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Response to the comments by J.H. Evans on ‘On the onset of void ordering in metals under neutron or heavy-ion irradiation’

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Abstract

Evans’s comments are related only loosely to the main body of our paper, which is devoted to the onset of void ordering: his Monte Carlo (MC) simulations of this early stage of ordering are in a qualitative agreement with our results. They question, however, the basic mechanisms of damage accumulation revealed by a number of scientists using various techniques over the years. Here we argue that his views are erroneous due to overlooking some essential features of the one-dimensional defect transport.

Keywords: void lattice; cascades; interstitial clusters; one-dimensional diffusion.

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Evans’s criticism of the assigning of the void spatial regularity found after electron irradiation in [1] to a bubble lattice refers to the analysis of Jäger and Trinkaus [2] described in the Introduction section in [3] as a part of the problem overview. We are sorry if we made an impression that we support their view, which we do not: loop punching from bubbles would not lead to ordering, of course. We do not have any interpretation of the observation made in [1], and do not even consider it as an established result for it has never been confirmed. We think that Jäger and Trinkaus might have a similar opinion: they did not include this result into Tables 1 and 2 [2] for void and bubble lattices, even though it was the only alloy of practical use.

The essence of Evans’s other comments on our paper [3], as well as conclusions of his recent publications [4-6], is that the one-dimensionally (1-D) of the diffusing clusters of self-interstitial atoms (SIAs) have inherent difficulties in forming perfect void lattices, which 2-D diffusing SIAs do not have. However attractive the idea of 2-D diffusion could be, there is no firm evidence of its existence. In the following we focus on two main points: the dimensionality of initial void ordering and the effect of box size on MC calculations.

Dimensionality of initial void ordering. The absence of void linear alignments during early stages of ordering can be explained by the instability of such structures due to the void coalescence described by Evans in [4]. For the sake of completeness, let us recall the mechanism of coalescence. Consider a line of equally spaced voids in a close-packed direction, where one void is shifted from the middle position between two other voids, say, to the right. Then, the free volume to the left void is larger, hence, more SIAs are produced there and interact with the void. As a result of the SIA annihilation at the void surface, the void’s centre of gravity should shift to the right, making a bigger distance even bigger. In other words, the linear alignments are physically unstable. In close-packed planes the void coalescence is prevented by the stabilising action of the SIA clusters moving in coplanar directions. In our paper [3] this is reflected by the fact that the most favourable conditions for destabilisation of homogeneous void arrangement correspond to formation of close-packed planes (equation (17)). Thus, the ordering mechanism is, indeed, linear, not planar, but the stability of ordered structures increases with increasing dimensionality, being unstable

for linear alignments. It follows that the dimensionality of initial ordering should not follow the dimensionality of SIA migration, in contrast to Evans's belief [5].

Effect of box size on MC calculations. In a partially formed void lattice, the 1-D mobile SIA clusters can be separated into two groups: a) those moving in free channels between voids with the mean free path (MFP) greater than the average distance between voids, and b) those moving between two nearest voids. The b-type SIAs lead to the void coalescence discussed above, whereas the a-type SIAs act against the latter, preventing coalescence and providing void ordering. The MFP is the characteristic distance from where on average the SIA clusters come to voids. If the simulation box is smaller than the MFP, then the relative contribution of a-type SIAs to void movement is artificially reduced: part of the a-type SIAs become unable to interact with voids, making perfection of a void lattice difficult, if possible. In a system containing randomly distributed voids of radius r and number density N , the MFP is equal to $(\pi r^2 N)^{-1}$, which gives $\sim 1.4 \mu\text{m}$ for $r \approx 1.5 \text{ nm}$ and $N \approx 10^{23} \text{ m}^{-3}$, as in sections 3.3 and 3.6 of Evans's paper [4]. (Note also that the MFP increases rapidly with increasing spatial correlations between voids, being infinite in a perfect void lattice with no other defects present.) Evans used a simulation box with a linear size of 215.4 nm, i.e. ~ 6.5 times smaller than the initial MFP, hence the failure to reproduce a perfect void lattice should not come as a surprise. Evans claims that '*the barrier for the precise alignment of voids – toward a perfect lattice – is a short range effect, and can be predicted from a trivially simple diagram*' [4]. The diagram mentioned is Figure 3 in [4] illustrating coalescence of voids due to interaction with the b-type SIA, which is indeed a short-range effect. Evans also described the stabilising effect of a-type SIAs, but failed to fully appreciate its long-range character with the corresponding dramatic effect of the size of simulation box. This is why, in contrast to Evans's view, void ordering by SIA clusters with the MFP smaller and bigger than the box size should be fundamentally different.

Evans raised two other issues, to which we respond only briefly. First, he noticed that void lattices are observed in bcc metals but the enhanced swelling near grain boundaries is not, which, in his view, undermines the role of 1-D migrating SIA clusters in the formation of void lattices. We think that this is not logical: grain boundary properties, for example, can be different in bcc compared to fcc crystals. Second, Evans noticed the importance of impurities, which we did not address. In fact, it is well known that oxygen, for example, increases the stability, hence concentration, of voids, which favours void lattice formation, as observed, e.g. in [7], and predicted by our model. Other impurity effects are either too lengthy to discuss here or beyond our understanding as yet.

The issues discussed above are but technical details of void lattice formation and can be verified by wisely chosen calculations. The differences in our views on the void lattice go deeper than that. So, Evans's view is close to the general perception of the void lattice as a separate phenomenon occurring in special circumstances, which is of pure academic interest, not for structural materials under conditions of practical importance. In contrast, we argue that it is just one particular type of a bigger class of spatial correlations caused by 1-D migrating SIA clusters, which are characteristic and permanent features of the microstructure formed in both pure metals and alloys under cascade damage conditions: the absence of void lattices indicates that correlations of voids with other defects prevail. As a consequence our paper [3] becomes an important supplement to another work [8], where we show that these correlations together with the radiation-induced segregation control void swelling in structural materials at high enough irradiation doses.

Finally we mention an important related topic which is the problem of swelling saturation in void lattices, as a potential for engineering radiation-resistant materials. Golubov already argued in 1980 [9] that "spatial ordering has no influence on the growth of

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voids in molybdenum”. Evans agreed with this view [6], stating that “the void lattice formation and void swelling must have separate mechanisms”. There is no satisfactory explanation for the phenomenon yet. In our forthcoming publication (in collaboration with Dr. B.N. Singh, Risø National Laboratory, Denmark) we argue that it originates from the lack of dislocation climb, which also seems to be a necessary condition for the formation of a perfect void lattice. The effect is due to distinguishing features of the interaction between 1-D migrating SIA clusters and dislocations and might exist in complex alloys too.

Despite differences in our views, we would like to express our appreciation for Dr. J.H. Evans’s work and thank him for initiating this discussion, which, we believe, will serve well in shaping the theoretical foundation of the observed phenomena.

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