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To cite this version:

Alexander V Barashev, Stanislav I Golubov. On the onset of void ordering in metals under neutron or heavy-ion irradiation. Philosophical Magazine, 2010, 90 (13), pp.1787-1797. 10.1080/14786430903482735 . hal-00587305

HAL Id: hal-00587305

https://hal.science/hal-00587305v1

Submitted on 20 Apr 2011

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Journal:	*Philosophical Magazine & Philosophical Magazine Letters*
Manuscript ID:	TPHM-08-Sep-0320.R2
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	02-Sep-2009
Complete List of Authors:	Barashev, Alexander; The University of Liverpool, Engineering Golubov, Stanislav; ORNL, Materials Science and Technology Division; University of Tennessee, Center for Materials Processing
Keywords:	kinetics, lattice defects, neutron irradiation, non-equilibrium phenomena, pattern-related phenomena, radiation effects
Keywords (user supplied):	displacement cascades, interstitial clusters

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On the onset of void ordering in metals under neutron or heavy-ion irradiation

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Formation of void lattices is observed in a number of metals and alloys under high-energy particle bombardment. Here we derive the conditions for destabilisation of homogeneous void arrangement using an approach developed for the description of lane formation in pedestrian crowds. The model is based on the Foreman's mechanism of void alignment due to one-dimensionally-migrating clusters of self-interstitial atoms. The results show that spatial correlations between voids should exist above some very small size, unless correlations with other defects prevail. It is shown that spatial correlations of voids with dislocations and second-phase precipitates should also evolve and provide a powerful driving force for further swelling.

Key words: void swelling, void lattice, displacement cascades, interstitial clusters.
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1. Introduction

The formation of a void lattice was first reported in 1971 by Evans [1] in molybdenum under nitrogen ion irradiation, by Kulchinski, Brimhall and Kissinger [2] in nickel under selenium ion bombardment and by Wiffen [3] in molybdenum, niobium and tantalum under neutron irradiation. Since then it was observed in bcc tungsten, the fcc Al, the hcp Mg, and some alloys. Jäger and Trinkaus [4] reviewed the characteristics of defect ordering, where many original references can be found, and analysed the theories proposed, including those based on the elastic interaction between voids, phase instability theory and low-dimensional atomic transport. They concluded that in cubic metals the void ordering is probably due to the one-dimensional (1-D) glide of self-interstitial atom (SIA) clusters along close-packed crystallographic directions. Two features of void ordering support this conclusion. First, that the symmetry and crystallographic orientation of a void lattice are always the same as those of the host lattice. And second, that the void lattices are formed under neutron and heavy-ion but not electron irradiation, *i.e.* when the primary damage is produced in displacement cascades. The only exception of void ordering during electron irradiation in a stainless steel containing a high concentration of nitrogen [5] was proposed to be most probably due to SIA loop punching from small nitrogen bubbles preferentially absorbing SIAs. Voids in hcp Mg (and bubbles in hcp Ti, Co, Zr and some Zr alloys) can order in planes parallel to the basal plane with variable void plane separation [6,7]. Jäger and Trinkaus concluded that for hcp metals a decision between 1-D or 2-D SIA transport proposed by Evans [8-10] was not possible at the moment due to the lack of a sufficient body of information. Now we know from molecular dynamics (MD) simulations using empirical potentials for the inter-atomic interaction that SIA clusters bigger than four SIAs in hcp Zr migrate one-dimensionally in the basal plane [11]. Hence, the observed planar void ordering in must also be accounted for using the same mechanism as for the void lattices in cubic metals.

It is worth noting that already in 1972 Foreman [12] suggested that voids are aligned along close-packed directions by 1-D SIA fluxes. Dubinko *et al*. [13] were first to study the effect of the glide of perfect interstitial loops due to interaction with voids on void lattice formation. Then, in 1992, Foreman *et al*. [14] discovered 1-D mobility of small SIA clusters in

MD studies of displacement cascades in copper. This finding resolved a serious problem of the theory called 'Singh-Foreman catastrophe' [15], that is, accumulation of a high density of immobile SIA clusters produced in displacement cascades that is not observed in experiments, and promoted formulation of the 'Production Bias Model' of radiation damage in its modern form. The model succeeds in explaining several striking observations, for example, enhanced swelling rates near grain boundaries [16] and in materials with small grain size [17], and under neutron compared to electron irradiation [18,19]. This is due to the recognition of two distinguishing features of defect production by high-energy recoils: first, the formation of SIA clusters directly in displacement cascades, as shown both experimentally [20] and in MD simulations [14,21,22] (see also review [23]); and, second, the 1-D mobility of SIA clusters [14,24-27].

After the review by Jäger and Trinkaus [4], several papers were published which exploited the Foreman's idea for the description of the void lattice. Some of them used Monte Carlo method to simulate void lattice formation (*e.g.* [28-30]). In our view, these attempts have not added much to the very Foreman's idea. This is mainly because they suffer from an intrinsic deficiency of the small box size compared to the mean-free path of the SIA clusters, which introduces methodological errors in the simulations, as partly discussed at the end of this paper. Two attempts were made to describe analytically the void lattice formation, but both failed in our view. In the analysis by Walgraef and Ghoniem [31], reactions of the 1-D diffusing SIA clusters with voids were incorporated incorrectly into the basic equation system (compare, *e.g.* equation system (1) in [31] with equations (5) and (6) in [18]). Another attempt was made by Semenov and Woo [32,33]. Their analysis was based on the assumption of the existence of the stationary size-distribution function of voids. This led to a conclusion that the formation of a void lattice is only possible if the fraction of the SIAs in the form of 1-D mobile clusters is less than 1% and thus less than the dislocation bias. However, as shown in [34], the stationary state does not exist for such a small fraction. In addition, the value of 1% is at least an order of magnitude smaller than that obtained in MD simulations [22].

In this paper we consider the void ordering in the framework of a model developed for the lane formation in pedestrian crowds [35]. It suits naturally to the description of the phenomenon, since, according to experiments, voids are first nucleated in a random arrangement and only then form a lattice, the perfection of which increases with increasing irradiation dose [4]. The main aim of the present work is to derive general conditions for the onset of void ordering, after which the conventional rate equations should not apply.

2. Analysis

2.1. *Basic equations*

We assume that the displacement cascades produce 3-D mobile single vacancies and SIAs and 1-D mobile SIA clusters. The fraction of the clustered SIAs is denoted by $\varepsilon_{\mathrm{i}}^{\mathrm{g}}$. We also assume that the void nucleation stage is over and the mobile defects interact only with already existing voids of the number density N and dislocations of the density ρ. The swelling rate is then [17]

$$\frac{dS}{d\phi} = p_{\mathrm{v}} - (1-\varepsilon_{\mathrm{i}}^{\mathrm{g}})p_{\mathrm{i}} - \varepsilon_{\mathrm{i}}^{\mathrm{g}} p_{\mathrm{cl}} = \\ = \frac{4\pi rN}{4\pi rN + Z_{\mathrm{v}}\rho} - (1-\varepsilon_{\mathrm{i}}^{\mathrm{g}})\frac{4\pi rN}{4\pi rN + Z_{\mathrm{i}}\rho} - \varepsilon_{\mathrm{i}}^{\mathrm{g}}\frac{\pi r^2 N}{\pi r^2 N + \pi\rho r_{\mathrm{d}}/2}, \qquad (1)$$

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where $S = 4\pi r^3 N/3$, r is the mean void radius, ϕ is the irradiation dose in displacements per atom, which accounts for intra-cascade recombination, p_j is the probability that a *j*-type defect is absorbed by a void, Z_v and Z_i are the capture efficiencies of dislocations for vacancies and single SIAs, respectively, and r_d is the dislocation capture radius for SIA clusters. The main purpose of writing equation (1) is to describe the reaction scheme and introduce probabilities p_j.

We use a mathematical model similar to that developed for the description of lane formation in pedestrian crowds [35]. With the total void density to be constant, the local density changes due to voids moving in and out of the local area and hence obeys a continuity equation

$$\frac{\partial N}{\partial \phi} = -div(N\mathbf{V} - D\nabla N), \tag{2}$$

where $\mathbf{V}$ is the mean velocity and D is the diffusion coefficient of voids, defined locally:

$$\mathbf{V} = \langle \sum_j \nu_j \Delta_j \rangle, \tag{3}$$

$$D = \frac{1}{6}\langle \sum_j \nu_j \Delta_j^2 \rangle. \tag{4}$$

Here, $j = \mathrm{v,i,cl}$ for the components corresponding to void collisions with vacancies, single SIAs and SIA clusters, respectively, Δ_j are the vectors of void displacements after collisions and the averaging is performed over voids in the local region. The collision frequencies are $\nu_\mathrm{v} = p_\mathrm{v}/\Omega N$, $\nu_\mathrm{i} = \left(1-\varepsilon_\mathrm{i}^\mathrm{g}\right)p_\mathrm{i}/\Omega N$ and $\nu_\mathrm{cl} = \varepsilon_\mathrm{i}^\mathrm{g} p_\mathrm{cl}/m\Omega N$, where Ω is the atomic volume and m is the mean number of SIAs in a cluster. In the following two sections, we derive the void velocity and diffusion coefficient as functions of microstructure parameters.

2.2. *Diffusion coefficient of void*

A void of radius r contains $M = 4\pi r^3/3\Omega$ vacancies and arrival of an additional vacancy to it should displace its centre of mass by a vector, which is approximately equal to

$$\Delta_\mathrm{v} = \frac{r\mathbf{n}}{M+1} \approx \frac{3\Omega}{4\pi r^2}\mathbf{n}, \tag{5}$$

where $\mathbf{n}$ is a unit vector normal to the void surface at the point of defect absorption. Here we use a conventional assumption that a defect is absorbed by a void at the point they touch each other and that the local surface diffusion is sufficient to keep void spherical (see, *e.g.* kinetic Monte Carlo simulations [28,30] and analytical treatment [36]). This issue was generally discussed by Balluffi [37] and the assumption seems reasonable for a small void at low temperature, when the void surface represents a highly distorted region and the surface diffusion is limited to distances of the order of a facet size. Arrival of an SIA to the same point should shift the void by the same distance but in the opposite direction $\Delta_\mathrm{i} = -\Delta_\mathrm{v}$, while a cluster of m SIAs should cause a proportionally larger displacement $\Delta_\mathrm{cl} = -m\Delta_\mathrm{v}$. Substituting these into equation (4), with the aid of equation (1) and taking $p_\mathrm{i} \approx p_\mathrm{v}$, one obtains

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$$D = \frac{3}{2N}\frac{\Omega}{\left(4\pi r^2\right)^2}\left[m\varepsilon_{\mathrm{i}}^{\mathrm{g}} p_{\mathrm{cl}} + (2-\varepsilon_{\mathrm{i}}^{\mathrm{g}})p_{\mathrm{v}}\right]. \tag{6}$$

2.3. *Void velocity*

The void velocity is determined by anisotropy of void collisions with mobile defects, hence by a nonzero $\nabla \nu_j$. Here, we assume that this anisotropy is due to existence of a gradient of void concentration $\nabla \nu_j \propto \nabla N$. An additional driving force due to gradient of void radius is ignored here for simplicity, to preserve the visual transparency of the original model of lane formation in pedestrian crowds (see also discussion in section 2.4 after equation (19)). Then, a component of the void velocity due to interaction with *j*-type defects can be calculated as an average over defects arrived to different points of the void surface

$$\mathbf{V}_j = \left\langle \frac{r}{\sigma}\int d\sigma \frac{\partial \nu_j}{\partial N}(\mathbf{n}\nabla N)\Delta_j \right\rangle_{L_j}. \tag{7}$$

Here, $\sigma = 4\pi r^2$ for 3-D and $\sigma = \pi r^2$ for 1-D migrating defects (separately for each cluster Burgers vector $\mathbf{b}_k$, $k=1$ to *n*, *n*=4 for the bcc and *n*=6 for the fcc crystal lattice), $d\sigma$ is the corresponding surface element and L_j is a characteristic size of the volume for averaging, which has replaced the averaging over different voids in the mean-field approach. For 3-D migrating vacancies and SIAs, this size is of the order of the mean-free path

$$L_{\mathrm{v,i}} \approx L_{\mathrm{3D}} \approx \left(4\pi r N + Z_{\mathrm{v}}\rho\right)^{-1/2}. \tag{8}$$

For 1-D migrating clusters, for each Burgers vector, it is of the order of the projection of the mean-free path L_{1D} on the direction of ∇N:

$$L_{\mathrm{cl}}^k = L_{\mathrm{1D}}^k \approx L_{\mathrm{1D}}\left|\cos\left(\mathbf{b}_k, \nabla N\right)\right|, \tag{9}$$

$$L_{\mathrm{1D}} = \left(\pi r^2 N + \pi\rho r_{\mathrm{d}}/2\right)^{-1}. \tag{10}$$

By performing the integration indicated in equation (7), one can obtain the following equations for the partial velocities:

$$N\mathbf{V}_{\mathrm{i}} = (1-\varepsilon_{\mathrm{i}}^{\mathrm{g}})A_{\mathrm{i}}\left\langle \nabla N\right\rangle_{L_{\mathrm{3D}}}, \tag{11}$$

$$N\mathbf{V}_{\mathrm{v}} = -A_{\mathrm{v}}\left\langle \nabla N\right\rangle_{L_{\mathrm{3D}}}, \tag{12}$$

$$N\mathbf{V}_{\mathrm{cl}} = \varepsilon_{\mathrm{i}}^{\mathrm{g}} A_{\mathrm{cl}}\frac{3}{4n}\sum_{k=1}^{n}\left\langle \nabla N + \left(\mathbf{e}_k, \nabla N\right)\mathbf{e}_k\right\rangle_{L_{\mathrm{1D}}^k}, \tag{13}$$

where $A_j = \left(p_j\right)^2/4\pi r N$ and $\mathbf{e}_k = \mathbf{b}_k/b$. As can be seen from equations (11) and (12), 3-D migrating SIAs and vacancies move voids towards regions of higher and lower void concentration, respectively, thus maximising their growth rate. The effect of SIA clusters is double fold. The first term in equation (13) is analogous to equation (11) for single SIAs and describes movement of voids along the void concentration gradient. The last term in the right-

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hand side of equation (13) describes movement of voids in the directions of the cluster Burgers vectors.

2.4. *Conditions for the onset of void ordering: a linear stability analysis*

Let us substitute equations (6) and (11)-(13) into equation (2) and analyse its stability to small variations of the void number density. Obviously, a homogeneous solution, N^{hom}, satisfies equation (2). To derive the basic conditions for its destabilisation, we apply the linear stability analysis and insert the *ansatz* $N = N^{\text{hom}} + \tilde{N}\exp(i\mathbf{qR} + a\phi)$, where $\mathbf{R}$ is the radius vector, $\mathbf{q}$ is a wave vector and a is the amplification factor. This results in the following equation

$$\frac{a}{q^2}e^{i\mathbf{qR}} = \varepsilon_{\text{i}}^{\text{g}} A_{\text{cl}} \frac{3}{4n}\sum_{k=1}^{n}\left[1+\cos^2\left(\mathbf{b}_k,\mathbf{q}\right)\right]\langle e^{i\mathbf{qR}}\rangle_{L_{1\text{D}}^k} + \\ + (1-\varepsilon_{\text{i}}^{\text{g}})A_{\text{i}}\langle e^{i\mathbf{qR}}\rangle_{L_{3\text{D}}} - A_{\text{v}}\langle e^{i\mathbf{qR}}\rangle_{L_{3\text{D}}} - De^{i\mathbf{qR}}. \tag{14}$$

We note that $3\sum_k \cos^2(\mathbf{b}_k,\mathbf{q}) = n$ in cubic structures, hence, for long waves, such that $q^{-1} >> L_{1\text{D}}$, equation (14) is reduced to (taking $p_{\text{i}} = p_{\text{v}}$ for simplicity)

$$\frac{a}{q^2} = \frac{\varepsilon_{\text{i}}^{\text{g}}}{4\pi rN}\left(p_{\text{cl}}^2 - p_{\text{v}}^2\right) - D < 0, \tag{15}$$

which is always negative since $p_{\text{cl}} \le p_{\text{v}}$ (voids do not shrink). For shorter wavelengths, we notice that the amplification factor a can be positive provided that two conditions are satisfied at the same time: (i) the third term in the right-hand side of equation (14) is zero and (ii) some of the terms of the sum are nonzero. The condition (i) requires $q^{-1} << L_{3\text{D}}$. The condition (ii) introduces limitations for both the magnitude and the direction of the wave vector. First, one needs $q^{-1} >> r$, otherwise all terms in the sum vanish. And, second, it requires $L_{1\text{D}}\left|\cos\left(\mathbf{b}_k,\nabla N\right)\right| << r$ for at least one *k*, *i.e.* the wave vector should be perpendicular to $\mathbf{b}_k$. The maximum a is achieved for a wave vector perpendicular to a plane containing any two Burgers vectors. In this case, two terms of the sum are nonzero, while the terms with other Burgers vectors are equal to zero, because their averaging is performed over distances $L_{1\text{D}}\left|\cos(\mathbf{b}_k,\nabla N)\right| \ge L_{3\text{D}}$.

Summarising the analysis presented above, we conclude that the most favourable conditions for destabilisation of the homogeneous solution are realised when

$$r << q^{-1} << L_{3\text{D}}, \tag{16}$$

$$\mathbf{q} \parallel [\mathbf{b}_k, \mathbf{b}_{k'}], \tag{17}$$

where $\mathbf{b}_k$ and $\mathbf{b}_{k'}$ ($k \ne k'$) are any two of *n* different Burgers vectors of the SIA clusters. These conditions define the void movement leading to formation of close-packed planes $\left[\mathbf{b}_k, \mathbf{b}_{k'}\right]$ of voids, and this is consistent with the observed isomorphism of the finally evolved void lattices and the host lattice structure. Substituting conditions (16) and (17) into equation (14), one obtains the destabilisation condition as

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$$a = q^2\left(3\varepsilon_{\mathrm{i}}^{\mathrm{g}} A_{\mathrm{cl}} / 2n - D\right) > 0\,. \tag{18}$$

Or, in a more explicit form, as

$$\frac{4\pi r^3}{3\Omega} > \frac{nm}{3}\left(1+\frac{\rho r_{\mathrm{d}}}{2r^2 N}\right)\left(1+\frac{2-\varepsilon_{\mathrm{i}}^{\mathrm{g}}}{\varepsilon_{\mathrm{i}}^{\mathrm{g}} m}\frac{p_{\mathrm{v}}}{p_{\mathrm{cl}}}\right). \tag{19}$$

Figure 1 shows the dependence of a critical void radius, above which voids start to order, on the void number density, given by equation (19). The calculations were performed for the bcc lattice (n=4), m=10, $\varepsilon_{\mathrm{i}}^{\mathrm{g}}$=0.5, $Z_{\mathrm{i}} = Z_{\mathrm{v}} = 1$ and two values of r_{d} and dislocation density shown in the figure. As can be seen from the figure, the critical void radius is very small, much smaller than the void saturation radius $\sim 2\pi r_{\mathrm{d}} / Z_{\mathrm{v}}$, predicted by equation (1) [16]. (The latter can readily be derived in the limiting case when the production bias is much higher than the dislocation bias: $\varepsilon_{\mathrm{i}}^{\mathrm{g}} >> B = Z_{\mathrm{i}} / Z_{\mathrm{v}} - 1$. For a comprehensive analysis, see an accompanying paper [38].)

[Insert figure 1 about here]

It is worth mentioning that the analysis presented here is similar to that used by Hähner and Frank [36]. The main difference is in consideration of a realistic mechanism for the lattice formation, which is supported by MD and first principal calculations, and is a requirement for explanation of some experimental data. Some better mathematical transparency of the present analysis is achieved by using several simplifying assumptions, for example that void velocity, equation (7), is proportional to the void concentration, while the contribution of the gradient of void radius is neglected. There are several reasons why gradients of void radius are not as important, but we have not found any concise explanation of this. Note, however, that according to the results obtained by Hähner and Frank, the fluctuations of void radii do not initiate instability, which supports our assumption. As far as we are concerned, Hähner and Frank were also the first to conclude that the void spacing in void lattices is likely to be determined by that in the disordered state, rather than be an 'intrinsic material parameter'. Although they used unrealistic mechanism for void ordering based on radiation-produced SIAs in metastable crowdion configuration, the main conclusion obtained in the present paper that void lattice should start for very small voids can be derived from their results in the limiting case, when the mean time before conversion of a crowdion to a dumbbell configuration is infinitely long: $\tau_{\mathrm{C}} \to \infty$. So, assuming that the sink strength of dislocations is negligible as compared to that of voids, which agrees with the experimental observations of void lattices, it can be obtained that void ordering should start at any void size and such wave vectors that perpendicular to the close-packed planes (*e.g.* {110} in the bcc crystal lattice) and which modulus satisfies the condition: $q^{-1} < L_{3\mathrm{D}}$. This is similar, but less stronger condition than the right-hand part of equation (16). The restriction corresponding to equation (19), which originates in diffusion of voids, is absent in the analysis by Hähner and Frank. Finally, the main important conclusion of the present work that the void ordering due to clusters of SIAs should start at very small voids is supported by their work, too.

Thus, the conditions for the onset of void ordering show that spatial correlations between voids should always be present, except for very early stages of irradiation, when voids are too small. Essentially, the real question is not why voids sometimes form super-lattices, but why they do not form them. We believe that we know the answer to the first question, although not all aspects of the process are yet understood. We suppose the answer to the latter question to be as follows. Spatial correlations always develop under cascade damage conditions. The void lattices represent only one type of such correlations, which is realised when the void number density is high enough. At lower void density, spatial correlations with other defects, *e.g.*

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second-phase precipitates and dislocations, are formed. Which correlations should prevail depends on the densities of different defects. In the analysis presented above we assumed that voids are correlated with each other rather than with other elements of microstructure. This is taken into account by assuming that the void velocity is caused by the gradient of void number density.

Let us derive applicability of this assumption for a system containing voids and edge dislocations. In the framework of the model considered, the probability that an SIA cluster has voids at both ends of its path is p_{cl}^2 and the probability that it has a void at one of the ends and a dislocation at the other end is $2p_{\mathrm{cl}}(1-p_{\mathrm{cl}})$. A void lattice should evolve if the former is much greater than the latter, *i.e.* when

$$r^2 N >> \rho r_{\mathrm{d}} . \tag{20}$$

Note that the dependence of the amplification factor on the defect densities in equation (18) is rather weak, hence it is most probable that this requirement determines the observed conditions for the void lattice formation, that is, high void and low dislocation density. The very absence of a void lattice, *i.e.* spatial correlations between voids, must be an indication that correlations of voids with other defects prevail.

2.5. *On spatial correlations between voids and other lattice defects*

It follows from the analysis that other microstructural features, *e.g.* dislocations and second-phase precipitates, must also be involved in shadowing of voids from the SIA clusters and establish spatial correlations with voids. So, for example, an existence of a gradient of dislocation density, should cause a void movement with the velocity given by equation (17), where N is replaced by ρ. The following analysis would be similar to that for void ordering and, if the inhomogeneity of the dislocation density is taken in the form $\rho = \rho^{\mathrm{hom}} + \tilde{\rho}\exp(i\mathbf{q}_{\mathrm{d}}\mathbf{R})$, the equation (18) for the amplification factor becomes

$$a = \frac{\tilde{\rho}}{\tilde{N}} q_{\mathrm{d}}^2 A_{\mathrm{d}}^2 \exp\left[i\left(\mathbf{q}_{\mathrm{d}} - \mathbf{q}\right)\mathbf{R} \right] - q^2 D , \tag{21}$$

where $A_{\mathrm{d}} = 3\varepsilon_{\mathrm{i}}^{\mathrm{g}} r_{\mathrm{d}} A_{\mathrm{cl}} / 4nr^2$. As can be seen, the first term in the right-hand side of equation (21) is real and positive if $\mathbf{q} = \mathbf{q}_{\mathrm{d}}$, *i.e.* when spatial positions of voids correlate with dislocations.

3. Concluding remarks

The conditions for the onset of void ordering have been analysed in the framework of a model developed for the lane formation in pedestrian crowds and Foreman's mechanism of void alignment due to 1-D migrating SIA clusters. The results show that *spatial correlations between voids should almost always be present unless correlations with other lattice defects of a higher density prevail*. The condition of high void / low dislocation density is thus necessary for void ordering, since it ensures the development of correlations between voids rather than between voids and other lattice defects, such as edge dislocations and second-phase precipitates. *The very absence of a void lattice must be an indication of the existence of correlations of voids with other defects.* An accompanying paper [38] is devoted to study the consequences of these correlations on void swelling and generally defect accumulation.

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Importantly, the critical void size for the onset of void ordering is much smaller than the void saturation radius predicted by the theory for voids distributed randomly. Hence, the saturation of swelling observed in void lattices cannot be a consequence of this, as was thought before [8,9]. This statement is also supported by a previous finding that the formation of the free channels between voids in void lattices provides the escape routes for the SIA clusters to dislocations and leads to a significant increase of the void saturation radius [39]. In addition it is shown in [35] that, in conditions when void ordering is observed, *i.e.* a high void density, the irradiation dose required for an ensemble of randomly distributed voids to reach the steady state is very large, about several hundred dpa, thus much higher than in experiments, which is ~10 dpa.

It is important that such spatial correlations provide a powerful mechanism for void growth and in an accompanying paper we argue that spatial correlations of voids with dislocations and second-phase precipitates should be a common feature under cascade-produced irradiation [38]. Association of large voids with various precipitates (G, η, Laves *etc.*) [40-45] and growth of voids in the compression side of edge dislocations [46,47] is well-known for a long time. Recently, an evidence for the correlations between voids and other defects has been observed by Kozlov, Portnykh *et al.* [48,49] in 20% cold-worked 16Cr–15Ni–2Mo–2Mn austenitic steel irradiated up to ~100 dpa in a BN-600 fast reactor in the temperature range 410 to 600ºC. The transmission electron microscopy has revealed voids of three main types: a-type associated with dislocations, b-type associated with G-phase precipitates and c-type, which were formed homogeneously in the matrix. The c-type voids were the smallest and made the smallest contribution to swelling, while the a-type voids were the largest.

It is relevant here to give arguments against apparently wrong interpretation of experimental data and some Monte Carlo results on void ordering by Evans [50], which led him to conclude that 2-D rather than 1-D SIA migration should be responsible for the void lattice formation. First, it is evident that a correct modelling of void ordering must use simulation boxes bigger than the mean-free path of 1-D migrating SIA clusters. This can be estimated using equation (10) and is typically of the order of micrometers, thus an order of magnitude longer than for 2-D diffusing objects. Evans used much smaller box size, which was suitable for 2-D but not for 1-D migrating defects, and his observation of an existence of a barrier for the precise alignment of voids due to 1-D motion of SIAs likely originates from this methodological error. Second, according to equations (16) and (17) of the present analysis, during early stages of void ordering, voids form close-packed planes rather than close-packed lines, in exact correspondence with experiments. Hence, Evans' expectation of 'the local ordering to be either along the relevant close-packed planes of along close-packed directions, depending on whether the SIA transport is planar or linear' is invalid. We also emphasise that, generally, substantial modelling and experimental evidence collected to date support 1-D rather than 2-D SIA transport.

Finally, we note that the considered spatial correlations tend to decrease the void-SIA collision frequency. The condition of the minimum of interaction intensity in the evolving structures is common in self-organisation processes and is considered as a generalisation of the Onsager principle of the minimal dissipation of entropy [35].

Acknowledgements

The authors express their gratitude to Dr B.N. Singh (RisØ National Laboratory, Denmark), Dr H. Trinkaus (Forschungscentrum Jülich, Germany), and Drs S.J. Zinkle, R.E. Stoller and Yu.N. Osetsky (Oak Ridge National Laboratory, USA) for careful reading and useful discussions of the manuscript. The research was sponsored by a research grant from the UK Engineering and the Physical Sciences Research Council and by EU-funded project FP 7 GetMat (A.V.B) and by the Office of Fusion Energy Sciences U.S. Department of Energy, under contract DE-AC05-00OR22725 with UT-Battelle, LLC (S.I.G).

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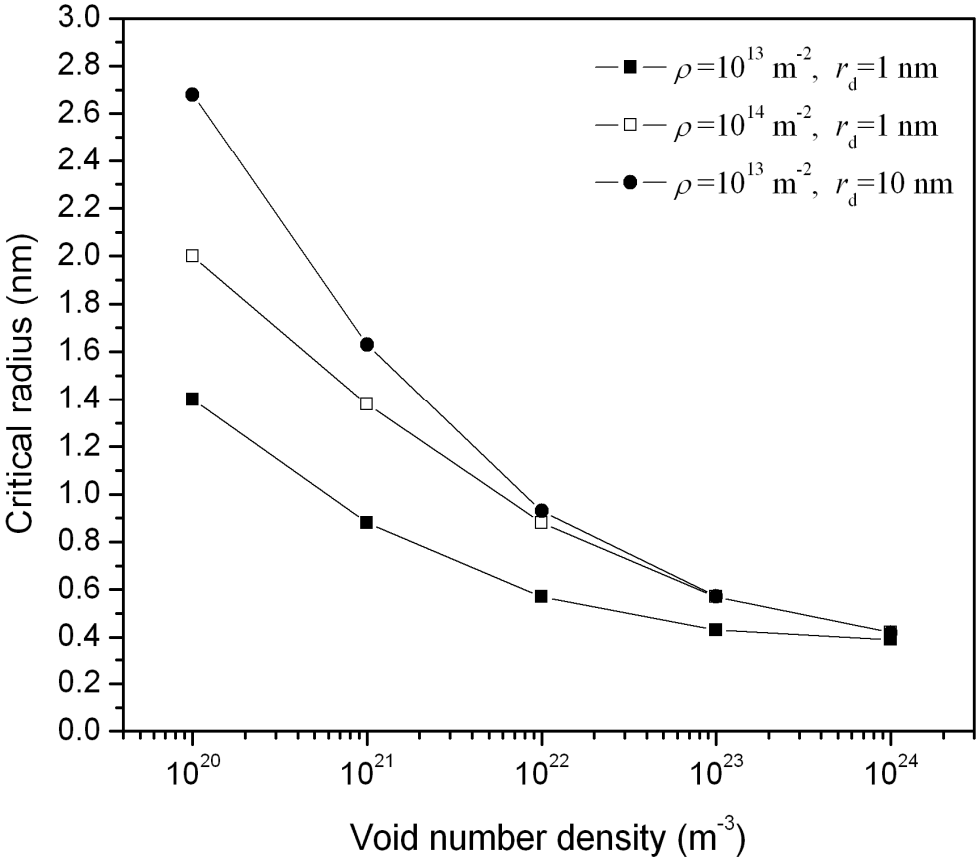
Figure 1. Dependence of the critical void radius for the onset of void ordering on the void number density.