The evolution of the nanoscale dissipative structures in a distribution of defects within the isothermally irradiated f.c.c. crystal

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A kinetic model for the influence of external noises such as fluctuations of the vacancies' generation rate and inhomogeneity of irradiated f.c.c. crystal on the formation of nanoscale modulated dissipative structure in a spatial distribution of vacancies is considered. The generation rate of vacancies all over the sites and a density of their dislocation-type sinks are modelled as independent random uniform stationary fields and with certain defined parameters of fluctuation correlations—spatial and temporal ones. Such stochastic fields can induce a spatial redistribution of vacancies that can lead to their density stationary uniform field or stochastic one. By the average value and correlation functions of these fluctuations, the conditions are determined for interacting fluctuations of the vacancies' density, under which this homogeneous random field becomes unstable in relation to the stochastic field with a spatially periodic mean distribution of vacancies' density. For instance, with f.c.c. nickel as a model of the irradiated functional material, the temperature dependence of spatial period $d(T)$ of the modulated dissipative structure of vacancies' subsystem in f.c.c. crystal is numerically forecasted and analysed, taking into account the total ('electrochemical' + 'strain-induced') interaction between vacancies. Such $d(T)$-dependence is also determined by the kinetic characteristics of vacancies' redistribution.

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1. Introduction

The main causes for the stochastic behaviour of radiation-defects’ density within the irradiated crystalline materials 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, 3].

In a given paper, the analysis of formation of the spatially periodic structure of the radiation point defects’ distribution that occurs due to non-linear interaction between the defects, which was carried out in Refs. [3–5] and extended to irradiated solids with fluctuating parameters [2, 3], is used to predict and consider the possible dissipative 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 [2–5] 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 [2, 3]. However, under certain conditions of irradiation, it becomes unstable due to the interaction of fluctuations of a defects’ density through the ‘strain-induced’ fields and ‘electrochemical’ interaction between defects. Because of these ones, a stochastic density field with a spatially periodic behaviour of its average value is formed [2, 3, 5].

Besides, in a given paper, the analogy between formations of the superlattice of nanovoids and the spatial ordered distribution of point defects (first of all, vacancies) is drawn. For the first time, such an analogy was noted by Chang [6, 7], using atomistic methods. In his opinion, vacancies are quasi-particles, which, due to their elastic interaction, array into superlattice of vacancies under radiation, *i.e.* interaction between vacancies is similar to interaction between atoms, as approved in Ref. [8–11], and vacancies have the same redistribution kinetics as for host-crystal atoms.

Formation of a superlattice of nanovoids is an intrinsic property of many crystalline materials under irradiation. This property is technologically important in respect to operations and maintenance of nuclear reactor materials as well as to applications of functional materials under irradiation, since a material having strong tendency to form a vacancy superlattice is expected to be resistant to the radiative swelling. Although nickel is of great technological importance because of its use as a host crystal for many functional materials, its defect-microstructure properties are not investigated as well as those of other f.c.c. metals. In attempt to obtain an understanding of the radiation-defects’ behaviour in course of formation of nanoscale modulated dissipative structures, in a given paper, the numerical calculations for f.c.c. Ni with vacancies are carried out.

2. Target setting and master 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 [2–5], the rate of generation of defects, $K(\boldsymbol{r},t)$, is considered to be a random uniform and stationary function of spatial coordinates ($\boldsymbol{r}$) and time (t), respectively. Its average, $\langle K(\boldsymbol{r},t)\rangle = K_0$, 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.* $\langle K(\boldsymbol{r},t)K(\boldsymbol{r}',t')\rangle = C_K(\boldsymbol{r}-\boldsymbol{r}',t-t')$, and their Fourier-transform components, *i.e.* the spectral densities, $G(\boldsymbol{k},t)$, are also supposed to be given functions [2, 3].

The defects migrate and are absorbed by sinks (for instance, by dislocations, dislocation loops, *etc.*). 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, the relevant atom-to-atom distances are large, and a total internal-energy contribution of interactions of self-interstitial atoms with each other and with vacancies is much weaker than contribution of interaction between vacancies [2–4]. Then, neglecting both the self-interstitial atoms' energy contributions and the recombination of mentioned point defects, the evolution of the density of 'slow' vacancies (v), $n(\boldsymbol{r},t)$, will be considered hereinafter and described by the following stochastic equation [2, 3]:

$$\frac{\partial n(\boldsymbol{r},t)}{\partial t} = K(\boldsymbol{r},t) - \beta(\boldsymbol{r})n(\boldsymbol{r},t) - (\nabla_r \cdot \boldsymbol{j}(\boldsymbol{r},t)) \tag{1}$$

($\nabla_{\boldsymbol{r}} \equiv \partial/\partial\boldsymbol{r}$ is the Hamilton differentiation operator 'nabla'; (...·...) symbolizes the scalar product). Here, $\beta(\boldsymbol{r}) = z_d\rho_d(\boldsymbol{r})D_v$ is the random field, which describes the probability of an absorption of point defect by sinks with density $\rho_d(\boldsymbol{r})$ and the preferable absorption coefficient z_d (i.e. a coefficient characterizing efficiency of interaction of vacancies with dislocations) [2, 3],

$$\boldsymbol{j}(\boldsymbol{r},t) = -D_v\left\{\nabla_r n(\boldsymbol{r},t) - \frac{n(\boldsymbol{r},t)\boldsymbol{F}(\boldsymbol{r},t)}{k_B T}\right\}$$

is a vacancy-flux density vector [2–5], where $D_v = D_0\exp(-E_m/\{k_B T\})$ 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, $\boldsymbol{F}(\boldsymbol{r},t) = -\nabla_{\boldsymbol{r}} \int W^{vv}(\boldsymbol{r}-\boldsymbol{r}')n(\boldsymbol{r}',t)\mathrm{d}\boldsymbol{r}'$ is the force of interaction between the vacancy located at the point $\boldsymbol{r}$ with all other vacancies with coordinates $\{\boldsymbol{r}'\}$ [2–5, 15], $W^{vv}(\boldsymbol{r}-\boldsymbol{r}') \approx \varphi^{vv}_{\mathrm{el.chem}}(\boldsymbol{r}-\boldsymbol{r}') + V^{vv}(\boldsymbol{r}-\boldsymbol{r}')$ is the energy of pairwise interactions of vacancies at the points $\boldsymbol{r}$ and $\boldsymbol{r}'$, which consists of, at least, two dominating contributions—'electrochemical' ($\varphi^{vv}_{\mathrm{el.chem}}(\boldsymbol{r}-\boldsymbol{r}')$) and 'strain-induced' ($V^{vv}(\boldsymbol{r}-\boldsymbol{r}')$) ones, which are basically of the cohesive and elastic natures at short-range and long-range distances $|\boldsymbol{r}-\boldsymbol{r}'|$ between vacancies, respectively [8–11, 16–18].

Pro hac vice, the master equation (1) may be solved with the use of periodic boundary conditions [2, 3]. (In this case, the characteristics of a stochastic field of the density of interstitial atoms are also simply determined.)

Further, it is assumed that temperature–concentration relationship is weak, and thermal changes can be neglected ($\frac{\mathrm{d}T}{\mathrm{d}t} \to 0$) due to effective heat exchange with thermostat and neglecting recombination of interstitial atoms with vacancies in course of the microstructure evolution.

In equation (1), separating the deterministic ($\bar{n}(\boldsymbol{r},t)$) and fluctuation-noise

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[*] By definition, migration-activation energy of vacancies is a height of the potential barrier separating the initial and final positions of the atom near vacancy, which is jumping into this vacant site [12–14]. As assumed within the model taking into account the effects of dilation in the vicinity of vacancy, for transition of the oscillating atom into the neighbouring vacancy, it is not required to impart additional energy to 'ascend' an intermediate neighbouring saddle of an intracrystalline potential relief, but it is sufficiently wait for such fluctuation, at which neighbouring atoms forming this saddle by their fields will part so that the saddle will 'sag', its height will go to zero, and the atom will pass into the neighbouring vacant site without obstruction. Energy of formation of such fluctuation, at which width of formed interstitial clearance is equal to diameter of the atom passing through it, can be estimated within the scope of the linear theory of elasticity taking into account anisotropy of a crystal, without adjustable parameters [12–14].

($\tilde{n}(\boldsymbol{r},t)$) components of $n(\boldsymbol{r},t)$, $K(\boldsymbol{r},t)$, $\beta(\boldsymbol{r})$, we have a following set of equations [2, 3]:

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

$$+\frac{D_v}{k_BT}\left(\nabla_{\boldsymbol{r}}\cdot\int\bar{n}(\boldsymbol{r},t)\bar{n}(\boldsymbol{r}',t)\nabla_{\boldsymbol{r}}W^{vv}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\right)+$$

$$+\frac{D_v}{k_BT}\left(\nabla_{\boldsymbol{r}}\cdot\int\left\langle\tilde{n}(\boldsymbol{r},t)\tilde{n}(\boldsymbol{r}',t)\right\rangle\nabla_{\boldsymbol{r}}W^{vv}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\right),\qquad(2)$$

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

$$+\frac{D_v}{k_BT}\left(\nabla_{\boldsymbol{r}}\cdot\int\tilde{n}(\boldsymbol{r},t)\bar{n}(\boldsymbol{r}',t)\nabla_{\boldsymbol{r}}W^{vv}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\right)+$$

$$+\frac{D_v}{k_BT}\left(\nabla_{\boldsymbol{r}}\cdot\int\bar{n}(\boldsymbol{r},t)\tilde{n}(\boldsymbol{r}',t)\nabla_{\boldsymbol{r}}W^{vv}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\right)+\left\langle\tilde{\beta}(\boldsymbol{r})\tilde{n}(\boldsymbol{r},t)\right\rangle-\tilde{\beta}(\boldsymbol{r})\tilde{n}(\boldsymbol{r},t)+$$

$$+\frac{D_v}{k_BT}\left(\nabla_{\boldsymbol{r}}\cdot\int\left\{\tilde{n}(\boldsymbol{r},t)\tilde{n}(\boldsymbol{r}',t)-\left\langle\tilde{n}(\boldsymbol{r},t)\tilde{n}(\boldsymbol{r}',t)\right\rangle\right\}\nabla_{\boldsymbol{r}}W^{vv}(\boldsymbol{r}-\boldsymbol{r}')\mathrm{d}\boldsymbol{r}'\right);\qquad(3)$$

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

$$\bar{n}(\boldsymbol{r},t)=\left\langle n(\boldsymbol{r},t)\right\rangle,\ K_0=\left\langle K(\boldsymbol{r},t)\right\rangle,$$

$$\beta_0=\left\langle\beta(\boldsymbol{r})\right\rangle,\ \tilde{n}(\boldsymbol{r},t)=n(\boldsymbol{r},t)-\bar{n}(\boldsymbol{r},t),\ \tilde{K}(\boldsymbol{r},t)=K(\boldsymbol{r},t)-K_0,\ \tilde{\beta}(\boldsymbol{r})=\beta(\boldsymbol{r})-\beta_0.$$

3. The stationary random uniform field of vacancies' density

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

$$K_0 - \beta_0 n_0 - \langle \tilde{\beta}(\boldsymbol{r})\tilde{n}_0(\boldsymbol{r},t)\rangle = 0. \tag{4}$$

Neglecting the fluctuations of a product of stochastic functions, we solve equation (3) and construct the correlation functions as follows [2]:

$$\langle \tilde{\beta}(\boldsymbol{r})\tilde{n}_0(\boldsymbol{r},t)\rangle = \bar{n}_0 \int \frac{G_\beta(\boldsymbol{k})}{\lambda(\boldsymbol{k};\bar{n}_0)} \mathrm{d}\boldsymbol{k}\,, \tag{5}$$

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

$$+\int \mathrm{d}\boldsymbol{k} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')+\lambda(\boldsymbol{k})(t_1-t_2)} \int_{-\infty}^{t_1-t_2} \mathrm{d}\tau_1 e^{-2\lambda(\boldsymbol{k})\tau_1} \int_{-\infty}^{\tau_1} \mathrm{d}\tau_2 G(\boldsymbol{k},\tau_2) e^{-\lambda(\boldsymbol{k})\tau_2}\,, \tag{6}$$

where

$$\lambda(\boldsymbol{k}) \equiv \lambda(\boldsymbol{k};\bar{n}_0) = -\left[k^2 D_v \left\{ 1 + \frac{\bar{n}_0 \tilde{W}^{vv}(\boldsymbol{k})}{k_B T} \right\} + \beta_0 \right],\ \tilde{W}^{vv}(\boldsymbol{k}) = \int W^{vv}(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \mathrm{d}\boldsymbol{r}\,.$$

The equations (4), (5) form a closed system for $n_0(\boldsymbol{r},t)$ and together with expression (6) completely describe a random homogeneous stationary field of the density of defects within the correlation approximation [2, 3].

4. Instability of a uniform distribution of vacancies in presence of fluctuations of the point-defects' generation rate and inhomogeneity of irradiated f.c.c. crystal

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 $\delta\bar{n}(\boldsymbol{r},t)\propto\exp\{\lambda_{\mathrm{f}}t+i\boldsymbol{k}\cdot\boldsymbol{r}\}$ (with a damping factor $\lambda_{\mathrm{f}}=\lambda_{\mathrm{f}}(\boldsymbol{k})$), and a perturbation of the fluctuation part is $\delta\tilde{n}(\boldsymbol{r},t)$ [2, 3]. Due to the anisotropy of f.c.c. crystal, the interaction-energy Fourier component, $\tilde{W}^{vv}(\boldsymbol{k})$, 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 $\boldsymbol{k}=\boldsymbol{k}_{\mathrm{c}}$ having the same direction. Among other factors, it allows to restrict the analysis of stability to one-dimensional perturbations by directing axis 0x along $\boldsymbol{k}_{\mathrm{c}}$. Substituting $\bar{n}(x,t)=\bar{n}_0+\delta\bar{n}(x,t)$ into equation (2) and $\tilde{n}(x,t)=\tilde{n}_0+\delta\tilde{n}(x,t)$ in equation (3), 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, 3]:

$$\frac{\partial\delta\bar{n}(x,t)}{\partial t}=-\beta_0\delta\bar{n}(x,t)-\left\langle\tilde{\beta}(x)\delta\tilde{n}(x,t)\right\rangle+D_v\frac{\partial^2}{\partial x^2}\delta\bar{n}(x,t)+$$

$$+\frac{D_v\bar{n}_0}{k_BT}\int\delta\bar{n}(x',t)\frac{\partial^2}{\partial x^2}W^{vv}(x-x')\mathrm{d}x'+$$

$$+\frac{D_v}{k_BT}\frac{\partial}{\partial x}\int\left\{\left\langle\tilde{n}_0(x,t)\delta\tilde{n}(x',t)\right\rangle+\left\langle\delta\tilde{n}(x,t)\tilde{n}_0(x',t)\right\rangle\right\}\frac{\partial}{\partial x}W^{vv}\left(x-x'\right)\mathrm{d}x', \qquad (7)$$

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

$$+\frac{D_v\tilde{n}_0}{k_BT}\frac{\partial^2}{\partial x^2}\int\delta\tilde{n}(x',t)W^{vv}(x-x')\mathrm{d}x'-\tilde{\beta}(x)\delta\bar{n}(x,t)+$$

$$+\frac{D_v}{k_B T}\frac{\partial}{\partial x}\left\{\tilde{n}_0(x,t)\int\delta\bar{n}(x',t)\frac{\partial W^{vv}(x-x')}{\partial x}\mathrm{d}x'+\delta\bar{n}(x,t)\int\tilde{n}_0(x',t)\frac{\partial W^{vv}(x-x')}{\partial x}\mathrm{d}x'\right\}.(8)$$

The set of equations (7), (8) has variable coefficients and is not closed, as it contains $\left\langle\tilde{\beta}(x)\delta\tilde{n}(x,t)\right\rangle$ and $\left\langle\tilde{n}_0(x,t)\delta\tilde{n}(x',t)\right\rangle$. Nevertheless, as in equation (8), the variable coefficients are only at $\delta\bar{n}(x,t)$, and we consider the relevant terms as inhomogeneity and find $\delta\tilde{n}(x,t)$, which is now a functional of $\delta\bar{n}(x,t)$. Then, we substitute it in equation (7) and, by averaging, obtain the following expression for a damping decrement of above-mentioned perturbations:

$$\lambda_{\mathrm{f}}(\boldsymbol{k})=\lambda(\boldsymbol{k})+$$

$$+\int\mathrm{d}\boldsymbol{k}'\frac{G_\beta(\boldsymbol{k}')}{\lambda_{\mathrm{f}}(\boldsymbol{k})-\lambda(\boldsymbol{k}-\boldsymbol{k}')}\left[\frac{\bar{n}_0 D_v S_1(\boldsymbol{k},\boldsymbol{k}')}{k_B T\lambda(\boldsymbol{k}')}+1\right]\left[\frac{\bar{n}_0 D_v S_2(\boldsymbol{k},\boldsymbol{k}')}{k_B T\lambda(\boldsymbol{k}')}+1\right]+S, \qquad (9)$$

where

$$S=\frac{D_v^2}{(k_B T)^2}\int_{-\infty}^{0}\mathrm{d}\tau_1\int_{-\infty}^{0}\mathrm{d}\tau_2\int_{-\infty}^{0}\mathrm{d}\tau_3\int\mathrm{d}\boldsymbol{k}S_1(\boldsymbol{k},\boldsymbol{k}')S_2(\boldsymbol{k},\boldsymbol{k}')\times$$

$$\times G(\boldsymbol{k}',\tau_1-\tau_2-\tau_3)\exp\{-\lambda(\boldsymbol{k}')(\tau_1+\tau_2)+[\lambda_{\mathrm{f}}(\boldsymbol{k})-\lambda(\boldsymbol{k}-\boldsymbol{k}')]\tau_3\},$$

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

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

In the derivation of expression (9), the statistical independence of $\tilde{\beta}(\boldsymbol{r})$ and $\tilde{K}(\boldsymbol{r},t)$ was supposed, *i.e.* their mutual correlation function and the relevant spectral density were taken to be equal to zero.

Evidently, the damping decrement λ_f is a function of $\boldsymbol{k}$. If the energy of thermal motion of vacancies (which is of the order of $\propto k_B T$ per vacancy) considerably exceeds the energy of their force interaction, $\lambda_f < 0$ for any mode [2–5]. Nevertheless, with decreasing temperature, the damping decrement (for some $\boldsymbol{k} = \boldsymbol{k}_c$) passing through zero becomes positive (as amplification factor), and the instability appears with respect to the transition to a probability distribution with an average value, which is spatially non-uniform with a period being equal to $2\pi/|\boldsymbol{k}_c|$ (figure 1) [2–5].

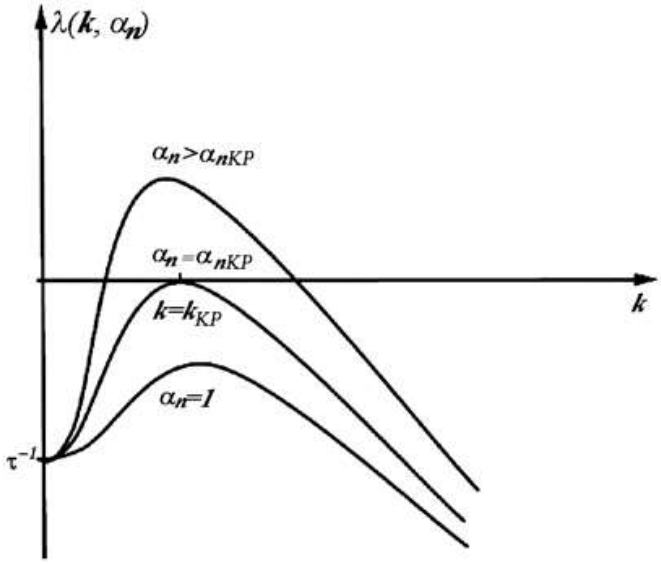

Figure 1. Schematic illustration of occurrence instability uniform distribution of vacancies [4].

5. Instability of a uniform distribution of vacancies in the absence of fluctuations of the point-defects' generation rate and inhomogeneity of irradiated f.c.c. crystal (deterministic model)

In the case of absence of external fluctuations, the rate of generation of point defects and fluctuations heterogeneity irradiated f.c.c. crystal, equation (1) is as follows [3–5, 15]:

$$\frac{\partial \bar{n}}{\partial t} = K_0 - \beta_0 \bar{n} - (\nabla_{\boldsymbol{r}} \cdot \boldsymbol{j}) . \tag{10}$$

Among steady-state solutions of equation (10), there is the following: $\bar{n} = \bar{n}_0 = n_{\mathrm{st}} \equiv K_0 / \beta_0 = K_0\tau$, where $\tau = (z_{\mathrm{d}}D_v\rho_{0\mathrm{d}})^{-1}$ is their lifetime with respect to the absorption of point defect by sinks (dislocations) with the density $\rho_{0\mathrm{d}} = \langle \rho_{\mathrm{d}}(\boldsymbol{r}) \rangle$ [3–5, 15]. In the irradiated sample, under the temperature decreasing, the role of interactions of vacancies becomes essential, and the uniform state of sample structure becomes unstable [3–5, 15]. This leads to the decomposition of the vacancies' subsystem, i.e. formation of the non-uniform spatial distribution of vacancies ($\bar{n}(\boldsymbol{r}) \neq \bar{n}_0$). To investigate stability of the uniform solution, let us treat the time evolution of its small perturbation:

$$\delta\bar{n}(\boldsymbol{r},t) \propto \exp(\lambda t + i\boldsymbol{k}\cdot\boldsymbol{r}). \tag{11}$$

Linearizing equation (10), one can obtain a spatial-dispersion equation [3–5, 15]:

$$\lambda(\boldsymbol{k},\alpha_{\boldsymbol{n}}) \equiv -D_v k^2 \left\{1 + \alpha_{\boldsymbol{n}}\tilde{U}(\boldsymbol{k})\right\} - \tau^{-1}, \tag{12}$$

where $\tilde{U}(\boldsymbol{k}) = \dfrac{\tilde{W}^{vv}(\boldsymbol{k})}{\tilde{W}^{vv}_{0\boldsymbol{n}}}$, $\tilde{W}^{vv}(\boldsymbol{k}) = \int W^{vv}(\boldsymbol{r})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\mathrm{d}\boldsymbol{r}$, $\tilde{W}^{vv}_{0\boldsymbol{n}} = \lim\limits_{k\to 0}\left|\tilde{W}^{vv}(k\boldsymbol{n})\right| > 0$,

$\alpha_{\boldsymbol{n}} = n_{\mathrm{st}}\tilde{W}^{vv}_{0\boldsymbol{n}} / (k_B T) > 0$ ($\boldsymbol{n} \equiv \boldsymbol{k}/k$) [3–5, 15].

The parameter $\alpha_{\boldsymbol{n}}$, which is proportional to the vacancies concentration and determined by the external source of defects (K_0) and temperature (T), will be called 'pumping parameter' [3–5, 15]. At low density of vacancies and/or high temperatures (when $\alpha_{\boldsymbol{n}} \to 0$), $\lambda(\boldsymbol{k}, \alpha_{\boldsymbol{n}}\to 0) \cong -D_v k^2 - \tau^{-1} < 0$, and the homogeneous state is stable [3–5, 15], *i.e.*, turning to expression (11) for the time dependent small spatial–time perturbation of stationary homogeneous distribution of vacancies' density, we can see that, when $\lambda(\boldsymbol{k}, \alpha_{\boldsymbol{n}}\to 0) < 0$, concentration inhomogeneities eventually 'resolve' because $\delta\bar{n}(\boldsymbol{r},t) \to 0$ at $t\to\infty$ [3–5, 15].

For certain directions of $\boldsymbol{k}$, $\tilde{U}(\boldsymbol{k}) < 0$. Thus, with parameter $\alpha_{\boldsymbol{n}}$ being exceeded above the threshold value $\alpha_{\boldsymbol{n}\mathrm{KP}}$ for some defined vector $\boldsymbol{k} = \boldsymbol{k}_{\mathrm{KP}}$, the value of $\lambda(\boldsymbol{k},\alpha_{\boldsymbol{n}})$ becomes positive [3–5, 15]. From the expression (11), it follows that in a condition $\lambda(\boldsymbol{k}, \alpha_{\boldsymbol{n}} \geq \alpha_{\boldsymbol{n}\mathrm{KP}} > 0) > 0$, the concentration heterogeneity increases with time, their perturbations grow at exponential law. Thus, the homogeneous state becomes unstable under growing modulated structure in distribution of vacancies with period $d = 2\pi/k_{\mathrm{KP}}$, where $\boldsymbol{k}_{\mathrm{KP}}$ is the (bifurcation) point of a new (additional to homogeneous) solution of the kinetic equation (10), given heterogeneity of concentration waves [3–5, 15]. The minimal value of $\alpha_{\boldsymbol{n}} = \alpha_{\boldsymbol{n}\mathrm{KP}}$ is a bifurcation point, at which the equation

$$\lambda(\boldsymbol{k}_{\mathrm{KP}}, \alpha_{\boldsymbol{n}\mathrm{KP}}) = -\left[D_v k_{\mathrm{KP}}^2 \left\{ 1 + \alpha_{\boldsymbol{n}\mathrm{KP}} \tilde{U}(\boldsymbol{k}_{\mathrm{KP}}) \right\} + \tau^{-1} \right] = 0 \tag{13}$$

has a solution at real $\boldsymbol{k}_{\mathrm{KP}} = k_{\mathrm{KP}}\boldsymbol{n}$ [3–5, 15], where k_{KP} is the condition

$$[\partial\lambda(\boldsymbol{k}, \alpha_{\boldsymbol{n}\mathrm{KP}})/\partial\boldsymbol{k}]\big|_{\boldsymbol{k}=\boldsymbol{k}_{\mathrm{KP}}} = \boldsymbol{0}\,. \tag{14}$$

The properties of an even function $\lambda(\boldsymbol{k};\alpha_{\boldsymbol{n}})$ are investigated in detail in Ref. [3, 4]. If $\alpha_{\boldsymbol{n}} < 1$, when $\tilde{U}(\boldsymbol{k}) < 0$, then $\lambda(\boldsymbol{k};\alpha_{\boldsymbol{n}}) < 0$. At $\alpha_{\boldsymbol{n}} = 1$ and at a point $\boldsymbol{k} = \pm\boldsymbol{k}_{\mathrm{m}}$, there is an extreme. $\boldsymbol{k}_{\mathrm{m}}$ monotonously increases with increasing $\alpha_{\boldsymbol{n}}$, and the value of $\lambda(\boldsymbol{k};\alpha_{\boldsymbol{n}})$ increases and becomes equal to zero at $\alpha_{\boldsymbol{n}} = \alpha_{\boldsymbol{n}\mathrm{KP}}$ and $\boldsymbol{k} = \pm\boldsymbol{k}_{\mathrm{m}} = \pm\boldsymbol{k}_{\mathrm{KP}}$ (see figure 1). At $\alpha_{\boldsymbol{n}} > \alpha_{\boldsymbol{n}\mathrm{KP}}$ near $\boldsymbol{k} = \pm\boldsymbol{k}_{\mathrm{KP}}$, the value of $\lambda(\boldsymbol{k};\alpha_{\boldsymbol{n}})$ become positive.

Thus, in the course of radiation, amplitudes will grow most quickly for those concentration waves, which wave vectors form beams of a star of a wave vector $\boldsymbol{k}_{\mathrm{KP}}$, and pumping parameter is not less $\alpha_{\boldsymbol{n}\mathrm{KP}}$ [3, 15]. All other, slower concentration waves, than wave with wave-vectors' beams of a star $\{\boldsymbol{k}_{\mathrm{KP}}\}$ will have a positive damping decrement only in the case, when $\alpha_{\boldsymbol{n}} > \alpha_{\boldsymbol{n}\mathrm{KP}}$ [3, 15].

From the equations (13) and (14) in the condition of approximation described below (see §6), the threshold $\alpha_{\boldsymbol{n}\mathrm{KP}}$ and critical value of wave-vector magnitude k_{KP} along the fixed direction $\boldsymbol{n}$ near $\boldsymbol{k} \cong \boldsymbol{0}$ for a cubic crystal may be found as follows (if $\rho_{0\mathrm{d}} = \langle \rho_{\mathrm{d}}(\boldsymbol{r}) \rangle$):

$$\alpha_{\mathbf{n}\mathrm{KP}} \cong -\frac{\tilde{W}^{vv}_{0\boldsymbol{n}}}{\tilde{w}^{vv}_{\boldsymbol{n}}} + \frac{2 z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) \tilde{W}^{vv}_{0\boldsymbol{n}}}{[\tilde{w}^{vv}_{\boldsymbol{n}}]^2} + \frac{2 \tilde{W}^{vv}_{0\boldsymbol{n}} \sqrt{z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) (z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) - \tilde{w}^{vv}_{\boldsymbol{n}})}}{[\tilde{w}^{vv}_{\boldsymbol{n}}]^2},$$

$$k_{\mathrm{KP}}(\boldsymbol{n}, \alpha_{\boldsymbol{n}\mathrm{KP}}) = \sqrt{\frac{-\tilde{W}^{vv}_{0\boldsymbol{n}} - \alpha_{\boldsymbol{n}\mathrm{KP}} \tilde{w}^{vv}_{\boldsymbol{n}}}{2 \alpha_{\boldsymbol{n}\mathrm{KP}} \tilde{\mathrm{B}}^{vv}(\boldsymbol{n})}},$$

where $\tilde{w}^{vv}_{\boldsymbol{n}} = \tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{0}) + \mathscr{A}^{vv}(\boldsymbol{n}) + Q^{vv}$ and $\tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) = \gamma^{vv}_0 + \mathscr{B}^{vv}(\boldsymbol{n})$ are the expansion coefficients in equation $\tilde{W}^{vv}(\boldsymbol{k}) \cong \tilde{w}^{vv}_{\boldsymbol{n}} + \tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) k^2 + \ldots$ [15] (see §6). Since, both the Fourier components of 'strain-induced' *v*–*v*-interaction energies and the Fourier components of 'electrochemical' *v*–*v*-interaction energies have negative minimum values for $\boldsymbol{k} \rightarrow \boldsymbol{0}$ along the direction [100] (or [010], or [001]) within the Brillouin zone (*BZ*) for f.c.c. crystal (see §6), then the threshold $\alpha_{[100]\mathrm{KP}}$ and critical value of wave vector along the direction [100] (or [010], or [001]), near $\boldsymbol{k} \cong \boldsymbol{0}$, may be found as follows [3–5, 15]:

$$\alpha_{[100]\mathrm{KP}} \cong 1 + \frac{2 z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}([100])}{\tilde{W}^{vv}_{0[100]}} + \frac{2 \sqrt{z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}([100]) \{ z_{\mathrm{d}} \rho_{0\mathrm{d}} \tilde{\mathrm{B}}^{vv}([100]) + \tilde{W}^{vv}_{0[100]} \}}}{\tilde{W}^{vv}_{0[100]}},$$

$$k_{\mathrm{KP}}([100], \alpha_{[100]\mathrm{KP}}) \cong \sqrt{\frac{(\alpha_{[100]\mathrm{KP}} - 1) \tilde{W}^{vv}_{0[100]}}{2 \alpha_{[100]\mathrm{KP}} \tilde{\mathrm{B}}^{vv}([100])}}.$$

The first (unit) term in the expression for $\alpha_{[100]\mathrm{KP}}$ contributes dominantly into the threshold $\alpha_{[100]\mathrm{KP}}$ magnitude [3–5, 15]. Thus, as long as $\tilde{\mathrm{B}}^{vv}([100]) \geq 0$ (see §6), the dissipative modulated structure in the distribution of vacancies in f.c.c. crystal appears in case of $\alpha_{[100]KP} > 1$. Period of dissipative modulated structure of vacancies' subsystem depends on parameters of kinetics of redistribution: diffusion coefficient, lifetime defects or z_d [3–5, 19, 20].

Between the dislocation sinks within the f.c.c. crystal, the vacancy concentration waves, $\bar{n}(\boldsymbol{r},t)$, can be in the form of three-dimensional superposition of two or three interpenetrating waves along the equivalent directions [100], [010] or [001] simultaneously:

$$\bar{n}(\boldsymbol{r},t) = \bar{n}_0 + \delta\bar{n}_1^{[001]}(z,t)\,, \tag{15a}$$

$$\bar{n}(\boldsymbol{r},t) = \bar{n}_0 + \delta\bar{n}_2^{[010]}(y,t) + \delta\bar{n}_2^{[001]}(z,t)\,, \tag{15b}$$

$$\bar{n}(\boldsymbol{r},t) = \bar{n}_0 + \delta\bar{n}_3^{[100]}(x,t) + \delta\bar{n}_3^{[010]}(y,t) + \delta\bar{n}_3^{[001]}(z,t)\,, \tag{15c}$$

where x, y, z—components of a vector of $\boldsymbol{r}$ in the directions of axes [100], [010], [001], respectively. Each of summand non-uniform functions, which are in the right parts of equations (15a)–(15c), describes one-dimensional modulation vacancies' subsystem along the direction of respective edge of f.c.c. cube [16] (see figures 2(a)–2(c)).

In the event of in-phase coincidence of crests of three interpenetrating synphased modulated vacancies' concentration waves simultaneously, conditions for 'nucleation' of nanovoids at sites spanned by ridges of waves appear (see figure 2(c)). Formation of such three-dimensional superposition of vacancies' concentration waves along the [100], [010] and [001] directions (see figures 2(a)–2(c)) at the same time (with the in-phase crossing of their crests) can be compared with the mechanism of formation of nanovoids within the irradiated f.c.c. crystal.

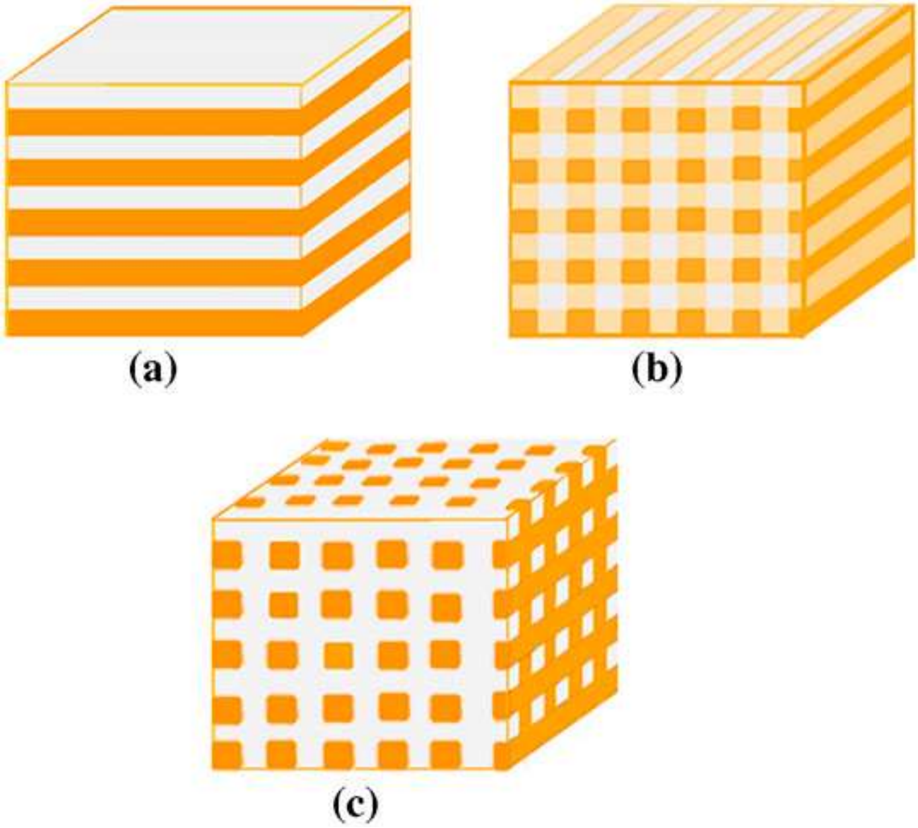

Figure 2. The schematic image of the one-dimensional (a), two-dimensional (b), or three-dimensional (c) modulated structure of vacancies' subsystem; crests of the concentration wave of atoms in metal f.c.c. crystal are designated by light ('grey') colour; crests of the concentration wave of vacancies' subsystem are designated by more dark ('orange') colour.

6. Interaction Parameters of Vacancies

Energy of total interaction between substitutional point defects, for instance, vacancies, in their solid solution within the relaxed (i.e., elastic-stress-free, but strained) host crystal can be presented conditionally as a sum [17, 18]:

$$W^{vv} \approx \varphi^{vv}_{\mathrm{el.chem}} + V^{vv},$$

where $\varphi^{vv}_{\mathrm{el.chem}}$ is an energy of 'electrochemical'-interaction contribution, which is caused by the 'direct' interaction of electric charges forming the point defects in unrelaxed (strain-free, but stressed) host crystal [8–11], and V^{vv} is an energy of the 'strain-induced' (or 'elastic') contribution, which is conditioned by the 'indirect' (host-crystal-specific) interaction between point defects as a result of interference of fields of the equilibrium static displacements of host-crystal atoms from their inherent sites, which occur due to the presence of point defects, in the relaxed (elastic-stress-free, but strained) host-crystal lattice [8, 16–18]. If a distance between the defects largely exceeds the host-lattice period *a*, the Fourier components, $\tilde{W}^{vv}(\boldsymbol{k})$, of the interaction energies for vacancies can be written as a power series [15, 16–18]:

$$\tilde{W}^{vv}(\boldsymbol{k}) \approx \tilde{V}^{vv}(\boldsymbol{k}) + \tilde{\varphi}^{vv}_{\text{el.chem}}(\boldsymbol{k}) \cong \tilde{w}^{vv}_{\boldsymbol{n}} + \tilde{\mathrm{B}}^{vv}(\boldsymbol{n})k^2 + \ldots, \qquad (16)$$

where $\tilde{V}^{vv}(\boldsymbol{k})$ is the Fourier component of ‘strain-induced’ *v*–*v*-interaction energies. Within the small finite region near $\boldsymbol{k} = \boldsymbol{0}$, $\tilde{V}^{vv}(\boldsymbol{k})$ may be represented as follows [16, 18, 21, 22]:

$$\tilde{V}^{vv}(\boldsymbol{k}) \cong \mathcal{A}^{vv}(\boldsymbol{n}) + \mathcal{B}^{vv}(\boldsymbol{n})k^2 + Q^{vv}.$$

Here, the well-known first term is based on the long-wave-limit approximation [16, 18, 21, 22]:

$$\mathcal{A}^{vv}(\boldsymbol{n}) = -\frac{9K^2\upsilon_0(L^v)^2(1+2\xi\tilde{\mathcal{X}}(\boldsymbol{n})+3\xi^2\tilde{\mathcal{Y}}(\boldsymbol{n}))}{\mathcal{D}(\boldsymbol{n})},$$

where L^v is a concentration coefficient of f.c.c.-lattice dilatation, $K = (C_{11} + 2C_{12})/3$ is a compressibility modulus, $\upsilon_0 = a^3/4$—atomic volume, $\xi = (C_{11} - C_{12} - 2C_{44})/C_{44}$ is an elastic-anisotropy factor, C_{11}, C_{12}, C_{44} are the elasticity moduli,

$\tilde{\mathcal{X}}(\boldsymbol{n}) = n_x^2n_y^2 + n_z^2n_y^2 + n_x^2n_z^2$, $\tilde{\mathcal{Y}}(\boldsymbol{n}) = n_x^2n_y^2n_z^2$,

$\mathcal{D}(\boldsymbol{n}) = C_{11} + \xi(C_{11} + C_{12})\tilde{\mathcal{X}}(\boldsymbol{n}) + \xi^2(C_{11} + 2C_{12} + C_{44})\tilde{\mathcal{Y}}(\boldsymbol{n})$ [16, 18, 21, 22]. The second term is a correction to this approximation [21, 22], and the third term is a gauge, which eliminates a ‘strain-induced’ self-action of the vacancies [23, 24].

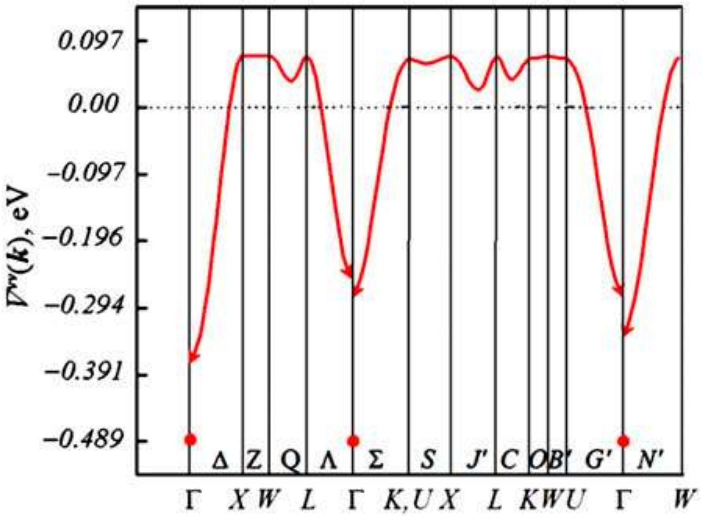

Figure 3. Dispersion curves for the Fourier components of ‘strain-induced’ *v*–*v*-interaction energies in f.c.c.-Ni along all the high-symmetry directions in reciprocal space, in particular, at the high-symmetry points, Γ, *X*, *W*, *L*, *K*(*U*), of the first Brillouin zone (with $L^v = -0.073$ estimated from data [25]); • — $\tilde{V}^{vv}(\mathbf{0})$ at $T = 300$ K.

The Fourier component of ‘strain-induced’ *v*–*v*-interaction energies has a minimum value (see figure 3) along the direction [100] within the first *BZ* (figure 4) for f.c.c. crystal:

$$\tilde{V}^{vv}(\mathbf{k}_{\|X\Gamma} \to \mathbf{0}) \cong -\frac{9K^2\upsilon_0(L^v)^2}{C_{11}} + \mathcal{B}^{vv}(\mathbf{n}_{\|X\Gamma})k^2 + Q^{vv};$$

$\mathcal{B}^{vv}(\mathbf{n}_{\|X\Gamma}) \cong \frac{9K^2a^4(L^v)^2M\omega_{\mathrm{L}X}^2}{256C_{11}^2}$ [22], $\omega_{\mathrm{L}X}$ is the temperature-dependent longitudinal phonon frequency at the *X*(100) point [26], *M* is a host atom mass.

Thus, the Fourier component of *v*–*v*-interaction energies along the direction

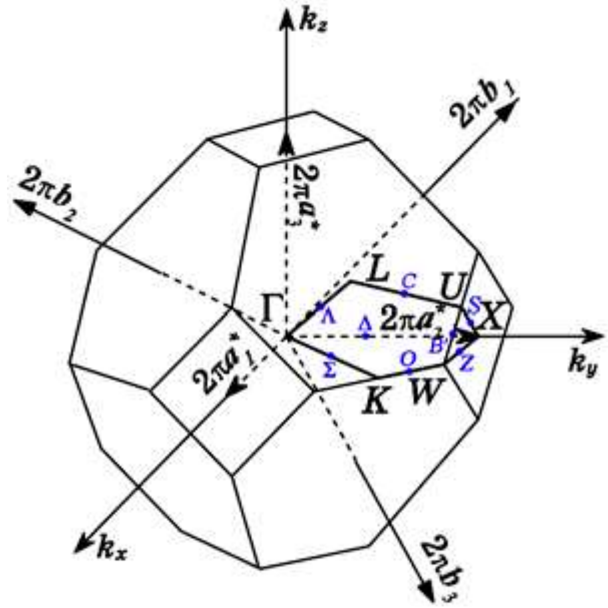

Figure 4. The first Brillouin zone of reciprocal space for f.c.c. lattice.

[100] within the small finite region near $\boldsymbol{k} = \boldsymbol{0}$ may be represented as follows:

$$\tilde{W}^{vv}(k[100]) \approx \tilde{W}^{vv}_{0[100]}\tilde{U}(k[100]) = \tilde{W}^{vv}_{0[100]}\{-1+\Psi([100])k^2\},$$

where $\Psi([100]) = \tilde{\mathrm{B}}^{vv}([100]) / \tilde{W}^{vv}_{0[100]}$.

In equation (16), $\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k})$ is the Fourier component of energies for direct ‘electrochemical’ *v*–*v*-interactions [24]. The dispersion curves for

$$\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k}) \cong 4\varphi^{vv}(r_{\mathrm{I}})\left[\cos(\frac{a}{2}k_x)\cos(\frac{a}{2}k_y) + \cos(\frac{a}{2}k_y)\cos(\frac{a}{2}k_z) + \right.$$

$$\left. + \cos(\frac{a}{2}k_x)\cos(\frac{a}{2}k_z)\right] + 2\varphi^{vv}(r_{\mathrm{II}})\left[\cos(ak_x) + \cos(ak_y) + \cos(ak_z)\right] +$$

$$+8\varphi^{vv}(r_{\mathrm{III}})\left[\cos(\frac{a}{2}k_x)\cos(\frac{a}{2}k_y)\cos(ak_z) + \cos(\frac{a}{2}k_y)\cos(\frac{a}{2}k_z)\cos(ak_x) + \right.$$

$$\left. + \cos(\frac{a}{2}k_z)\cos(\frac{a}{2}k_x)\cos(ak_y)\right] + 4\varphi^{vv}(r_{\mathrm{IV}})\left[\cos(ak_x)\cos(ak_y) + \right.$$

$$+\cos(ak_y)\cos(ak_z)+\cos(ak_x)\cos(ak_z)\Big]+4\varphi^{vv}(r_{\mathrm{V}})\times$$

$$\times\Big[\cos\left(a(k_x+k_y)\right)\cos\left(\frac{a}{2}(k_x-k_y)\right)+\cos\left(a(k_x+k_z)\right)\cos\left(\frac{a}{2}(k_x-k_z)\right)+$$

$$+\cos\left(a(k_y+k_z)\right)\cos\left(\frac{a}{2}(k_y-k_z)\right)+\cos\left(a(k_x-k_z)\right)\cos\left(\frac{a}{2}(k_x+k_z)\right)+$$

$$+\cos\left(a(k_x-k_y)\right)\cos\left(\frac{a}{2}(k_x+k_y)\right)+\cos\left(a(k_y-k_z)\right)\cos\left(\frac{a}{2}(k_y+k_z)\right)\Big]+$$

$$+8\varphi^{vv}(r_{\mathrm{VI}})\cos(ak_x)\cos(ak_y)\cos(ak_z)\ +\ldots$$

along all the high-symmetry directions within the 1st *BZ* are presented in figure 5.

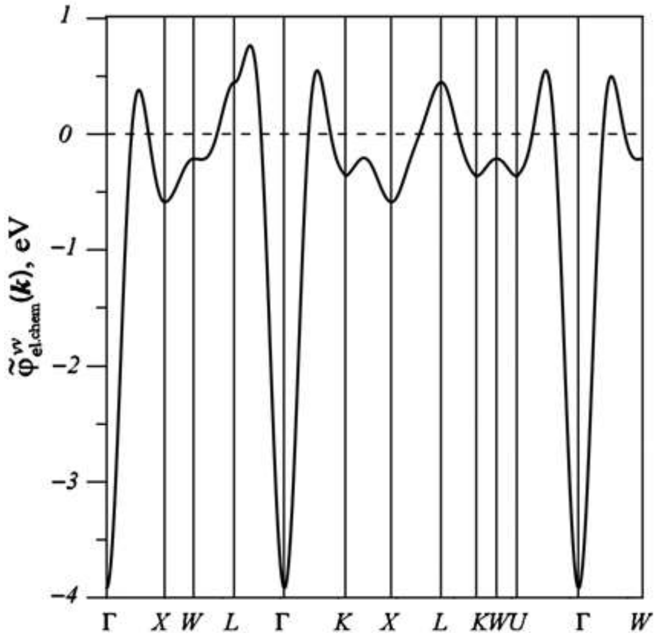

Figure 5. Dispersion curves for the Fourier components of 'electrochemical' *v*–*v*-interaction energies along all the high-symmetry directions in reciprocal space, using the Machlin potential [27] with cohesive energy $\varepsilon = -4.45$ eV/atom [28, 29] at $T = 300$ K and with taking into account for 6 coordination spheres only.

($\varphi^{vv}(r_{\mathrm{I}})$, $\varphi^{vv}(r_{\mathrm{II}})$, …, $\varphi^{vv}(r_{\mathrm{VI}})$ are the 'electrochemical' *v*–*v*-interaction energies at the first, second, …, sixth, … coordination shells.)

Within both the long-wavelength approximation and the approach developed in Refs. [8–11, 18],

$$\tilde{\varphi}^{vv}_{\text{el.chem}}(\boldsymbol{k}) \cong \tilde{\varphi}^{vv}_{\text{el.chem}}(\boldsymbol{0}) + \gamma^{vv}_0 k^2 + \ldots,$$

where

$$\tilde{\varphi}^{vv}_{\text{el.chem}}(\boldsymbol{0}) = \sum_{\boldsymbol{r}\in\{\boldsymbol{r}_{\text{I}},\boldsymbol{r}_{\text{II}},\ldots\}} \varphi^{vv}_{\text{el.chem}}(|\boldsymbol{r}|) \approx$$
$$\approx 12\varphi^{vv}(r_{\text{I}}) + 6\varphi^{vv}(r_{\text{II}}) + 24\varphi^{vv}(r_{\text{III}}) + 12\varphi^{vv}(r_{\text{IV}}) + 24\varphi^{vv}(r_{\text{V}}) + 8\varphi^{vv}(r_{\text{VI}}) + \ldots,$$

$$\gamma^{vv}_0 = -\frac{1}{6} \sum_{\boldsymbol{r}\in\{\boldsymbol{r}_{\text{I}},\boldsymbol{r}_{\text{II}},\ldots\}} |\boldsymbol{r}|^2 \varphi^{vv}_{\text{el.chem}}(|\boldsymbol{r}|) \approx$$
$$\approx -a^2\{\varphi^{vv}(r_{\text{I}}) + \varphi^{vv}(r_{\text{II}}) + 6\varphi^{vv}(r_{\text{III}}) + 4\varphi^{vv}(r_{\text{IV}}) + 10\varphi^{vv}(r_{\text{V}}) + 4\varphi^{vv}(r_{\text{VI}}) + \ldots\}.$$

Dependence of the energy of ‘electrochemical’ *v*–*v*-interaction in f.c.c. crystal on normalized distance *r*/*a*, with taking into account interaction in the real 28 coordination spheres over sites, is plotted in figure 6.

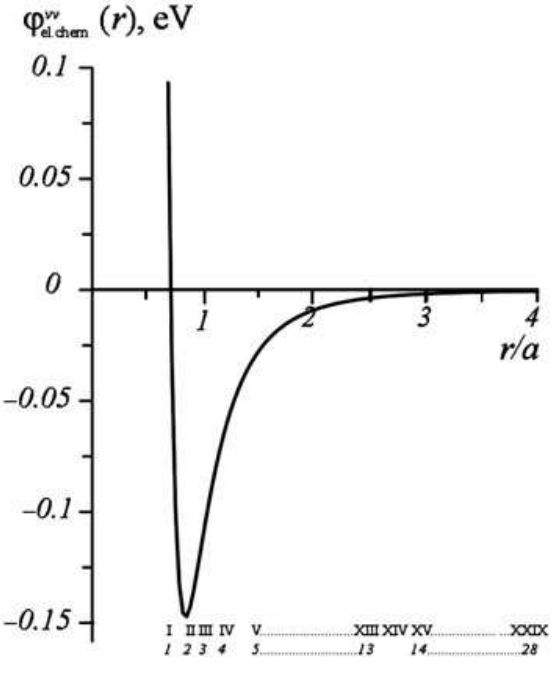

Figure 6. Dependence of the energy of ‘electrochemical’ interaction of vacancies in f.c.c. crystal describing by the Machlin potential [27] (with cohesive energy ε = −4.45 eV/atom [28, 29]) depending on normalized distance $r(300\text{ K})/a(300\text{ K})$ between them.

As known, there is a simple relationship between the ordinal number of the coordination sphere, $N_{(\mathrm{n})}$, and its radius, R_n, for f.c.c. lattice [30–33]: $R_\mathrm{n} = r_\mathrm{I}(N_{(\mathrm{n})})^{1/2} = a(2N_{(\mathrm{n})})^{1/2}/2$. Unfortunately, it is broken (because of specific 'removal of a crystallographic degeneracy') at XIV-th, XXX-th, … spheres! Really, for three-dimensional f.c.c. lattice, the ordinal number of the real coordination sphere and its radius are defined by the Miller indices $\{h_\mathrm{n}k_\mathrm{n}l_\mathrm{n}\}$: $2N_{(\mathrm{n})} = h_\mathrm{n}^2 + k_\mathrm{n}^2 + l_\mathrm{n}^2$, $2R_\mathrm{n}/a = \sqrt{h_\mathrm{n}^2 + k_\mathrm{n}^2 + l_\mathrm{n}^2}$. Evidently, the doubled numbers of XIV-th, XXX-th, … coordination spheres, 2×XIV, 2×XXX, …, do not consist of the three squares of integers $\{h_\mathrm{n}k_\mathrm{n}l_\mathrm{n}\}$ simultaneously. According to Refs. [30–33], these ordinal numbers correspond to so-called 'zero' coordination spheres, on which the sites of f.c.c. lattice do not take place (*i.e.*, their coordination numbers are equal to zero).

As shown, moduli of energies of 'electrochemical' *v*–*v*-interaction quickly decrease with increasing distance r_n (monotone for n ≥ II; figure 6) ('short-range interaction'). Meanwhile the 'strain-induced' of their interactions has a significantly long-range nature and quasi-oscillating character [22]. The function $\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k})$ at $\boldsymbol{k} = \boldsymbol{0}$ is analytic (*i.e.* $\lim\limits_{\boldsymbol{k}\to\boldsymbol{0}} \tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k}) = \tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{0})$) (figure 5). The function $\tilde{V}^{vv}(\boldsymbol{k})$ to a point $\boldsymbol{k} = \boldsymbol{0}$ is nonanalytic (see Ref. [22]): $\lim\limits_{\boldsymbol{k}\to\boldsymbol{0}} \tilde{V}^{vv}(\boldsymbol{k}) \neq \tilde{V}^{vv}(\boldsymbol{0})$ (figure 3).

In spite of that, the energy of 'strain-induced' *v*–*v*-interaction has the long-range nature and quasi-oscillating character, the value of its energy is much less than 'electrochemical' *v*–*v*-interaction energy. Thus, the energy of 'electrochemical' *v*–*v*-interaction has a main contribution to the interaction energy between vacancies in the f.c.c. Ni.

However, the Fourier components of 'electrochemical' interaction *v*–*v*-interaction energies near $\boldsymbol{k} = \boldsymbol{0}$ do not depend on the direction $\boldsymbol{n}$. Therefore, calculations of dispersive curves for the Fourier components of 'strain-induced' *v*–*v*-interaction energies are also important, as from their analysis, it is possible to reveal in what direction can be formed vacancies' concentration waves.

The Machlin potential $\varphi^{\mathrm{NiNi}}(r) = -A_{\mathrm{NiNi}}r^{-4} + B_{\mathrm{NiNi}}r^{-8}$ [27] (of cohesive character) for $T > 0$ K (but in terms of f.c.c.-lattice spacing a_0 at $T = 0$ K, cohesive energy ε_0, and lattice sums $S_4 \cong 25.338$, $S_8 \cong 12.80193$, where $A_{\mathrm{NiNi}} = -\varepsilon^0 a_0^4 S_4^{-1}$, $B_{\mathrm{NiNi}} = -\varepsilon^0 a_0^8 S_8^{-1}/8$ [18, 27, 34]) extends significantly beyond the limits of the 1st coordination sphere (with radius $r_{\mathrm{I}} = a/\sqrt{2}$) (figure 6). As result, the dependence of $\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k}) \approx \tilde{\varphi}^{\mathrm{NiNi}}_{\mathrm{el.chem}}(\boldsymbol{k})$ is extreme (at least, locally) not only at the high-symmetry points, but also within the whole of 1st BZ (figure 5). The corresponding character of dispersion curves $\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{k})$ hypothetically promotes expansion to a variety of the long-wave dissipative modulated structures in distribution of vacancies, which can be formed under favourable conditions.

7. Characteristics of dissipative modulated structures of vacancies' subsystem in the absence of fluctuations of the point-defects' generation rate and inhomogeneity of irradiated f.c.c. crystal

In a given paper, estimates for the following values of parameters for f.c.c. Ni with vacancies and their (dislocation) sinks: $z_{\mathrm{d}} = 1$, $\rho_{0\mathrm{d}} \cong 5\cdot10^{-8}$ Å^{-2} [20, 35, 36], and for example at 1500 K $\tau \cong 1.33\cdot10^{-4}$ s were carried out. Energy of activation of migration and pre-exponential factor in the Arrhenius formula for coefficient of diffusion of vacancies, D_v, were expected equal 1.3 eV and $3.5\cdot10^{15}$ Å^2 s^{-1} [20, 35], respectively.

Experimental data on elasticity moduli, $C_{11}(T)$, $C_{12}(T)$, $C_{44}(T)$, and consistent estimation of concentration-dilatation coefficient, L^v, are presented in Ref. [37] and Ref. [25], respectively. $\tilde{\varphi}^{vv}_{\mathrm{el.chem}}(\boldsymbol{0})$, γ_0^{vv} were estimated with use of interatomic potential for f.c.c. Ni in Ref. [27].

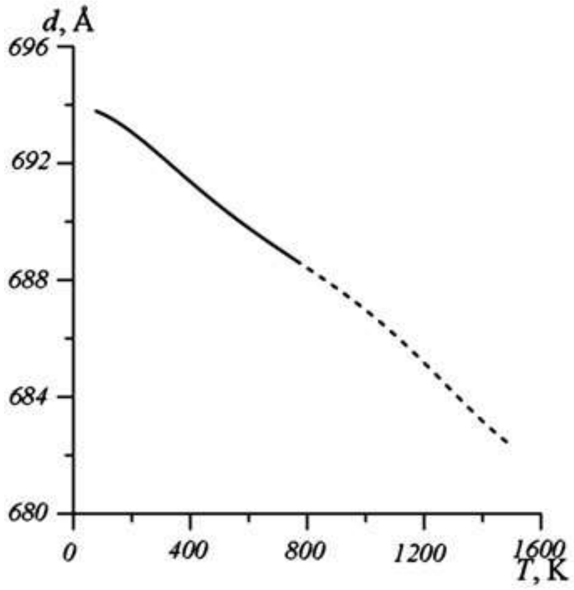

Figure 7. Temperature dependence of the modulated-structure nanoscale period in the distribution of vacancies *d*(*T*), when ρ_{0d} = const $\cong 5\cdot10^{-8}$ Å^{-2} [36]. (The dashed line in figure shows the *d*(*T*) dependence obtained by extrapolation of the curves presenting experimental data on elastic moduli [37] and coefficient of thermal expansion [38, 39] outside the range of their determinations.)

Predicted temperature dependence of the period of the dissipative modulated structure of vacancies' subsystem, which can be appear the first in quality of the inhomogeneity solution (15) of the equation (10) are presented in figure 7. (The dashed line in figure 7 shows the *d*(*T*) dependence obtained by extrapolation of the curves presenting experimental data on elastic moduli [37] and coefficient of thermal expansion [38, 39].)

The energy of 'electrochemical' interaction is a main contribution into energy of parameter $\tilde{W}^{vv}_{0\boldsymbol{n}} = \lim_{k\to 0}\left|\tilde{W}^{vv}(k\boldsymbol{n})\right|$ in the relations for a critical value of the wave vector and the period of the dissipative modulated structure in the distribution of vacancies, *d*(*T*). It determines the temperature dependence of the period *d*(*T*).

The energy of 'electrochemical' *v*–*v* interaction has a non-monotonic character, (see figure 6) depending on the normalized distance, *r*/*a*, between vacancies. The absolute value of their 'electrochemical'-interaction energy grows with temperature elevation on the first coordination sphere and it is not compensate in $\tilde{W}^{vv}_{0[100]}$ decrease of moduli of such energies on the following spheres. Period (nanoscale) of the dissipative modulated structure of vacancies' subsystems can a slightly decrease (by < 2%) with temperature increasing in the conditions of constancy of density of dislocations (formation of dissipative modulated structures of vacancies' subsystems is made easier) (figure 7).

The nanoscale period of dissipative of modulated structure of vacancies' subsystem depends on the density of dislocations. As known, dislocation density is decreasing with temperature increasing [40–43]. In a given paper, to analyse the influence of the density of dislocation on the period, the experimental data of the temperature dependence of the density of dislocations and their approximation (by different processing conditions) are used (Ref. [40–43]). One of such temperature dependence of the experimental data of density of dislocation on the temperature $\rho_{0d}(T)$, and its approximations is presented in figure 8 [43]:

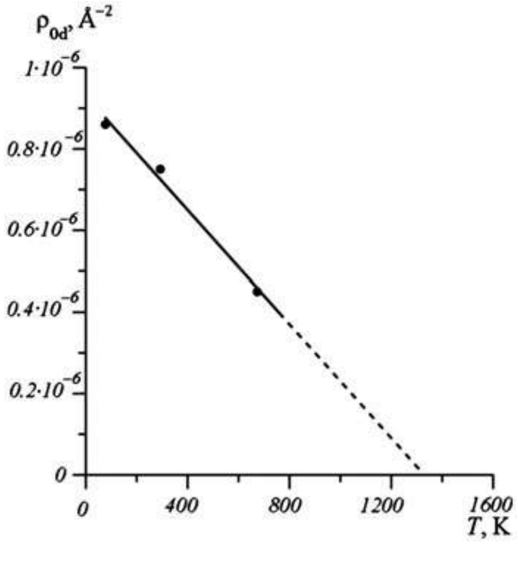

Figure 8. Temperature dependence of the dislocation density, $\rho_{0d}(T)$ for f.c.c. single crystal Ni [43] at the minimum extents of deformation by compression with orientation of an axis of compression [001]. (The dashed line in figure shows the $\rho_{0d}(T)$ dependence, which is obtained by extrapolation of a curve plotted with experimental data on a density of dislocations.)

$$\rho_{0\text{d}} \cong \rho_{77\ \text{K}} + \rho_1 (T - 77\ \text{K}), \qquad (17)$$

where $\rho_{77\ \text{K}} \cong 0.87 \cdot 10^{-6}$ Å^{-2}, $\rho_1 \cong -6.995 \cdot 10^{-10}$ Å$^{-2} \cdot$K^{-1} (figure 8).

Accounting empirical temperature dependence of density of dislocations leads to increasing period of the dissipative modulated structure with temperature, which is caused by the entropy factor and ‘electrochemical’ interaction of vacancies (figure 9).

Therefore, decrease of density of dislocation $\rho_{0\text{d}}(T)$ with temperature increasing blocks formation (spatially ordered) of dissipative modulated structure of vacancies’ subsystem. However, at increase in density of dislocations from 10^{-6} Å^{-2} to 10^{-4} Å^{-2}, (nanoscale) period of the dissipative modulated structure of vacancies’ subsystem decreases from 10^3 Å to 10^2 Å.

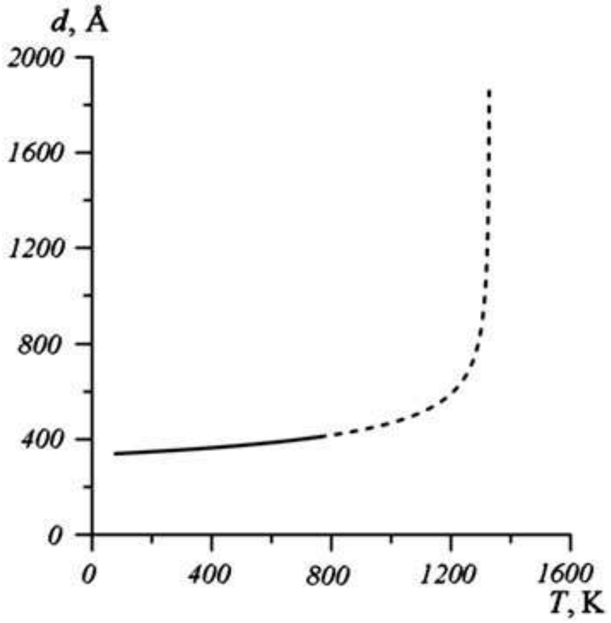

Figure 9. Temperature dependence of the modulated-structure period in the distribution of vacancies with approximation of dislocation density $\rho_{0\text{d}}(T)$ for expression (17). (In figure 8, see an explanation for dashed line.)

The nanoscale period of modulated of dissipative structures of vacancies’ subsystem depends on the rate of defect generation K_0. With increase the rate of generation of defects, such as vacancies, K_0, the temperature range of the existence of the period

$d(T)$ is expanded (figure 10). The dissipative modulated structure of vacancies' subsystem becomes probable at $T < T_{\mathrm{KP}}$ = 360–820 K in depending on the rate of defect generation ($K_0 = 10^{-8}$–10^{-2} dpa·s^{-1}), values of coefficient of diffusion of vacancies and density of dislocation (figure 10).

Figure 10 shows the region of instability of homogeneous vacancy distribution in the coordinates of critical temperature and radiation intensity ($\propto K_0$). The corresponding coordinate plane is divided into two parts by the curve: in the region I, the homogeneous distribution is unstable, whereas in region II, it is stable. At temperatures and radiation intensities, which fall within the region I, the periodic distribution of vacancies' subsystem density should set in.

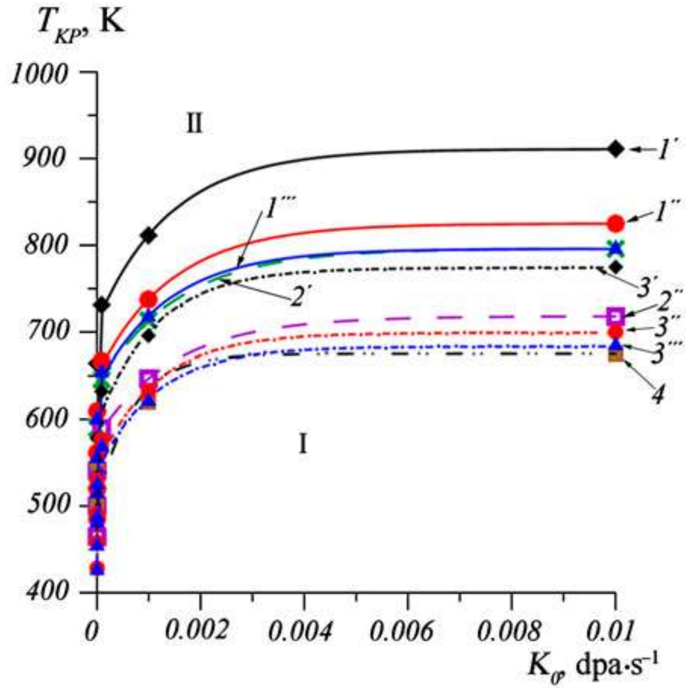

Figure 10. Regions (in)stability of the homogeneous distribution of vacancies in f.c.c. crystal with respect to its inhomogeneous perturbations in terms of the radiation intensity and the critical temperature of a sample: I—region of instability, II—region of stability; (solid lines—$D_v = 1\cdot10^{15}\exp\{(-1.4\text{ eV})/(k_B T)\}$ [Å^2·s^{-1}] [44, 12], dashed lines—$D_v = 3.5\cdot10^{15}\exp\{(-1.3\text{ eV})/(k_B T)\}$ [Å^2·s^{-1}] [35, 12], dashed lines with point—$D_v = 6\cdot10^{15}\exp\{(-1.3\text{ eV})/(k_B T)\}$ [Å^2·s^{-1}] [45, 12] for cases: (*1*′, *2*′, *3*′)—dislocation density $\rho_{0d} \cong 5\cdot10^{-8}$ Å^{-2} [36], (*1*″, *2*″, *3*″)—with taking into account the empirical dependence $\rho_{0d}(T)$ (17), (*1*‴, *3*‴)—dislocation density $\rho_{0d} \cong 0.75\cdot10^{-6}$ Å^{-2} [43]. (4)—the dividing curve is given according to work [12] for comparison.

The range of stability of the dissipative modulated structure of vacancies' subsystem a little expands, taking into account the decreasing temperature dependence of density of dislocations (figure 10). Decrease of mobility of vacancies promotes shift of range of stability of such structure in coordinates of the critical temperature (T_{KP}) and the rate of defect generation K_0 sideways more high temperatures (figure 10). The curves in figure 10 determine the order of magnitude for threshold values of $K_0(T_{\mathrm{KP}})$, when instability occurs.

In addition, we will note that, in applied models, isothermal conditions of self-organization of the dissipative modulated structure of vacancies' subsystem in irradiated f.c.c. crystal are considered. The quantitative results obtained within their scopes can be satisfactory not always as influence of external fluctuations (radius of spatial correlation of fluctuations of rate of generation of vacancies, time of correlation of fluctuations of rate of vacancies' generation, and variation factor of rate of vacancies' generation), which are always in real-life environment of irradiation, is not considered. Nevertheless, despite of this, the present model decently describes the phenomenon at qualitative level.

Let us note that, in regard to nanovoids, it can be assumed that the energy of interaction of nanovoids is given by only their 'strain-induced' interaction energy within the continuum approximation in the long-wavelength limit [15, 16, 18]: $\tilde{w}_{\boldsymbol{n}}^{vv} \Rightarrow \tilde{w}_{\boldsymbol{n}} \cong \mathcal{A}^{vv}(\boldsymbol{n}) + Q^{vv}$, $\tilde{\mathrm{B}}^{vv}(\boldsymbol{n}) \Rightarrow \tilde{\mathrm{B}}(\boldsymbol{n}) \cong \mathcal{B}^{vv}(\boldsymbol{n})$. (Within the continuum approximation, the nanovoids are considered as finite objects, and one can use the lattice-statics method for $\boldsymbol{k} \to \boldsymbol{0}$ only, *i.e.* within the long-wave approximation.) Correspondingly, for comparison, the temperature dependence of the nanoscale superlattice period in the distribution of nanovoids is shown in figure 11.

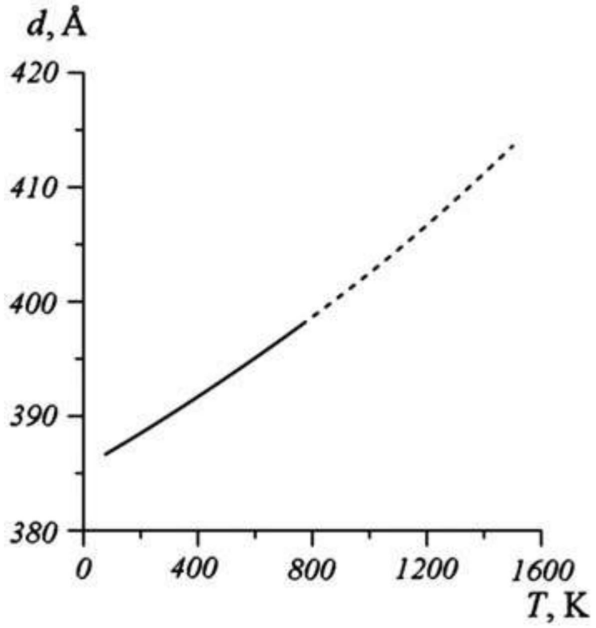

Figure 11. Dependence of the superlattice period in the distribution of microvoids on T with coefficient of a concentration dilatation of f.c.c.-Ni $L^p \cong 0.0146$ [46] because of presence of voids. (In figure 7, see an explanation for dashed line.)

Period of a superlattice in the distribution of nanovoids is increasing with temperature that was indirectly confirmed in Refs. [45, 47–52] for some irradiated b.c.c. and f.c.c. metals.

8. Dissipative modulated structures of vacancies' subsystem in presence of fluctuations of the point-defects' generation rate

The expressions obtained for the determination of n_0 (see equations (4), (5)), critical values of parameters, and a period of the structure, which arises (see equation (9)), are non-linear and depend on integrated properties of an interaction potential and corresponding spectral densities. The influence of fluctuations of the rate of a defects' generation and heterogeneity of an irradiated crystal within the approximations taken is independent, the corrections defined by them are included in (5) and (9) as additive terms. An average value of the density of defects in contrast to a damping decrement $\lambda_f(\boldsymbol{k})$ depends only on fluctuations of the density of sinks (through $G_\beta(\boldsymbol{k})$) but not on the fluctuations of a defect-production rate: its correlation functions or spectral densities. In the absence of random heterogeneity of sinks, the expression for an average density of defects [2] $\bar{n}_0 = K_0 / \beta_0$ formally coincides with the expression obtained in a deterministic approximation if all quantities are substituted by their averages.

The joint accounting for the stationary external fluctuations and non-linear interaction of vacancies causes qualitatively new results, namely, the vanishing or, on the contrary, arising sets of possible uniform random fields of the defects' density, each of which can be realized [2].

When the external fluctuations become negligible, equations (4), (5) and (9) turn into relations obtained within the scope of the deterministic model (see §5 and Refs. [2, 15]). As the influence of $\tilde{K}(\boldsymbol{r},t)$ and $\tilde{\beta}(\boldsymbol{r})$ is additive, their role is analysed in [53], and the statistical characteristics of random homogeneous stationary distributions of defects are obtained in Ref. [54], here let us consider the conditions for a spatially-periodic (inhomogeneous) distribution of the defects' density to arise in their stochastic formation [2]. To obtain further results, a form of a spectral density should be rendered concrete.

For the Gauss temporal spectrum with $\ln\{G(\boldsymbol{k},t)/G(\boldsymbol{k},t)\} \propto t^2$, there will always 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_{corr}, and the time of their correlation, τ_{corr}, is much less of all characteristic times of a problem. Then for the component in (9) caused by fluctuations we have

$$S \approx \frac{D_v^2}{2(k_B T)^2} \int \mathrm{d}\boldsymbol{k}' \frac{G(\boldsymbol{k}')S_1(\boldsymbol{k},\boldsymbol{k}')S_2(\boldsymbol{k},\boldsymbol{k}')\tau_{\text{corr}}}{\lambda(\boldsymbol{k}')\{\lambda(\boldsymbol{k}')+\lambda(\boldsymbol{k}-\boldsymbol{k}')\}}. \tag{18}$$

The radius of correlation of fluctuations and the time of correlation of fluctuations may be represented by definition as follows [55, 56]:

$$r_{\text{corr}} = \frac{\int \left\langle K(\boldsymbol{r},t)K(\boldsymbol{r}+\Delta\boldsymbol{r},t)\right\rangle \mathrm{d}(\Delta\boldsymbol{r})}{\left\langle K^2(\boldsymbol{r},t)\right\rangle},$$

$$\tau_{\text{corr}} = \frac{\int \left\langle K(\boldsymbol{r},t)K(\boldsymbol{r},t+\Delta t)\right\rangle \mathrm{d}(\Delta t)}{\left\langle K^2(\boldsymbol{r},t)\right\rangle}.$$

$r_{\text{corr}} < 10^4$–10^6 Å (< order of size of displacement cascade, *i.e.* the maximum distance at which stages may cross overlap and we can enter deterministic and fluctuation components of the density of generated defects) and $\tau_{\text{corr}} \leq 10^2$–$10^4$ ps (≤ order of time of development cascades) [55].

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

As substantiated in the end of §4, the integrand in (18), decreasing with an increase of k as k^2 is localised within the interval $[-|\boldsymbol{k}_{\text{m}}|, |\boldsymbol{k}_{\text{m}}|]$ ($|\boldsymbol{k}_{\text{m}}| \leq |\boldsymbol{k}_{\text{KP}}|$). The damping decrement λ_{f} will become zero at $\alpha_{\boldsymbol{n}} \leq \alpha_{\text{KP}}$, because the numerator of an integrand in (18) is non-negative within the interval $(-|\boldsymbol{k}_{\text{KP}}|, |\boldsymbol{k}_{\text{KP}}|)$ ($\boldsymbol{k}_{\text{KP}} \equiv k_{\text{KP}}\boldsymbol{n}$), and $S > 0$ [2]. In a numerator of an integrand in equation (18), we will be restricted to the first term of an expansion, and in $\lambda(\boldsymbol{k},\alpha)$, to the second term because it determines point of a minimum

$\boldsymbol{k}_\mathrm{m}$. Going to (18) from an integration to the summation and taking into account that $G(\boldsymbol{0},0)=\left\langle \tilde{K}^2\right\rangle r_\mathrm{corr}\tau_\mathrm{corr}$, then, substituting (18) into (9) and keeping the terms of the same order of smallness, we find [2]:

$$\alpha_{[100]\mathrm{KP}} \Rightarrow \alpha_{[100]\mathrm{c}} \equiv \frac{K_{0\mathrm{c}}\tilde{W}^{vv}_{0[100]}(T)}{\beta_0(T)k_BT} \cong \alpha_{[100]\mathrm{KP}} - \frac{1}{2}\sqrt{b(T)\left(\rho_{0\mathrm{d}}(T)\right)^{5/4}\left(\Psi(T)\right)^{-1/4}}\,,$$

$$k_\mathrm{KP} \Rightarrow k_\mathrm{c} \cong k_\mathrm{KP}(T)\sqrt{1-\frac{1}{4}\sqrt{b(T)\left(\rho_{0\mathrm{d}}(T)\right)^{1/4}\left(\Psi(T)\right)^{-5/4}}}\,,$$

where

$$b(T)=r_\mathrm{corr}\tau_\mathrm{corr}D(T)\frac{\left\langle \tilde{K}^2\right\rangle}{K_0^2},\;\; \Psi(T)=\frac{\tilde{\mathrm{B}}^{vv}([100])}{\tilde{W}^{vv}_{0[100]}}\,.$$

Hence, under fluctuations at issue, the spatial period of such a dissipative structure is determined by kinetic characteristics too (besides of irradiation parameters).

Correspondingly, the temperature dependences of a nanoscale period of modulated structure of vacancies' subsystem with taking into account empirical temperature dependence of density of dislocations, $\rho_{0\mathrm{d}}(T)$, and influence of external fluctuations of rate of generation of defects, which are characterized by the correlation radius r_corr, correlation time τ_corr, and coefficient of variation $\sqrt{\left\langle \tilde{K}^2\right\rangle}/K_0$, are presented in figures 12(a), 12(b). (The dashed line in figures 12(a), 12(b) shows the dependence $d(T)$, obtained by extrapolation of the curves presenting experimental data on elastic moduli [37], coefficient of thermal expansion [38, 39] and dislocation density [43], outside boundary of range their determination.)

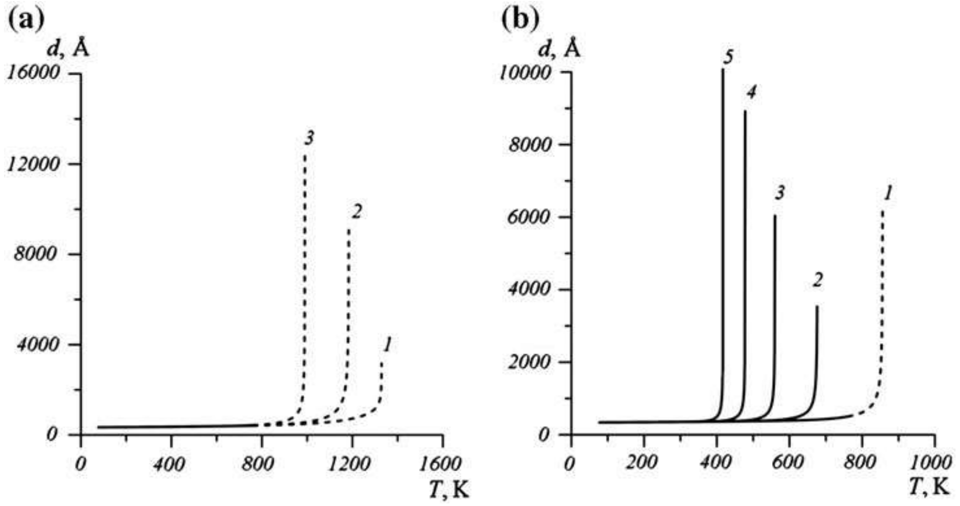

Figure 12. Temperature dependence of the nanoscale dissipative modulated-structure period of vacancies' subsystem with coefficient of diffusion of vacancies $D_v = 3.5\cdot10^{15}\exp\{(-1.3\text{ eV})/(k_BT)\}$ [Å$^2\cdot$s^{-1}] [35] and dislocation density, $\rho_{0d}(T)$ (17) (*a*) with fluctuations at the fixed values of ($\sqrt{\langle\tilde{K}^2\rangle}/K_0 = 1$) and the correlation time $\tau_{\text{corr}} = 10^4$ ps fluctuations, but at their various correlation radius r_{corr} (*1*—$r_{\text{corr}} = 10$ Å, *2*—$r_{\text{corr}} = 10^2$ Å, *3*—$r_{\text{corr}} = 10^3$ Å); (*b*) at the fixed values of correlation radius $r_{\text{corr}} = 10^2$ Å and correlation time $\tau_{\text{corr}} = 10^4$ ps, but at different value of the fluctuations $\sqrt{\langle\tilde{K}^2\rangle}/K_0$ (*1*—10, *2*—10^2, *3*—10^3, *4*—10^4, *5*—10^5

At high temperatures, the presence of fluctuations leads to the destruction of the dissipative modulated structure of vacancies' subsystem, which manifests itself in increase of temperature period. Fluctuations of rate of generation of defects are reducing with temperature decreasing. The dissipative modulated structure of vacancies' subsystem is formed in the conditions of radiation always. Due to superfast material cooling, it can be recorded even after the stopping of radiation [20].

Thus, the presence of both external fluctuations of the rate of generation of radiation point defects such as vacancies and inhomogeneities in the distribution of sinks (*e.g.*, dislocations) in f.c.c. crystal leads to a narrowing of the range of stability of dissipative modulated structures in the spatial distribution of density of vacancies' subsystem (figures 12(a), 12(b)).

Conclusions

For the description of occurrence of the dissipative modulated structures of vacancies' subsystem in an irradiated f.c.c. crystal, the mechanism obviously based on openness and non-equilibrium of the system and on nonlinearity character of bindings of vacancies with an environment is considered. For the first time, contributions to interaction between the generated vacancies, which are determined by both indirect long-range 'strain-induced' interaction (in particular, on far distances, of 'elastic' character) and 'direct' short-range 'electrochemical' interaction (basically, of the cohesive nature on close distances), are simultaneously considered. Interactions between vacancies cause instability of their uniform distribution and play a crucial role in the mechanism of formation of the modulated structures of vacancies' subsystem.

By the example of f.c.c. Ni lattice, the dispersion curve for the Fourier components of 'electrochemical' *v*–*v*-interaction energies is numerically calculated, taking into account features of such 'direct' interaction (in particular, its isotropy and attractive character). As found, at least, at distances of the several first coordination spheres' radii, considerable values of corresponding energies (in comparison with energies of 'strain-induced' interaction between the vacancies) provide domination of 'electrochemical' contribution (of cohesion nature) to the Fourier components of total *v*–*v*-interactions near the *BZ* centre of the reciprocal space for f.c.c. lattice.

The case of isothermal conditions of self-organization of formation precursor of the nanovoids' superlattice—the modulated structure in distribution of the vacancies generated by radiation, due to instability of their uniform distribution as a result of interaction between them in irradiated f.c.c. crystal, is considered.

The temperature dependences of the period of the dissipative modulated structures in distribution of vacancies and nanovoids are evaluated within the deterministic model.

As confirmed numerically, in conditions of the lack of both the fluctuations of generally non-uniform distributions of vacancies and their sinks and the fluctuations of rate of generation of vacancies within the irradiated f.c.c. crystal, instability of uniform distribution of vacancies is determined by a set of some parameters. These are: (i) the diffusivity of vacancies (and their migration-activation energy), (ii) the characteristic lifetime of vacancies before absorbing by sinks, (iii) a coefficient characterizing the efficiency of interaction of vacancies with sinks, and (iv) the Fourier components of energies of total ('strain-induced' and 'electrochemical') interactions between the vacancies corresponding to vicinity of the centre of the Brillouin zone of reciprocal space of f.c.c. lattice. Under the above-mentioned fluctuations, the condition of instability of uniform distribution of vacancies is also characterized by the correlation parameters: (v) an effective radius of spatial correlation of fluctuations of rate of generation of vacancies, (vi) a time of correlation of fluctuations of rate of vacancies' generation, and (vii) a variation coefficient for rate of vacancies' generation.

Period of dissipative modulated structure of vacancies' subsystem (including nanoscale period) decreases with temperature increasing in the conditions of constancy of density of dislocations that is determined, first of all, by the 'electrochemical' interactions of vacancies in absence of both the external fluctuations of nonzero rate of generation of radiation point defects such as vacancies and the internal fluctuations of inhomogeneity of irradiated f.c.c. crystal such as dislocations.

As revealed, the period $d(T)$ of the stationary dissipative modulated structures of vacancies' subsystem essentially depends on density of sinks for vacancies. The account of empirical temperature dependence of density of dislocations as sinks for vacancies in f.c.c. crystal reveals an expansion of the temperature range of stationary presence of the modulated structure with a finite nanoscale period. As numerically shown, the account of empirical temperature dependence of dislocation density, namely, the decreasing of dislocation density with increasing temperature, leads to increasing period $d(T)$ of dissipative modulated structure of vacancies' subsystem. This is caused by an entropy factor and 'electrochemical' interactions between the vacancies.

For the first time, an influence of temperature dependence of density of dislocation sinks for vacancies and energy parameters of vacancies' interactions in f.c.c. crystal on other characteristics of the modulated structures of vacancies' subsystem (in particular, on a critical temperature of their initiation) is taken into account. As shown, for the case of account of temperature dependence of the sinks' density for vacancies, the estimated value of critical temperature of formation of dissipative structure is rising.

As demonstrated, the parametric dependence of the nanoscale period d of the stationary dissipative modulated structures of a subsystem of vacancies on rate of their generation is nonlinear and can correspond to deterioration or improvement of functional properties of a material, depending on radiation intensity. With increasing the rate of generation of vacancies in f.c.c. crystal, the temperature range of stability of their modulated structures is extending.

As confirmed, the period of the stationary dissipative modulated structures of a vacancies' subsystem parametrically depends in non-linear way on the diffusion coefficient of vacancies in f.c.c. crystal. Reduction of mobility of vacancies promotes shift of a range of stability of dissipative modulated structures of the vacancies' subsystem towards higher temperatures.

As quantitatively confirmed, unlike the modulated structures arising in closed vacancies' subsystem of f.c.c. crystal by spinodal mechanism of relaxation (see Refs. [57, 58]), the period of the stationary (dissipative) modulated structure of the open nonequilibrium subsystem of vacancies in an irradiated f.c.c. crystal is essentially determined by both their kinetic parameters (diffusivity, characteristic time of a life before absorption by sinks, and coefficient characterizing efficiency of interaction of vacancies with dislocations) and characteristics of an irradiation (first of all, by its intensity and rate of generation of point defects by it).

In the case of nanovoids, within the continuum approximation, the period of a superlattice in the distribution of nanovoids is increasing with temperature, since it is determined only by their ‘elastic’ interaction.

Besides, nonlinear dependence of the period $d(T)$ of the stationary dissipative modulated structures of vacancies’ subsystem on parameters of correlation of external fluctuations is numerically investigated, namely, on radius of spatial correlation (of fluctuations of rate of vacancies’ generation), time of correlation (of fluctuations of rate of vacancies’ generation), and variation factor (of rate of vacancies’ generation). Investigation of fluctuations of vacancies’ generation rate shows that, with increase in radius of spatial correlation (of fluctuations of rate of generation of vacancies) and/or in a variation factor (of rate of generation of vacancies), the temperature range of stationary presence of the dissipative modulated structures of vacancies’ subsystem (with the finite period $d(T)$) in an f.c.c. crystal is narrowed.

For comparison, the hypothesis is numerically confirmed and illustrated as regards the possibility of formation of a superlattice (of the finite period) from ‘elastically’ interacting nanovoids after their ‘nucleation’ in vicinities of those sites of (irradiated) f.c.c. crystal, in which density of (clustered) vacancies is increased in the certain interval of temperatures.

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