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SPLITTING VACANCY VOIDS IN THE GRAIN BOUNDARY REGION BY A POST-CASCADE SHOCK WAVE

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Abstract. The structural transformation of vacancy voids in the grain boundary region of the bicrystal under the influence of post-cascade shock waves is studied with the aid of molecular dynamics simulations. It is shown that the void may be split into two parts or completely displaced. This effect depends on the relative position of the void and grain boundary dislocations. Also shown is a seamless transfer of vacancy clusters through the tilt grain boundary.

1. Introduction

The materials used for manufacturing various engineering parts are generally polycrystals composed of individual grains. Under the influence of irradiation the point defects and various transmutants such as inert gases are formed. At low temperatures the interstitials, having higher mobility compared with the vacancies, migrate to the drains which are grain boundaries and form impurity segregation reinforcing dislocations. As a result, the yield strength of the material increases. An increase in temperature, which leads to an increase in the diffusion mobility of vacancies and void formations over the grain boundaries, is the cause of the radiative embrittlement. Thus, the grain boundaries play an important role when considering the various radiation-induced phenomena.

Problems of the radiation-induced void formation in materials have been the objective of much research [1–4].

The present study investigates the influence of such factors as temperature, intensity of irradiation, fluence, the presence of structural imperfections, and the presence of gases and non-gaseous impurities on the radiation-induced void formation. Vast accumulation of experimental material made possible to build models of the phenomenon and form the basis of the theory. It is necessary to highlight among the theoretical models the model of diffusion-deformation instability [5, 6], whereby the excess vacancies are the source of elastic tensile stresses. Reduced Gibbs energy gives rise to upward diffusion phenomena if these stresses are taken into account and, as a result, formation of voids. The proposed model is developed to overcome the difficulties encountered in describing the initial stage of void formation, as well as explaining the reasons why the vacancy satiety is realized in the form of voids instead of vacancy loops.

In the study of the evolution of defect structures in the material susceptible to radiation, it is necessary to take into account another important factor, the possibility of post-cascade

the crystallite was divided into two equal grains, each of which is rotated relative to the crystallographic direction < 111 >. The axis of rotation passes through the lattice point at the center of the grain. To get the misorientation angle θ one of the grains was rotated by an angle $\theta/2$, and the second one by $-\theta/2$ (see Fig. 1a). Then, the atoms in the boundary region were removed so that the grain boundaries are parallel to each other (see Fig. 1b), then both the grains approached each other by a distance corresponding to the distance between the lattice sites in the X direction of the calculated cell (see Fig. 1c). After such manipulations some atoms could be placed on a critically short distance, so prior to the structural relaxation the atoms with the distances to the nearest neighbor less than the minimum in the simulated crystal structure were removed from the calculated cell.

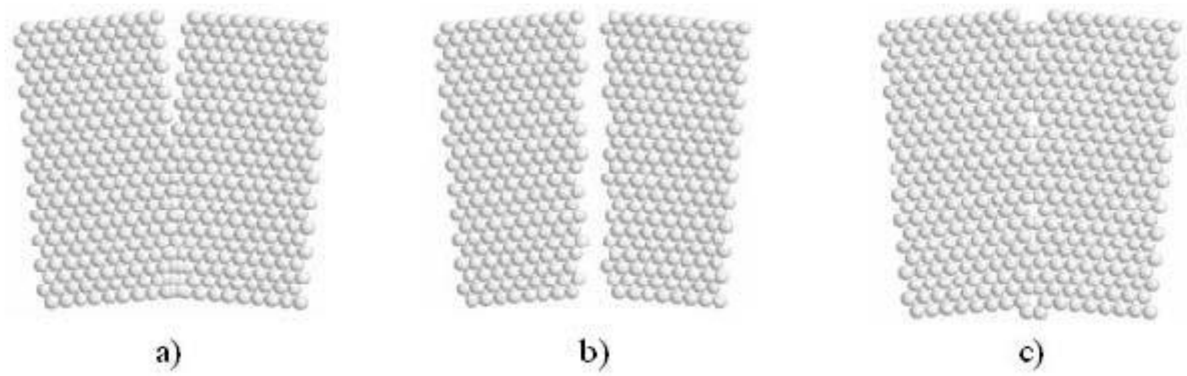

Fig. 1. The process of creating a model of symmetrical tilt grain boundaries: (a) rotation of grains, (b) pruning, (c) shift.

In order to minimize the energy of the boundary the hard shift of one grain, as a single entity relative to the other in a direction parallel to the boundary plane, can be done so that the boundary atoms were in a position of a local minimum of potential energy. In the future, we will be considering both the models of the borders, with and without the shift.

Thus, the "atomic" relaxation was used for the first model, when each atom is moved under the influence of all the forces acting on it until it reaches the minimum amount of energy of all pair wise interactions.

And for the second model, the relaxation was carried out in two stages: the "hard" relaxation, when as a result of the shift the sum of interactions is minimized, but each atom still occupies its site in its grain, and then "atomic" relaxation takes place [21].

The waves were generated by assigning the speed along the direction *X* to the atoms located at the border of the cell. The close-packed directions were chosen because due to the focusing mechanism of energy, a spherical wave is transformed into fragments of plane waves propagating exactly along the close-packed directions [22, 23].

After performing a specified number of steps of the computer experiment there followed the structural relaxation of the system at 0 K. The renderer of the superimposed close-packed rows, consisting of lines connecting the atoms in the three close-packed directions, was used to visualize the resulting structure.

3. Results and discussion

When considering a system of two crystallite, which misorientation leads to the formation of grain boundary area, one of the main characteristics is the specific energy of the grain boundaries γ defined as the energy difference between the single crystal and bicrystal containing the same number of atoms per unit area of the grain boundary. Specific energies of the grain boundaries, determined at various grain misorientation angles for the used models with and without the shift, are shown in Table 1.

minimum is observed in the case where the center of the void is aligned with the dislocation core. When considering the larger angle of misorientation, the void size and the number of dislocations led to the fact that there was always crossing of the void and the dislocation core, so the dependency is more uniform.

In what follows we consider only the low-angle boundaries, as at larger angles is difficult to identify the location of individual grain boundary dislocations and, as a consequence, it is difficult to determine the effect of a single dislocation on the void.

Consider the effect of the shock wave on the structural transformation of the void, placed between the two grains. The alignment of the vacancy void between the dislocation cores is the most precarious position of all possible at the grain boundary. This study demonstrated that in this case the shock waves can shift part of the void from its original position (see Fig. 3). In order to shift the void, the center of which coincides with the core of the grain boundary dislocation, more intensive shock waves are required (see Fig. 4).

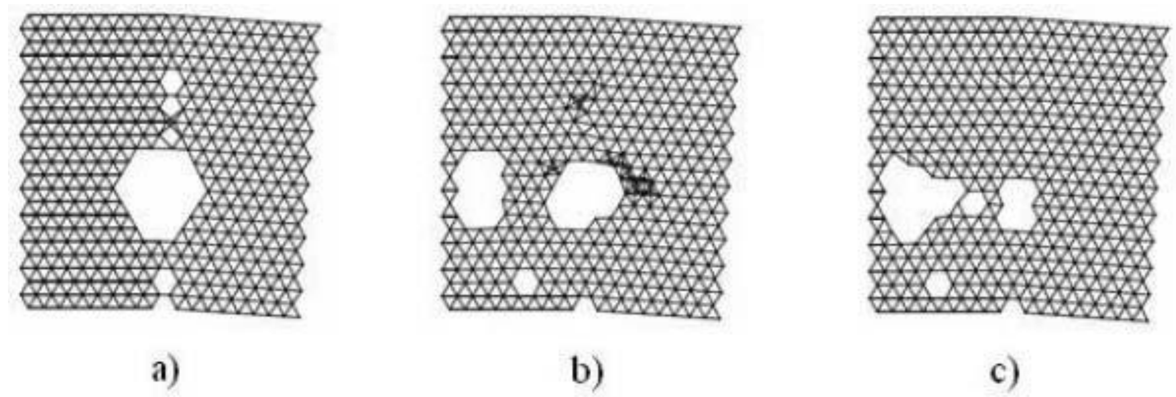

Fig. 3. (a) A detail of plane <111> of the considered block with the void located between the cores of grain boundary dislocations at the beginning of the experiment, (b) after passing of the six shock waves at a speed of 4000, and (c) 7000 m/sec. The waves propagate from left to right relative to the figure.

As follows from Figs. 3b and 3c, the increase in the velocity of the wave increases the number of the vacancies shifted from its original position. Note that the calculation cell temperature was set at 300 K, which is not sufficient to dissolve the voids by diffusion processes. This temperature was maintained throughout the experiment, because the wave-induced excess energy was absorbed by the thermostat.

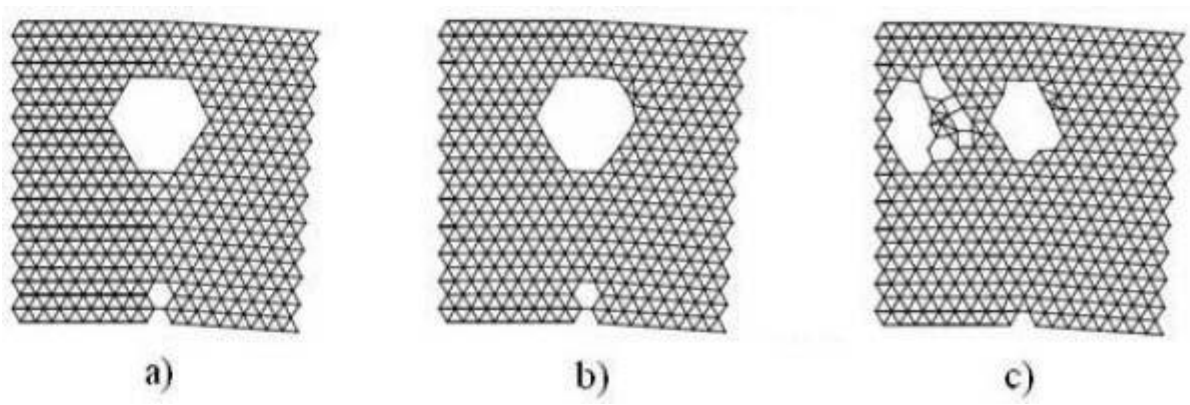

Fig. 4. (a) A detail of plane <111> of the calculated block with a void, whose center is aligned with the core of the grain boundary dislocation at the beginning of the experiment, (b) after passing the six shock waves at a speed of 4000, and (c) 7000 m/sec. The waves propagate from left to right relative to the figure.

blocs with different grain misorientation.

As can be seen from Fig. 5, at low angles of misorientation the wave overcomes the border with virtually no loss of speed. Besides, when using a model with a shift the velocity drops sharply at the border. This is due to the disruption in focusing of atomic collisions. Another reason for disfocusing can be intersection of the cores of the grain boundary dislocations. However, it can be assumed that the shock wave affects the structural transformation of the vacancy voids in polycrystalline, at a low angle of the grain misorientation. Let us verify this hypothesis experimentally. To do this, we create a void in one of the grains of the bicrystal, while the source of the waves is in the second grain. The experimental results with the considered block having a misorientation angle of grains four degrees are shown in Fig. 6.

As shown in Fig. 6, a group of vacancies which splits from the void under the influence of the shock waves and can be transferred through the grain boundary.

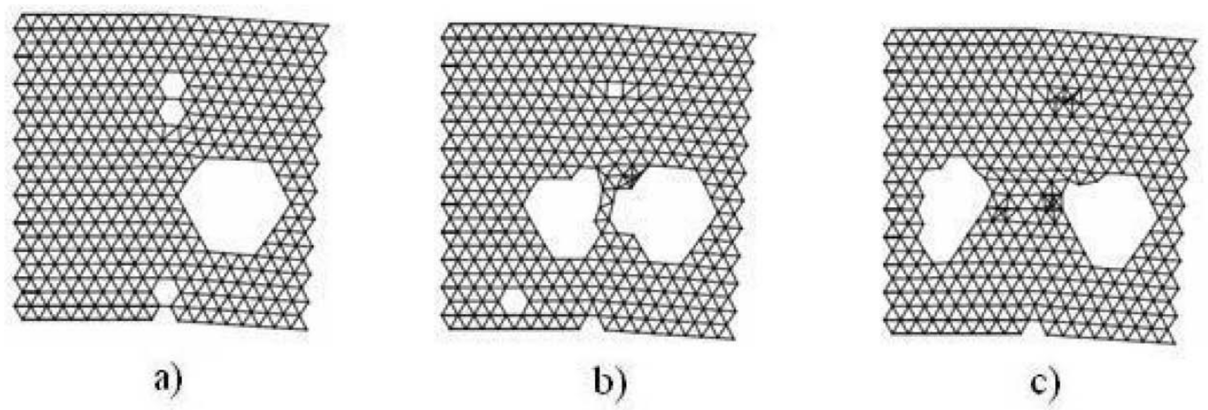

Fig. 6. (a) A detail of plane <111> of the considered block with the void located in one of the grains at the beginning of the experiment, and also after the shock wave passes (b) five times and (c) nine times at a velocity of 7000 m/sec.
The waves propagate from left to right relative to the figure.

4. Conclusions

The study showed that the post-cascade shock waves can cause fragmentation of vacancy void into the individual components when placing it in the grain boundary region. In many ways manifestation of this effect depends on the relative positions of the void and the grain boundary dislocations. Also shown is a seamless transfer of vacancy clusters through the tilt grain boundary.

It is known that the dissolution of the void can be done through consecutive vacancy evaporation or due to the diffusion flow of material deep into the void. The process of reducing the dimensions of the void under the influence of shock waves, described in this paper, does notfit into the framework of the given mechanisms. Therefore, we call it dynamic dissolution, as it is initiated by high-speed cooperative atomic displacements.

The obtained results can be used in radiation material science as well as predicting the behavior of materials under extreme operating conditions. In particular, it is known that the main ways to reduce the radiation swelling of construction materials are to change the structural state of the materials by alloying and through mechanical and thermal treatments. It is possible that this work may contribute to the development of new methods to control swelling.

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