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Statistical Characteristics of Distribution of Radiation-Induced Defects under Random Generation

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***Abstract*—**We consider fluctuations of defects density taking into account their interaction. Stochastic field of displacement generation rate gives random defect distribution. We determinate statistical characteristics (mean and dispersion) of random field of point defect distribution as function of defect generation parameters, temperature and properties of irradiated crystal.

***Keywords*—**Irradiation, Primary Defects, Interaction, Fluctuations.

I. Introduction

THE essential property changes in structural materials are induced by irradiation [1].

The main reason of this is radiation-induced defects of the material structure. Defect generation due to irradiation gives rise to microstructural evolution and results in changes in material properties. When a high-energy particle collides with lattice atoms in a solid, the displacement reactions produce non-equilibrium point defects within a range of nanometer for several picoseconds. The radiation damage event is concluded when the displaced atom (also known as the primary knock-on atom, PKA) comes to rest in the lattice as an interstitial atom. This event lasts about 10^{-11} s. Then such defects diffuse over macroscopic length and time scales and forms a new secondary structure by interacting with other point and extended defects. This secondary structure of defects significantly alters the materials properties.

Amount of defects produced by one high-energy particle and their distribution inside material depends on type and energy of particle. If it is low energy, only separate defects is generated. If energy is high enough, cascades of defects and tracks are formed.

Passing through material high-energy particle can produce one or several primary knock-on atoms from the lattice sites. In turn they displace other atoms of lattice, etc. As result one or more dense cascade of atomic displacements are generated. Such cascades contain from a few hundred to tens of thousands of displaced atoms. Ones of them are separate point defects (interstitial atoms and vacancies), other ones create small clusters. The interstitial atoms, vacancies and their small clusters are distributed inside cascade area in a random way.

Development of secondary structure of radiation-induced defects depends on primary defect distribution. Distribution of primary defects is formed as result of a large number of collisions between high-energy particles and atoms of solid; sequential diffusion and drift due to long-range interaction.

The real distribution of defects formed during irradiation cannot be represented in the form of uniformly distributed single Frenkel pairs over the volume. Nature of defect generation is inherently stochastic function because place and time of each collision are random events. Defect distribution after each collision is random function of time and coordinates too.

In the present article we obtain statistical characteristics of stochastic distribution of radiation-induced defects which need to describe development of secondary structure of the radiation-induced damage. We take into account long-range interaction between point defects and absorption point defects by extended ones which can consider as sinks for point defects. The long-range interaction can be of different nature. For big distances which are much more lattice distance it is an elastic interaction first of all [2].

II. Model and Basic Equations

Let us consider an irradiated crystal under stationary conditions of irradiation. The crystal defects (vacancies, interstitial atoms) are created and accumulated in the crystal as a result of irradiation. Defects are created by random way. The rate of defect generation is spatially homogeneous and stationary stochastic field. All characteristics of this field are assumed well-known. Radiation-induced defects have a finite lifetime because they are mobile enough and can be absorbed by different kinds of sinks for example by dislocations, grain boundaries, and so on. The absorption of interstitial atoms is much more than vacancies since the diffusion of the interstitial atoms is much quicker than the one of the vacancies. Thus the concentration of the interstitial atoms is much more than the vacancy concentration. It allows us to neglect recombination and take into account the defects of only one type.

Each defect is a centre of dilatation. So the defects interact by means of elastic forces [3]-[5]

$$F(r,r') = -\nabla U(r,r') \quad (1)$$

where $U(r,r')$ is potential of interaction.

For example here is potential for cubic crystal lattice

$$U(r,r') = \frac{3\Delta v^2}{8\pi|r-r'|^3}\left(\frac{\overline{K}}{C_{11}}\right)^2 C_a \Phi(\vartheta_x,\vartheta_y,\vartheta_z) \quad (2)$$

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where

$$\Phi(\vartheta_x, \vartheta_y, \vartheta_z) = \left[-3 + 5\left(\cos^4(\vartheta_x) + \cos^4(\vartheta_y)\right) + \cos^4(\vartheta_z)\right]$$

The force between defects in vicinity of point ***r*** and all other defects is

$$F(r) = -n(r)\nabla_r\left(\int U(r - r')\,n(r')dr'\right) \qquad (3)$$

We assume here that all forces are additive. Here *n* is concentrations of defects, *U(**r-r'**)* is potential of their interaction.

If defects' distribution is homogenous, the force equals zero.

We can take into account influence of the interaction between defects on diffusion by means of introduction the forces in flux of defects the following way

$$j = -D\left(\nabla n - \frac{n(r)F(r)}{kT}\right) \qquad (4)$$

Now flux of defects ***j*** depends on gradient of defects and force between defects. Here *T* is the crystal temperature, *k* is Boltzmann's constant.

Defects' density *n* changes due to generation by irradiation (*K)*, annealing ***(n/τ)*** and diffusion (div***j)***

$$\frac{\partial n}{\partial t} = div(J) + K(\vec{r}, t) - \beta n \qquad (5)$$

Substituting (4) in (5) gives

$$\frac{\partial n}{\partial t} = div\left(D\nabla n - \frac{Dn\vec{F}(r)}{T}\right) + K(\vec{r}, t) - \beta n \qquad (6)$$

where *K(**r**,t)* is stochastic field of defect generation rate, $\beta(T) = \rho_d D(T)$ is the inverse lifetime of defects with respect to absorption by sinks (dislocations), and the average dislocation density is ρ_d. $D = D_0 \exp(-E_m / T)$ is the diffusion coefficient of defects, E_m - migration energy. The average value, *K*, of defect generation rate, $K(\vec{r}, t)$, the spatial and temporal correlation functions, $<K(r_1,t_1)\ K(r_2,t_2)>$, and spectral density, *G(k,t),* of defect generation rate are assumed to be known.

It is well known that a periodical change of microstructure is developed due to non-linear elastic interaction between radiation defects [6]-[8]. When external fluctuations are small stochastic equations turn into deterministic ones. In this case the formation of periodical dissipative structures was described via self-organization formalism in [9], [10].

In the present work the external fluctuations is taken into account and statistical characteristics of defects distribution are found. The problem is solved in the approximation of the microscopic equations averaged sinks and within correlation theory [11].

III. Average and Dispersion

Averaging (6) gives that the average defect concentration is stationary homogenous defects' distribution and is equal to $\bar{n} = K/\beta$.

Separating in (1) deterministic (average) $\bar{n}$ and random parts $\tilde{n}(r,t)$ gives

$$\frac{\partial \tilde{n}}{\partial t} = div\left(D\nabla\tilde{n} - \frac{D\tilde{n}\vec{F}(r)}{T}\right) + \tilde{K}(\vec{r}, t) - \beta\tilde{n}$$

Being interested in a stationary homogeneous random field defect density, we build the correlation function of the density of defects:

$$< \tilde{n}(\vec{r}_1, t_1)\tilde{n}(\vec{r}_2, t_2) >= \\ = \int_{-\infty}^{t_1} d\tau_1 \int_{-\infty}^{t_2} d\tau_2 \int_{-\infty}^{\infty} d\vec{k}\,G(\vec{k}, \tau_1 - \tau_2)e^{-\lambda(\vec{k})(t_1 + t_2 - \tau_1 - \tau_2) + i\vec{k}(\vec{r}_1 - \vec{r}_2)}$$

where

$$G(\vec{k}, \Delta t) = \frac{1}{(2\pi)^3}\int < \tilde{K}(\vec{r}_1, t)\tilde{K}(\vec{r}_1 + \vec{r}, t + \Delta t) > e^{-i\vec{k}\vec{r}}d\vec{r} \ ,$$

,

$$\lambda(\vec{k}) = k^2 D(1 - \frac{\bar{n}V(\vec{k})}{T}) + \beta ,$$

and

$$V(\vec{k}) = \left(\int_{-\infty}^{\infty} d\vec{r}\,U(r)e^{-i\vec{k}\vec{r}}\right) \Bigg/ \lim_{k \to o}\left(\int_{-\infty}^{\infty} d\vec{r}\,U(r)e^{-i\vec{k}\vec{r}}\right)$$

Taking in (2) $t_1 = t_2, \vec{r}_1 = \vec{r}_2$,.we obtain the dispersion of distribution of defects density.

Let us assume that at one unit of time in the unit of a crystal's volume, *m* actions defect formation are happening in moments of time ***t***, and, hence, in the points of example ***r***. The number *m* is a random value and has a Poisson distribution. The points $\vec{r}_i$ and moments of time t_i are also random values which are distributed uniform. In each action of defects formation in the region of volume $\Delta v = \Delta x \Delta y \Delta z$ with the centre at $\vec{r}_i$ at the time t_i a random number of defects $k_i \Delta v \Delta t$ is formed. Later on we shall consider that the defects distribution inside each region is uniform, and the sizes Δx, Δy, Δz and duration of time *Δt* for each of the actions are the same.

At the value *λ(k)* tending to zero (under a certain *k*) the dispersion of defects density increases up to infinity. This means that the stationary uniform defects density field is not stable and can take place not for every occurrence of radiation. The loss of stability of stationary uniform defects distribution is connected to the arising of preference of the defects drift above the diffusion. If the time between the two actions of defect movement (due to their interaction) is a lot higher than the development time of each of them $\delta t >> \Delta t$, then together with the increase the value δt the correlation function decreases exponentially with characteristic time $\lambda^{-1}(\vec{k})$.

In case when Δt is smaller than all of the characteristic times in the problem which responds to the limit $\Delta t \to 0$ at constant defect generation rate ($K = const$) the fluctuations of the defects density becomes δ-correlated. Such approximation can be used in the formation of single defects and low energy cascades.

At constant increase of the average speed of defects formation-dispersion density of their distribution decreases as $\overline{m}$ increases.

Numerical evaluation of the value of the relative defects density show that at $\overline{K} = 10^{-4}$ dpa/s, T=800 K and the number of displacements in the centre of the cascade of every thousand's atom, the relation $\langle \tilde{n}^2 \rangle / \overline{n}^2$ has a value $1.5 \cdot 10^{-3}$, at. $T = 900K$ - $3 \cdot 10^{-1}$, and at $T = 1000K$ - 4, but that is not within the performed approximations.

IV. Conclusion

The examination of the stochastic nature of the defect distribution in irradiated crystals shows that fluctuations of defect density can be large enough. During stationary irradiation the defect density can reach much higher values than the expected steady-state values. It can lead to change of typical operation and an accident, e.g. for a nuclear reactor.

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