k R(\mathbf{k}) = R(k_c) = -\frac{D_0 \bar{c}_v(1 - \bar{c}_v)}{k_B T} \left(\tilde{w}_{n_c} + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right)^2 \frac{1}{4\tilde{\mathcal{B}}(\mathbf{n}_c)} < 0.$$

The modulated structure of vacancies' subsystem is formed along the crystallographic direction, which is parallel to corresponding direction \mathbf{n}_c of the highest growth rate of inhomogeneity-wave amplitude and is characterized by the wave vector of a magnitude k_c [22].

If both the Fourier components of indirect anisotropic 'strain-induced' $v-v$ -interaction energies, $\tilde{V}^{vv}(\mathbf{n}) > 0$ (Fig. 2, *a*), and the Fourier components of 'mixing' energies for the direct '(electro)chemical' $v-v$ -interactions, $\tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k})$, have $\min_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{V}^{vv}(\mathbf{k}) < 0$ in case of an elastic-anisotropy factor $\xi > 0$ (see definitions in Sec. Calculation of Interaction Parameters...), *e.g.*, for the b.c.c.-Mocystal, and $\min_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) = \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) < 0$ (Fig. 3, *a*), respectively, within the first Brillouin zone (*BZ*; Fig. 1) for a b.c.c. host crystal, and, in particular,

$$\begin{aligned} \tilde{V}^{vv}(\mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_p} \rightarrow \mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_N} \rightarrow \mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_H} \rightarrow \mathbf{0}) < 0 < \\ < \tilde{V}^{vv}(\mathbf{k}_H) = \tilde{V}^{vv}(\mathbf{k}_N) = \tilde{V}^{vv}(\mathbf{k}_p), \end{aligned}$$

then, for such a crystal, k_c for \mathbf{k}_c along the direction $\mathbf{n}_c \parallel [111]$ near $\mathbf{k} \cong \mathbf{0}$ can be determined as follows:

$$|\mathbf{k}_c| = k_c \approx \sqrt{-\left[\mathcal{A}^{vv}(\mathbf{n}_{c\parallel[111]}) + \mathcal{Q}^{vv} + \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] \frac{1}{2[\mathcal{B}^{vv}(\mathbf{n}_{c\parallel[111]}) + \gamma_0]}} = \frac{2\pi}{d}.$$

Contrariwise, in case of an elastic-anisotropy factor $\xi < 0$ (see Sec. Calculation of Interaction Parameters...), *e.g.*, for the b.c.c.-Fe crystal, $\min_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{V}^{vv}(\mathbf{k}) < 0$, and, in particular,

$$\begin{aligned} \tilde{V}^{vv}(\mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_H} \rightarrow \mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_N} \rightarrow \mathbf{0}) < \tilde{V}^{vv}(\mathbf{k}_{\downarrow\uparrow\mathbf{k}_p} \rightarrow \mathbf{0}) < 0 < \\ < \tilde{V}^{vv}(\mathbf{k}_H) = \tilde{V}^{vv}(\mathbf{k}_N) = \tilde{V}^{vv}(\mathbf{k}_p), \end{aligned}$$

as well as $\min_{\mathbf{k} \rightarrow \mathbf{0}} \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{k}) = \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) < 0$ (Fig. 3, *a*) within the first Brillouin zone.

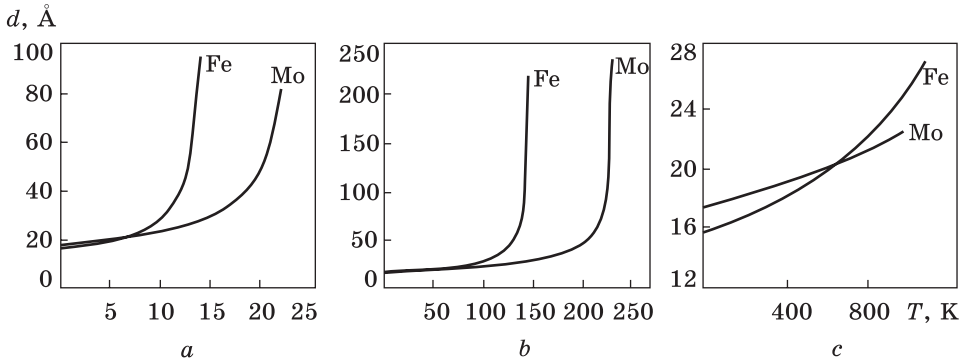


Fig. 6. The temperature dependence of the period of modulation of distribution of vacancies occurring by means of the spinodal mechanism for three average relative concentrations in the post-irradiated b.c.c.-Mo and b.c.c.-Fe crystals: $\bar{c}_v = 10^{-4}$ (a), $\bar{c}_v = 10^{-3}$ (b), $\bar{c}_v = 10^{-2}$ (c)

lounin zone for a b.c.c. host crystal. Then, k_c for \mathbf{k}_c along the direction $\mathbf{n}_c \parallel [100]$ near $\mathbf{k} \approx 0$ can be determined as follows:

$$|\mathbf{k}_c| = k_c \approx \sqrt{-\left[\mathcal{A}^{vv}(\mathbf{n}_{c\parallel[100]}) + Q^{vv} + \tilde{\varphi}_{\text{el.chem}}^{\text{mix}}(\mathbf{0}) + \frac{k_B T}{\bar{c}_v(1 - \bar{c}_v)} \right] \frac{1}{2[\mathcal{B}^{vv}(\mathbf{n}_{c\parallel[100]}) + \gamma_0]}} = \frac{2\pi}{d}.$$

As interaction between vacancies, competing with an entropic factor, begins manifest itself in structure formation only at relative vacancies' concentrations of an order of 10^{-4} – 10^{-2} , there is a threshold character in appearance of the periodic modulated structure. Its period is defined by parameters of specified '(electro)chemical' and 'strain-induced' v - v -interactions. With increase in average relative concentration of 'residual' vacancies, the temperature range of advantage of the modulated structure of their subsystem extends (Fig. 6).

Conclusions

As revealed by means of the statistical-thermodynamics analysis, modulated structure of the closed 'residual'-vacancies' subsystem characterized by the nanoscale period d (Fig. 6) can arise only at the initial stage of spinodal decomposition of 'solid solution' of 'residual' vacancies in a host crystal. Within the scope of the Cahn–Khachaturyan concept [22], structural parameters of this process are defined by an entropy factor, energy parameters of vacancies' interactions, and external conditions (temperature T , concentration of 'residual' vacancies \bar{c}_v), but do not depend obviously on kinetics parameters of 'solution', for instance, on the coefficient of diffusion of vacancies.

As shown, in case of positive factor of elastic anisotropy, $\xi > 0$ (for instance, for the Mo, Nb, W crystals), the modulated structure can be formed by vacancies' layers, which are perpendicular to the [111] direction. In case of negative factor of elastic anisotropy, $\xi < 0$ (for example, for the b.c.c.-Fe crystal), the modulated structure could be formed by vacancies' layers, which are perpendicular to the [100] direction, at sufficiently low temperatures below T_c .

Taking into account '(electro)chemical' interactions of vacancies as well as their 'strain-induced' interactions, the temperature and concentration dependences of the nanoscale period d of respective modulated structures of vacancies' subsystem are analysed. As established, the temperature elevation leads to increase in the period $d(T)$ of such a structure (Fig. 6) due to an entropy factor as well as temperature dependences of both the energy parameters of '(electro)chemical' interactions of vacancies and the elasticity moduli of a host b.c.c.- Me crystal ($Me = Mo$ or Fe). With increasing average concentration of vacancies, \bar{c}_v , the temperature interval of existence of the modulated structure of their subsystem is extended.

Remark. The main novelty of presented results is the inequality $\lim_{\mathbf{k} \rightarrow 0} \tilde{w}(\mathbf{k}) \neq \tilde{w}(\mathbf{0}) \equiv \tilde{w}_n$ taken into account in a model at issue.

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МОДУЛЮВАННЯ РОЗПОДІЛУ ВЗАЄМОДІЙНИХ ВАКАНСІЙ У ПРУЖНЬО АНІЗОТРОПНИХ ОЦК-КРИСТАЛАХ ПІСЛЯ ОПРОМІНЕННЯ

Розглянуто спинодальний механізм можливого формування надгратниці нанопор в об'ємно-центрованому кубічному (ОЦК) кристалі після опромінення. Проаналізовано критерій формування модульованої структури із взаємодійних вакансій у пружньо анізотропних ОЦК-кристалах. Оцінено залежність періоду модульованої структури розчину вакансій в ОЦК-Мо та ОЦК-Fe від температури. Як показано, у випадку позитивного фактора анізотропії пружності ($\xi > 0$ для Мо, Nb, W) модульовані структури можуть бути сформовані в напрямку [111], а у випадку негативного фактора анізотропії пружності ($\xi < 0$ для ОЦК-Fe) модульовані структури можуть бути сформовані в напрямку [100]. Період модульованої структури в просторовому розподілі вакансій, утвореної через спинодальний механізм (у закритій системі вакансій), зростає з температурою і визначається ентропійним чинником, «(електро)хімічною» взаємодією вакансій і пружніми властивостями ОЦК-кристалу.

Ключові слова: вакансії, «деформаційна» взаємодія, «(електро)хімічна» взаємодія, спинодальний розпад, модульована структура

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МОДУЛИРОВАНИЕ РАСПРЕДЕЛЕНИЯ ВЗАИМОДЕЙСТВУЮЩИХ ВАКАНСИЙ В УПРУГО АНИЗОТРОПНЫХ ОЦК-КРИСТАЛЛАХ ПОСЛЕ ОБЛУЧЕНИЯ

Рассмотрен спинодальный механизм возможного формирования сверхрешётки нанопор в объёмно-центрированном кубическом (ОЦК) кристалле после облучения. Проанализирован критерий формирования модулированной структуры из взаимодействующих вакансий в упруго анизотропных ОЦК-кристаллах. Оценена зависимость периода модулированной структуры раствора вакансий в ОЦК-Мо и ОЦК-Fe от температуры. Как показано, в случае положительного фактора упругой анизотропии ($\xi > 0$ для Mo, Nb, W) модулированные структуры могут быть сформированы в направлении [111], а в случае отрицательного фактора упругой анизотропии ($\xi < 0$ для ОЦК-Fe) модулированные структуры могут быть сформированы в направлении [100]. Период модулированной структуры в пространственном распределении вакансий, образованной посредством спинодального механизма (в закрытой системе вакансий), растёт с температурой и определяется энтропийным фактором, «(электро)химическим» взаимодействием вакансий и упругими свойствами ОЦК-кристалла.

Ключевые слова: вакансии, «деформационное» взаимодействие, «(электро)химическое» взаимодействие, спинодальный распад, модулированная структура.