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Influence of Fluctuations of the Point-Defects' Generation Rate and Inhomogeneity of Irradiated F.C.C. Crystal on the Temperature Dependence of the Dissipative-Structure Period in a Spatial Distribution of Radiation Vacancies

O.V. Oliinyk[1,*], V.A. Tatarenko[1,†], P.O. Selyshchev[2], Y.B. Park[3]

[1] *G. V. Kurdyumov Institute for Metal Physics, Department of Solid State Theory, 36 Academician Vernadsky Blvd., UA-03680 Kyyiv-142, Ukraine*
[2] *University of Pretoria, Department of Physics,Private Bag X20, 0028 Hatfield, South Africa*
[3] *Department of Materials Science and Metallurgical Engineering, Nano Materials Research Center, Sunchon National University, Sunchon 540-742, Korea*

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A kinetic model for the influence of external noise, such as fluctuations of the point-defects' production rate and inhomogeneity of irradiated f.c.c. crystal, on the formation of modulated defect-distribution structure is considered. Defect-production rate and density of sinks for point defects are simulated as independent uniform and stationary stochastic fields with certain parameters. The interaction between vacancies is taken into account. Such stochastic fields can induce a spatial point-defects' distribution, which is a stationary uniform stochastic field. Its mean value and correlation functions are estimated, and restricting conditions are determined when this stochastic field becomes unstable because of interaction between defect-density fluctuations and a stochastic field with a spatially-periodic mean value is formed. A formula for evaluating its spatial period is analysed. This geometrical parameter of such a dissipative structure is determined also by kinetic characteristics.

Keywords: Vacancies, Dissipative structure, 'Electrochemical' interaction, Strain-induced interaction.

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1. INTRODUCTION

The main causes for the stochastic behaviour of radiation-defects' density are external ones. Firstly, these are fluctuations of the rate of defects' generation. Secondly, it is the random distribution of various imperfections of a crystal lattice, which serve as sinks for the point defects. Because of these, the fluctuations of the density of radiation point defects are essentially non-equilibrium. Unlike the thermodynamic fluctuations, they do not decrease in inverse proportion to a system size and can reach the noticeable values [1]. The role of random disturbances becomes especially important for systems with non-linear feedbacks between their elements, and for processes, which have a threshold character and bifurcation points [2].

In a given work, the analysis of the formation of the spatially-periodic structure of the radiation point-defects' distribution that occurs due to non-linear interdefect interaction, which was carried out in Refs. [3-5] and extended to irradiated solids with fluctuating parameters [2], is used to predict and consider the possible modulated structure in a spatial distribution of radiation defects formed in irradiated f.c.c. crystal. To describe the probabilistic nature of a point-defects' distribution, it is suggested to be a stochastic field, and for its description a stochastic differential equation is used. If the rate of production of defects and density of their sinks are modelled by the relevant random uniform stationary fields, the random distribution of point defects can also be homogeneous and stationary. However, under certain conditions of irradiation, it becomes unstable due to the interaction of fluctuations of a defects' density through the strain-induced ('elastic') fields and 'electrochemical' interaction between defects. Because of this, a stochastic field with a spatially-periodic behaviour of its average value is formed.

2. THE BASIC EQUATIONS

We consider an f.c.c. crystal in which due to an external irradiation the vacancies and self-interstitial atoms are randomly formed. Right after [2], the rate of generation of defects, $K(\mathbf{r}, t)$, is considered to be a random uniform and stationary function of spatial coordinates ($\mathbf{r}$) and time (t), respectively. Its average, $\langle K(\mathbf{r},t)\rangle = K_0(\approx 0.5\cdot 10^{-3} - 5\cdot 10^{-3}\mathrm{s}^{-1})$ and variance are the constants and supposed to be predetermined. Correlation functions of this field depend only on a difference of respective arguments, i.e. $\langle K(\mathbf{r},t)K(\mathbf{r}+\Delta\mathbf{r},t+\Delta t)\rangle = f(\Delta\mathbf{r},\Delta t)$, and their Fourier-transform components, i.e. the spectral densities, $G(\mathbf{k}, t)$, are also supposed to be given functions. The defects migrate and are absorbed by sinks (for instance, by dislocations, dislocation loops, *etc.*) with the density $\rho_{\mathrm{d}} = \rho_{\mathrm{d}}(\mathbf{r})$. As, due to the 'fast' migration of intrinsic interstitial atoms during the relaxation, their concentration in a bulk is rapidly decreasing, a residual concentration of self-interstitial atoms is comparatively small, atom-to-atom distances are large, and a total contribution of their interactions between themselves and with vacancies is much more weaker than contribution of interaction between vacancies. Then, neglecting both the former and the recombination of these point defects, the evolution of the density of 'slow' va-

* neutrino@ukr.net
† tatar@imp.kiev.ua

cancies (v), $n(\mathbf{r}, t)$, will be considered hereinafter and described by the following stochastic equation [2, 6]:

$$\frac{\partial n(\mathbf{r},t)}{\partial t} = K(\mathbf{r},t) - \beta(\mathbf{r})n(\mathbf{r},t) - (\nabla_{\mathbf{r}} \cdot \mathbf{j}(\mathbf{r},t)) \qquad (1)$$

($\nabla_{\mathbf{r}} = \partial/\partial\mathbf{r}$ is the Hamilton differentiation operator 'nabla'; (...·...) symbolizes the scalar product). Here $\beta(\mathbf{r}) = z_d D \rho_d(\mathbf{r})$ is the uniform random field, which describes the probability of an absorption of point defect by sinks [2], with $\langle\beta(\mathbf{r})\rangle = \beta_0$, the factor $z_d \approx 1$ for a vacancy, and the spectral density – $G_\beta(\mathbf{k})$,

$$\mathbf{j}(\mathbf{r},t) = -D\left\{\nabla_{\mathbf{r}} n(\mathbf{r},t) - \frac{n(\mathbf{r},t)\mathbf{F}(\mathbf{r},t)}{k_B T}\right\} \qquad (2)$$

is a vacancy-flux density vector [2, 5, 6], where $D = D_0\exp(-E_m/\{k_B T\})$ is the vacancy-diffusion coefficient (diffusivity), E_m is the migration-activation energy, T is the temperature of an irradiated specimen, k_B is the Boltzmann constant, $\mathbf{F}(\mathbf{r},t) = -\nabla_{\mathbf{r}}\int W^{vv}(\mathbf{r}-\mathbf{r}')n(\mathbf{r}',t)d\mathbf{r}'$ is the force of interaction between the vacancy located at the point $\mathbf{r}$ with all other vacancies with co-ordinates $\{\mathbf{r}'\}$, $W^{vv}(\mathbf{r} - \mathbf{r}')$ is the pairwise-interaction energy of vacancies at the points $\mathbf{r}$ and $\mathbf{r}'$.

Separating in (1) the deterministic and fluctuation-noise components of $n(\mathbf{r}, t)$, $\beta(\mathbf{r})$, and $K(\mathbf{r}, t)$, we have a following set of equations [2, 6]:

$$\frac{\partial \bar{n}(\mathbf{r},t)}{\partial t} = K_0 - \beta_0(\mathbf{r})\bar{n}(\mathbf{r},t) - \left\langle\tilde{\beta}(\mathbf{r})\tilde{n}(\mathbf{r},t)\right\rangle + D\Delta\bar{n}(\mathbf{r},t) +$$

$$+\frac{D}{k_B T}\ \nabla_{\mathbf{r}}\cdot\int \bar{n}(\mathbf{r},t)\bar{n}(\mathbf{r}',t)\nabla_{\mathbf{r}}W^{vv}(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\ +$$

$$+\frac{D}{k_B T}\ \nabla_{\mathbf{r}}\cdot\int \left\langle\tilde{n}(\mathbf{r},t)\tilde{n}(\mathbf{r}',t)\right\rangle\nabla_{\mathbf{r}}W^{vv}(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\ , \qquad (3)$$

$$\frac{\partial \tilde{n}(\mathbf{r},t)}{\partial t} = \tilde{K}(\mathbf{r},t) - \beta_0\tilde{n}(\mathbf{r},t) - \tilde{\beta}(\mathbf{r})\bar{n}(\mathbf{r},t) + D\Delta\tilde{n}(\mathbf{r},t) +$$

$$+\frac{D}{k_B T}\ \nabla_{\mathbf{r}}\cdot\int \tilde{n}(\mathbf{r},t)\bar{n}(\mathbf{r}',t)\nabla_{\mathbf{r}}W^{vv}(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\ +$$

$$+\frac{D}{k_B T}\ \nabla_{\mathbf{r}}\cdot\int \bar{n}(\mathbf{r},t)\tilde{n}(\mathbf{r}',t)\nabla_{\mathbf{r}}W^{vv}(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\ +$$

$$+\left\langle\tilde{\beta}(\mathbf{r})\tilde{n}(\mathbf{r},t)\right\rangle - \tilde{\beta}(\mathbf{r})\tilde{n}(\mathbf{r},t) +$$

$$+\frac{D}{k_B T}\ \nabla_{\mathbf{r}}\cdot\int\ \tilde{n}(\mathbf{r},t)\tilde{n}(\mathbf{r}',t) - \left\langle\tilde{n}(\mathbf{r},t)\tilde{n}(\mathbf{r}',t)\right\rangle\ \nabla_{\mathbf{r}}W^{vv}(\mathbf{r}-\mathbf{r}')d\mathbf{r}'\ , \qquad (4)$$

where $\Delta \equiv (\nabla_{\mathbf{r}}\cdot\nabla_{\mathbf{r}})$ is the Laplace operator, and

$$\tilde{n}(\mathbf{r},t) = n(\mathbf{r},t) - \bar{n}(\mathbf{r},t), \tilde{\beta}(\mathbf{r},t) = \beta(\mathbf{r}) - \beta_0,$$

$$\tilde{K}(\mathbf{r},t) = K(\mathbf{r},t) - K_0\,.$$

3. THE RANDOM UNIFORM STATIONARY FIELD OF DEFECTS' DENSITY

Amongst the solutions of Eq. (1) or the set of Eqs. (3) and (4), there can be a solution, which is a random uniform stationary field – $n_0(\mathbf{r}, t)$. The average density of vacancies for it, $\langle n_0(\mathbf{r},t)\rangle = \bar{n}_0$ is constant in space and in time, and the correlation function of a defects' density depends only on a difference of arguments [2].

Then, for the average value n_0, we have [2]

$$K_0 - \beta_0 n_0 - \left\langle\tilde{\beta}(\mathbf{r})\tilde{n}_0(\mathbf{r},t)\right\rangle = 0. \qquad (5)$$

Neglecting the fluctuations of a product of stochastic functions, we solve Eq. (4) and construct the correlation functions as follows [2]:

$$\left\langle\tilde{\beta}(\mathbf{r})\tilde{n}_0(\mathbf{r},t)\right\rangle = \bar{n}_0\int\frac{G_\beta(\mathbf{k})}{\lambda(\mathbf{k};n_0)}, \qquad (6)$$

$$\left\langle\tilde{n}_0(\mathbf{r},t_1)\tilde{n}_0(\mathbf{r}',t_2)\right\rangle = \bar{n}_0^2\int\frac{G_\beta(\mathbf{k})\cdot e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}d\mathbf{k}}{\lambda^2(\mathbf{k};n_0)} +$$

$$+\int d\mathbf{k}e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')+\lambda(\mathbf{k})(t_1-t_2)}\int_{-\infty}^{t_1-t_2}d\tau_1 e^{-2\lambda(\mathbf{k})\tau_1}\int_{-\infty}^{t_1}d\tau_2 G(\mathbf{k},\tau_2)e^{-\lambda(\mathbf{k})\tau_2}, \qquad (7)$$

where $\lambda(\mathbf{k}) \equiv \lambda(\mathbf{k};\bar{n}_0) = -\left[k^2 D\left\{1 + \frac{\bar{n}_0\tilde{W}^{vv}(\mathbf{k})}{k_B T}\right\} + \beta_0\right]$,

$$\tilde{W}^{vv}(\mathbf{k}) = \int W^{vv}(\mathbf{r})\exp(-i\mathbf{k}\cdot\mathbf{r})d\mathbf{r}\,. \qquad (8)$$

The equations (5), (6) form a closed system for $n_0(\mathbf{r}, t)$ and together with expression (7) completely describe a random homogeneous stationary field of the density of defects within the correlation approximation.

For the determination of stability conditions for a random uniform stationary field, let us consider the evolution of a small perturbation of a probability distribution of the density of vacancies, at which the perturbation of average value is $\delta\bar{n}(\mathbf{r},t)$ ($\propto\exp\{\lambda_f t + i\mathbf{k}\cdot\mathbf{r}\}$ with a damping factor $\lambda_f = \lambda_f(\mathbf{k})$), and a perturbation of the fluctuation part is $\delta\tilde{n}(\mathbf{r},t)$ [2]. Due to the anisotropy of an f.c.c. crystal, the interaction-energy Fourier component, $\tilde{W}^{vv}(\mathbf{k})$, reaches a minimum value for a particular crystallographic direction. Therefore, with a change of parameters, for instance, the temperature of an irradiated specimen (and/or its content), one of the modes will become unstable with a wave vector $\mathbf{k} = \mathbf{k}_c$ having the same direction. Among other factors, it allows to restrict the analysis of stability to one-dimensional perturbations by directing Ox axis along $\mathbf{k}_c$. Substituting $\bar{n}(x,t) = \bar{n}_0 + \delta\bar{n}(x,t)$ into Eq. (3) and $\tilde{n}(x,t) = \tilde{n}_0 + \delta\tilde{n}(x,t)$ in Eq. (4), we obtain the equations of the evolution of small perturbations of the average value and fluctuations of a homogeneous stationary random distribution of point defects [2, 6]

$$\frac{\partial\delta\bar{n}(x,t)}{\partial t} = -\beta_0\delta\bar{n}(x,t) - \left\langle\tilde{\beta}(x)\delta\tilde{n}(x.t)\right\rangle + D\frac{\partial^2}{\partial x^2}\delta\bar{n}(x.t) + \frac{Dn_0}{k_B T}\int\delta\bar{n}(x',t)\frac{\partial^2}{\partial x^2}W^{vv}(x-x')dx' +$$

$$+\frac{D}{k_BT}\frac{\partial}{\partial x}\int \left\langle \tilde{n}_0(x,t)\delta\tilde{n}(x',t)\right\rangle + \left\langle \delta\tilde{n}(x,t)\tilde{n}_0(x',t)\right\rangle \frac{\partial}{\partial x}W^{vv}\ \ x-x'\ dx', \tag{9}$$

$$\frac{\partial\delta\tilde{n}(x.t)}{\partial t} = -\beta_0\delta\bar{n}(x,t) + D\frac{\partial^2}{\partial x^2}\delta\tilde{n}(x,t) +$$

$$+\frac{Dn_0}{k_BT}\frac{\partial^2}{\partial x^2}\int \delta\tilde{n}(x',t)W^{vv}(x-x')dx' - \tilde{\beta}(x)\delta\bar{n}(x,t) +$$

$$+\frac{D}{k_BT}\frac{\partial}{\partial x}\left\{\tilde{n}_0(x,t)\int \delta\bar{n}(x',t)\frac{\partial W^{vv}(x-x')}{\partial x}dx' + \delta\bar{n}(x,t)\int \tilde{n}_0(x',t)\frac{\partial W^{vv}(x-x')}{\partial x}dx'\right\}. \tag{10}$$

The set of Eqs. (9), (10) has variable coefficients and is not closed, as it contains $\left\langle\tilde{\beta}(x)\delta\tilde{n}(x,t)\right\rangle$ and $\left\langle\tilde{n}_0(x,t)\delta\tilde{n}(x',t)\right\rangle$ [2]. But, as in Eq. (10), the variable coefficients are only at $\delta\bar{n}(x,t)$ we consider the relevant terms as a inhomogeneity and find $\delta\tilde{n}(x,t)$, which is now a functional of $\delta\bar{n}(x,t)$. Then, we substitute it in Eq. (9) and by averaging obtain the following expression for a damping decrement of above-mentioned perturbations [2]:

$$\lambda_{\rm f}(\mathbf{k}) = \lambda(\mathbf{k}) + \int d\mathbf{k}'\frac{G_\beta(\mathbf{k}')}{(\lambda_{\rm f}(\mathbf{k})-\lambda(\mathbf{k}-\mathbf{k}'))}\left[-\frac{n_0DS_1(\mathbf{k},\mathbf{k}')}{k_BT\lambda(\mathbf{k}')}-1\right]\left[-\frac{n_0DS_2(\mathbf{k},\mathbf{k}')}{k_BT\lambda(\mathbf{k}')}-1\right]+S\,, \tag{11}$$

where

$$S = \frac{D^2}{(k_BT)^2}\int_{-\infty}^{0}d\tau_1\int_{-\infty}^{0}d\tau_2\int_{-\infty}^{0}d\tau_3\int d\mathbf{k}S_1(\mathbf{k},\mathbf{k}')S_2(\mathbf{k},\mathbf{k}')G(\mathbf{k}',\tau_1-\tau_2-\tau_3)\exp\{-\lambda(\mathbf{k}')(\tau_1+\tau_2)+(\lambda_{\rm f}(\mathbf{k})-\lambda(\mathbf{k}-\mathbf{k}'))\tau_3\},$$

$$S_1(\mathbf{k},\mathbf{k}') = ((\mathbf{k}-\mathbf{k}')\cdot\{\mathbf{k}\tilde{W}^{vv}(\mathbf{k})-\mathbf{k}'\tilde{W}^{vv}(\mathbf{k}')\}),$$

$$S_2(\mathbf{k},\mathbf{k}') = (\mathbf{k}\cdot\{\mathbf{k}'\tilde{W}^{vv}(\mathbf{k}')-(\mathbf{k}'-\mathbf{k})\tilde{W}^{vv}(\mathbf{k}-\mathbf{k}')\}).$$

In the derivation of expression (11), the statistical independence of $\tilde{\beta}(\mathbf{r})$ and $\tilde{K}(\mathbf{r},t)$ was supposed, *i.e.* their mutual correlation function and the relevant spectral density were taken to be equal to zero. Evidently, the damping decrement $\lambda_{\rm f}$ is a function of $\mathbf{k}$. If the energy of thermal motion of vacancies considerably exceeds the energy of their force interaction, $\lambda_{\rm f}<0$ for any mode. Nevertheless, with decreasing temperature for some $\mathbf{k}=\mathbf{k}_{\rm c}$ (where $\tilde{W}^{vv}(\mathbf{k}_{\rm c})<0$), the damping decrement passing through zero becomes positive (as amplification factor), the instability in relation to the transition to a probability distribution with an average, the period of spatial change of which being equal to $2\pi/|\mathbf{k}_{\rm c}|$ [2].

We consider the conditions for a spatially-periodic (inhomogeneous) distribution of the defects' density to arise in their stochastic formation. To obtain further results a form of a spectral density should be rendered concrete. For the Gauss temporal spectrum $G(\mathbf{k},t)\propto\exp(-\sigma t^2)$, there will be an unstable mode and the homogeneous stationary random field of a defects' density will not be realized. Let us consider the case when fluctuations of a rate of defect-production in time and in space are statistically independent and small so that the period of a structure of a defects' density which arises is close to a deterministic one and much more than a radius of their correlation, $r_{\rm cor}$, and the time of their correlation, $\tau_{\rm cor}$, is much less of all characteristic times of a problem. Then for the component in (11) caused by fluctuations we have [2]

$$S = \frac{D^2}{2(k_BT)^2}\int d\mathbf{k}'\frac{G(\mathbf{k}')S_1(\mathbf{k},\mathbf{k}')S_2(\mathbf{k},\mathbf{k}')\tau_{\rm cor}}{\lambda(\mathbf{k}')(\lambda(\mathbf{k}')+\lambda(\mathbf{k}-\mathbf{k}'))}. \tag{12}$$

In the stochastic description, it is not possible to reduce parameters $\bar{n}_0$, $\tilde{W}_{\mathbf{0}}^{vv}$, T to the one parameter—$\alpha=\bar{n}_0\tilde{W}_{\mathbf{0}}^{vv}/(k_BT)$, where $\tilde{W}_{\mathbf{0}}^{vv}=\max\limits_{\{\mathbf{n}\}}\lim\limits_{\mathbf{k}\to\mathbf{0}}\left|\tilde{W}^{vv}(\mathbf{k})\right|$. We will search for conditions of the development of instability by changing K_0 ($\lambda_{\rm f}$ depends on K_0 only through α), and the temperature and coefficient of a variation of the rate of a creation of displacements $\sqrt{\left\langle\tilde{K}^2\right\rangle}/K_0$ will be considered as fixed [2].

Correspondingly, the radius of correlation and the time of correlation may be evaluated as follows [7, 8]**:**

$$r_{\rm cor} = \frac{\int\left\langle K(\mathbf{r},t)K(\mathbf{r}+\Delta\mathbf{r},t)\right\rangle d(\Delta\mathbf{r})}{\left\langle K^2(\mathbf{r},t)\right\rangle},$$

$$\tau_{\rm cor} = \frac{\int\left\langle K(\mathbf{r},t)K(\mathbf{r},t+\Delta t)\right\rangle d(\Delta t)}{\left\langle K^2(\mathbf{r},t)\right\rangle}.$$

A condition of the development of instability obtained without taking into account the fluctuations is the following:

$$\lambda(\mathbf{k};\alpha)\equiv-\left[k^2D\ 1+\alpha\tilde{U}(\mathbf{k})\ +\beta_0\right]=0\,, \tag{13}$$

$\tilde{U}(\mathbf{k}) = \tilde{W}^{vv}(\mathbf{k}) / \tilde{W}_{\mathbf{0}}^{vv}$. The properties of an even function $\lambda(\mathbf{k}; \alpha)$ are investigated in detail in [3, 5]. If $\alpha < 1$, then $\lambda(\mathbf{k}; \alpha) < 0$. At $\alpha = 1$ at a point $\mathbf{k} = \mathbf{k}_m$, there is a extremum. $|\mathbf{k}_m|$ monotonously increases with increasing α, and the value of $\lambda(\mathbf{k}_m; \alpha)$ increases and becomes equal to zero at $\alpha = \alpha_{cr}$ and $\mathbf{k} = \mathbf{k}_{cr}$ [2, 6]. Because of this the integrand in (12), decreasing with an increase of k as $\propto k^2$ is localised within the interval $(-|\mathbf{k}_m|, |\mathbf{k}_m|)$ provided that $|\mathbf{k}_m| \le |\mathbf{k}_{cr}|$. The damping decrement λ_f will become zero at $\alpha \le \alpha_{cr}$, because the numerator of an integrand in (11) is non-negative within the interval $(-|\mathbf{k}_m|, |\mathbf{k}_m|)$, and $S > 0$ [2]. It is also clear from this consideration that in a region of stability $\lambda(\mathbf{k}; \alpha) < 0$ for all $\mathbf{k}$.

The value of $\mathbf{k}_{cr}$ is that, for the large-scale inhomogeneity of sinks' distribution when k_0 is small, $\tilde{W}^{vv}(\mathbf{k}_{cr}) \approx \tilde{W}_{\mathbf{n}}^{vv} \equiv \lim_{\mathbf{k}\to\mathbf{0}} \tilde{W}^{vv}(\mathbf{k})$, where $\mathbf{k} \to \mathbf{0}$ along the direction $\mathbf{n}_{cr} \equiv \mathbf{k}_{cr}/|\mathbf{k}_{cr}|$. If a distance between the defects largely exceeds the host-lattice period, the Fourier components, $\tilde{W}^{vv}(\mathbf{k})$, of the interaction energies for vacancies can be written as a power series:

$$\tilde{W}^{vv}(\mathbf{k}) \approx \tilde{V}^{vv}(\mathbf{k}) + \tilde{\varphi}^{vv}_{\text{el.chem}}(\mathbf{k}) \cong \tilde{w}^{vv}_{\mathbf{n}} + \tilde{\beta}^{vv}(\mathbf{n})k^2 + \ldots \quad (14)$$

$\tilde{V}^{vv}(\mathbf{k})$ is the Fourier component of strain-induced v–v-interaction energies. Within the small finite region near $\mathbf{k} \cong \mathbf{0}$, $\tilde{V}^{vv}(\mathbf{k})$ may be represented as follows [9, 10]: $\tilde{V}^{vv}(\mathbf{k}) \cong A^{vv}(\mathbf{n}) + B^{vv}(\mathbf{n})k^2 + Q^{vv}$. Here, the well-known first term is based on the long-wave-limit approximation [9, 10]; the second term is a correction to this approximation [10, 11], and the third term is a gauge, which eliminates a strain-induced self-action of the vacancies [9, 12]. The coefficient $B^{vv}(\mathbf{n})$ was derived in revised form in Ref. [11]. $\tilde{\varphi}^{vv}_{\text{el.chem}}(\mathbf{k})$ is the Fourier component of energies for direct 'electrochemical' v–v-interactions. Within both the long-wavelength approximation and the cohesive-energy-estimation approach developed in Refs. [13–17], $\tilde{\varphi}^{vv}_{\text{el.chem}}(\mathbf{k}) \cong \tilde{\varphi}^{vv}_{\text{el.chem}}(\mathbf{0}) + \gamma^{vv}k^2$ [17], $\tilde{\beta}^{vv}(\mathbf{n}) \cong B^{vv}(\mathbf{n}) + \gamma^{vv}$ is the expansion coefficient in Eq. (13) ($\mathbf{n} \equiv \mathbf{k}/k$), $\tilde{w}_{\mathbf{n}} \cong A^{vv}(\mathbf{n}) + Q^{vv} + \tilde{\varphi}^{vv}_{\text{el.chem}}(\mathbf{0})$.

As shown in Ref. [17], the coefficient $B^{vv}(\mathbf{n})$ and hence, $\tilde{\beta}^{vv}(\mathbf{n})$ have the minimum values along the direction (100) for f.c.c. crystal, when $\mathbf{k} \to \mathbf{0}$. The Fourier component of v–v-interaction energies along the direction (100) within the small finite region near $\mathbf{k} = \mathbf{0}$ may be represented as follows:

$$\tilde{W}(\mathbf{k}) \approx \tilde{W}^{vv}_{\mathbf{0}}(-1 + \mathscr{B}^{vv}(100)k^2),$$

where $\mathscr{B}^{vv}(100) = \tilde{\beta}^{vv}(100) / \tilde{W}^{vv}_{\mathbf{0}}$.

In a numerator of an integrand in (12), we will be restricted to the first term of an expansion, and in, $\lambda(\mathbf{k}; \alpha)$ (13), to the second term because it determines $\mathbf{k}_m$ [2]. Going to (12) from an integration to the summation and taking into account $G\ \mathbf{0},0\ = \langle\tilde{K}^2\rangle r_{\text{cor}}\tau_{\text{cor}}$ [2], then substituting (12) into (11) and keeping the terms of the same order of smallness, we find [2]

$$\alpha_c \equiv \frac{K_{0c}\tilde{W}^{vv}_0}{\beta(T)k_BT} = \alpha_{cr} - \frac{1}{2}\sqrt{b(T)\rho_d^{5/4}\mathscr{B}^{vv}(100)^{-1/4}},$$

$$k_c^2 = k_{cr}^2\left(1 - \frac{1}{4}\sqrt{b(T)\rho_d^{1/4}\mathscr{B}(100)^{-5/4}}\right),$$

where $b(T) = r_{\text{cor}}\tau_{\text{cor}}D(T)\langle\tilde{K}^2\rangle / K_0^2$ [2].

REFERENCES

1. V. Herstemke and R. Lefebvre, *Noise-Induced Transitions* (Moscow: Mir: 1987) (in Russian).
2. P. A. Selishchev, *Metallofiz. Noveishie Tekhnol.* **21** No9, 11 (1999) (in Russian)
3. V.J. Sugakov, *Preprint ITF-84-70*, ITPh AS Ukr.SSR, Kiev, 1984 (in Russian).
4. P. A. Selishchev, V. I. Sugakov, *Radiat. Eff. and Defects in Solids* **133**, 231 (1995).
5. V.J. Sugakov, *Fundamentals of Synergetics*, (Kyyiv: Oberegy: 2001) (in Ukraine).
6. P. A. Selishchev, *Self-Organization in Radiation Physics*, (Kiev: Aspekt-Poligraf: 2004) (in Russian).
7. P.A. Selishchev, D.V. Shchur, *Bulletin of Kyiv University. Ser. Phys-Math. Science* **2**, 505 (1999) (in Ukraine).
8. I. A. Kvasnikov, *Thermodynamics and Statistical Physics. Theory of Non-Equilibrium Systems* (Moscow: MGU: 1987) (in Russian).
9. A.G. Khachaturyan, *Theory of Structural Transformations in Solids* (Mineola, NY: Dover Publications, Inc.: 2008).
10. A.A. Katsnelson, A.I. Olemskoi, *Microscopic Theory of Nonhomogeneous Structures* (Moscow: Mir Publ.: 1990).
11. O.V. Oliinyk, V.A. Tatarenko, S.M. Bokoch, *Metallofiz. Noveishie Tekhnol.* **33** No10, 1383 (2011) (in Ukrainian); Erratum, *ibidem*, **34** No1, 137 (2012).
12. V.A. Tatarenko, C.L. Tsinman, *Physics of Real Crystals*, 244 (Kiev: Naukova Dumka: 1992) (in Russian).
13. V.G. Weizer and L.A. Girifalco, *Phys. Rev.* **120** No3, 837 (1960).
14. R. Yamamoto and M. Doyama, *J. Phys. F: Metal Phys.* **3** No8, 1524 (1973).
15. W.A. Harrison, *Pseudopotentials in the Theory of Metals* (New York: W.A. Benjamin, Inc.: 1966).
16. W.A. Harrison, *Solid State Theory* (New York: McGraw-Hill: 1970).
17. O.V. Oliinyk, V.A. Tatarenko, *J. Nano- Electron. Phys.* **4** No1, 01023 (2012).