

Breather mechanism of the void ordering in crystals under irradiation

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ABSTRACT

The void ordering has been observed in very different radiation environments ranging from metals to ionic crystals. In the present paper the ordering phenomenon is considered as a consequence of the energy transfer along the close packed directions provided by self-focusing discrete breathers. The self-focusing breathers are energetic, mobile and highly localized lattice excitations that propagate great distances in atomic-chain directions in crystals. This points to the possibility of atoms being ejected from the void surface by the breather-induced mechanism, which is similar to the focuson-induced mechanism of vacancy emission from voids proposed in our previous paper. The main difference between focusons and breathers is that the latter are stable against thermal motion. There is evidence that breathers can occur in various crystals, with path lengths ranging from 10^4 to 10^7 unit cells. Since the breather propagating range can be larger than the void spacing, the voids can shield each other from breather fluxes along the close packed directions, which provides a driving force for the void ordering. Namely, the vacancy emission rate for “locally ordered” voids (which have more immediate neighbors along the close packed directions) is smaller than that for the “interstitial” ones, and so they have some advantage in growth. If the void number density is sufficiently high, the competition between them makes the “interstitial” voids shrink away resulting in the void lattice formation. The void ordering is intrinsically connected with a saturation of the void swelling, which is shown to be another important consequence of the breather-induced vacancy emission from voids.

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1. Introduction

Void ordering is observed in a number of bcc metals (Mo, W, Nb and Ta), the fcc metals Ni and Al, the hcp Mg, and some alloys, *e.g.* stainless steel, under neutron and heavy-ion irradiations (see *e.g.* reviews [1–3]). A similar phenomenon is observed under electron irradiation of ionic crystals, such as natural fluorite (CaF_2), where calcium colloids nucleate and grow randomly, and subsequently form a simple cubic superlattice, which copies the fluorine crystal lattice. Since fcc calcium crystallites are coherent with CaF_2 structure, they can be viewed as voids in the fluorine sub-lattice. The void ordering is often accompanied by a saturation of the void swelling, which makes an understanding of the underlying mechanisms to be both of scientific significance and of practical importance for nuclear engineering.

Currently the most popular void ordering concept is based on the mechanisms of *anisotropic interstitial transport* along the close packed directions [3–6] or planes [7]. In these models, anisotropic diffusion of self-interstitial atoms (SIA) or propagation of small SIA loops along the close packed directions makes the competition be-

tween growing voids to be dependent on spatial void arrangements.

A common difficulty inside the concept of anisotropic SIA transport is the explanation of saturation and even reduction in the void swelling accompanying the void lattice formation [8].

In the present paper, the ordering phenomenon is considered as a consequence of *the energy transfer* along the close packed directions provided by long propagating self-focusing breathers [9–11]. In Section 2, a modification to the rate theory is shortly reviewed, which includes the mechanisms of vacancy emission from voids due to the void interaction with focusons [12] and unstable Frenkel pairs [13]. In Section 3, the long propagating self-focusing breathers are considered as an alternative mechanism for the void ordering and swelling saturation.

2. Mechanisms of vacancy emission from voids

It is known that a considerable part of the primary knock-on atom energy is spent on the production of *unstable Frenkel pairs* and *focusons* [13]. Focusons transfer energy along close packed directions of the lattice, but there is no interstitial transport by a focusing collision. In an ideal lattice a focuson does not produce de-

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fects along its path. However, if the focuson has to cross an extended defect (ED), such as a void surface, a vacancy may be produced in its surroundings as has been demonstrated in [14] by means of MD simulations. The focuson propagation range in ideal lattice, l_f^0 , decreases with increasing lattice temperature due to random thermal atomic displacements. So the efficiency of the vacancy production by this mechanism decreases with increasing temperature.

Another mechanism of the radiation-induced vacancy emission from EDs is based on the production of unstable Frenkel pairs (UFPs) near EDs. An ED such as a void or a dislocation is surrounded by a region of a radius R_{cap} , in which a point defect is unstable since it is captured by the ED athermally [15]. The capture radius for self-interstitial atoms is larger than the one for vacancies due to the lower migration energy and stronger interaction with ED. If a regular atom in the region $R_{cap}^v < r < R_{cap}^i$ gets an energy $E > E_v$ it may move to an interstitial position, where it can be athermally captured by the ED, leaving behind it a stable vacancy. The process can be described as an effective emission of a vacancy by the ED due to its interaction with an UFP. As the energy of the system is increased as a result of vacancy formation, the minimum transferred energy, E_v , should exceed the energy of vacancy formation, which is considerably lower than the energy of stable Frenkel pair formation.

These mechanisms have been incorporated in the rate theory [12,13] by modifying the so called *local equilibrium concentrations of vacancies*, c_v^{eq} , which are determined by the rates of vacancy emission from EDs due to thermal or radiation-induced fluctuations of energy states of atoms surrounding the EDs. Generally, c_v^{eq} is given by the sum of the thermal and the radiation-induced constituents

$$c_v^{eq} = c_v^{th} + c_v^{irr}, \quad c_v^{th} = \exp(-E_v^f/k_B T), \quad (1)$$

$$c_v^{irr} = K_F b l_F^0 / D_v + K_{UFP} b (R_{cap}^i - R_{cap}^v) / D_v, \quad (2)$$

where K_F is the effective production rate of focusons and K_{UFP} is the UFP production rate, E_v^f is the vacancy formation energy at a given ED and D_v is the vacancy diffusion coefficient, b is the interatomic spacing.

Now the void growth (or shrinkage) rate is given by the usual expression of the rate theory

$$dR/dt = [Z_{i,v}^V D_v \bar{c}_v - Z_{i,v}^V D_v c_v^{eq} - Z_{i,v}^V D_i \bar{c}_i] / R, \quad (3)$$

where $Z_{i,v}^V$ is the void capture efficiency for vacancies (subscript “v”) and SIAs (subscript “i”), $\bar{c}_{i,v}$ is the mean concentration of point defects determined by the rate equations. As can be seen from Eqs. (2) and (3), the product $D_v c_v^{irr}$ determines the rate of the void *radiation-induced* dissolution/shrinkage. The latter does not depend on temperature, and it is determined by the production rates of focusons and UFPs, and by the material parameters, such as the focuson propagation range, and the SIA-vacancy capture range difference. Assuming $R_{cap}^i - R_{cap}^v \approx b$ one finds that the UFP effect dominates over the focuson effect if $l_F^0 < 50b$, which is likely to be the case due to the instability of focusons against thermal vibrations [13]. However, there exists another, essentially non-linear, mechanism of the excitation propagation over great distances, which is called self-focusing discrete breathers.

3. Breather mechanism of the void shrinkage

As the incident focuson energy is dispersed but the available kinetic energy still far exceeds that of phonons, atoms experience large displacements from their equilibrium positions, while remaining at their original lattice sites. Propagation of the corresponding lattice vibrations may be governed by nonlinear forces.

This may result in formation of a vibrational particle-like soliton, which can propagate great distances in atomic-chain directions in crystals. It was shown theoretically that the presence of surrounding lattice prevents the propagation of Toda-like solitons but allows the propagation of breather-like solitons (or so called discrete breathers (DB) [9–11]. According to molecular dynamic simulations, the DBs are mobile, highly anharmonic longitudinal vibrations that are sharply localized in longitudinal direction and practically across one atomic distance in the transverse direction. The main difference between focusons and breathers is that the latter are stable against thermal motion. There is evidence that DBs can occur in various crystals, with path lengths ranging from 10^4 to 10^7 unit cells. Specifically, when a crystal of muscovite (an insulating solid with a layered crystal structure) was bombarded at a given point, atoms were ejected from remote points on another face of the crystal, lying in atomic-chain directions at more than 10^7 unit cells distance from the site of bombardment [11]. There is evidence that breathers can occur in non-layered crystals, but with shorter path lengths of order 10^4 unit cells. This was reported in connection with radiation damage studies in diffusion of interstitial ions in austenitic stainless steel [10]. This points to the possibility of atoms being ejected from the void surface by the breather-induced mechanism, which is similar to the focuson-induced mechanism of vacancy emission from voids. This would modify the void “solubility limit”, which is determined by c_v^{irr} given now by the expression similar to Eq. (2) but depending on the breather production rate, K_B , and the path length, l_B :

$$c_v^{irr} \approx K_B b l_B / D_v. \quad (4)$$

The demonstrated stability of breathers against thermal motion and ubiquitous occurrence makes this mechanism a promising candidate for the explanation of the radiation-induced void dissolution at decreasing irradiation temperature [16,17] and related phenomena such as the void lattice formation and swelling saturation [8].

According to the present theory, ordering phenomena might be a natural consequence of the energy transfer along the close packed directions provided by DBs. If the DB length is larger than the void spacing, the voids shield each other from the DB fluxes along the close packed directions, which provides a driving force for the void ordering, as illustrated in Fig. 1.

The emission rate for “locally ordered” voids (which have more immediate neighbors along the close packed directions) is smaller than that for the “interstitial” ones, and so they have some advan-

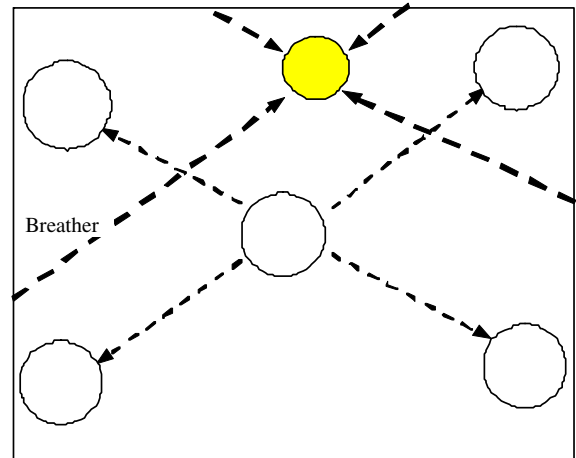


Fig. 1. Illustration of the dissolution of a void in the “interstitial” position due to the absorption of breathers coming from larger distances as compared to “regular” voids that shield each other from the breather fluxes along the close packed directions.

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