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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

shock waves [7–9]. The development of atomic collision cascade to the point at which the Maxwell Speed Distribution of the colliding particles occurs at the time of the order of 10^{-12} sec, while for the uniform dispersion of energy in terms of the cascade of waves in the lattice the required time is 10^{-11} sec [8]. The sudden expansion of intensely heated cascade region can result in a shock wave. Even in the absence of the temperature required for the start of diffusion processes, the propagation of post-cascade shockwaves leads to a number of interesting effects such as flow of a defect-free material with agitated atoms of the medium, the anomalous mass transfer, diffusionless processes, phase transformations, and the sharp increase in the number of displacements per atom in the volume of material [9–13].

In some earlier publications [14–17], the authors studied the behavior of vacancy voids under the influence of post-cascade shock waves in monocrystals. The study showed that the shock waves can cause displacements of voids as well as their splitting or dissolution. This dissolution can be carried out even at temperatures insufficient to start thermal activation diffusion mechanism. Besides, when there are voids in certain locations, the shock waves can initiate integration of them. Moreover, these processes can also take place at relatively low temperatures, insufficient to start the so-called heat-induced coalescent. The number of vacancies as well as the temperature at which these processes occur affects the processes of structural transformation. An investigation of the effect of deformation of the considered block showed that under compression the impact of the surface energy of the voids increases, causing the waves to activate the processes, which in some cases can lead to the merging of individual voids. Extension leads to stabilization of the voids as a result of which the shock waves cause the displacement of individual voids.

The aim of this study is to determine the effect of the post-cascade shock waves on the processes of structural changes in polycrystalline vacancy voids.

2. Description of the experiment

The small dimensions o fthe domain under examination in this study makes difficult to observe it directly. Therefore, the computer simulation is best suited for this task. The method of molecular dynamics was selected as a method of computer simulation because it allows one to conduct experiments with preset speeds of atoms and compare the dynamics of investigated processes with the real time. The study was conducted with the help of the software simulation package XMD [18]. The apparent advantages of this package are a wide range of supported options, the relative ease of use and access to the source code. As a potential function of the interatomic interaction the Johnson potential was used, calculated in the framework of the embedded atom method [19]. The integration step was five phot-seconds.

The temperature of the considered cell was set by assigning random speeds to the atoms according to the Maxwell-Boltzmann distribution for a given temperature. The simulation was performed at a constant temperature.

In order to maintain the temperature of the cell the Andersen thermostat was used [20], where the atoms of the system are colliding with some virtual particles, resulting in a reduced speed of real particles.

The simulated gold crystal was in a shape of parallelepiped. The orientation of crystallites was set as follows: the X-axis is directed along the crystallographic direction <110>, the axis Y – along <112>, and Z - <111>.

To create a void in the crystal a sphere was set with a certain radius. Then the center of the sphere was made coincident with the one of the lattice sites, and all the atoms that fall into this volume were removed. After removal of the atoms the structural relaxation of the cell was performed until the system reached a state of minimum energy.

In the present work symmetrical tilt grain boundaries are considered. To create them

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.

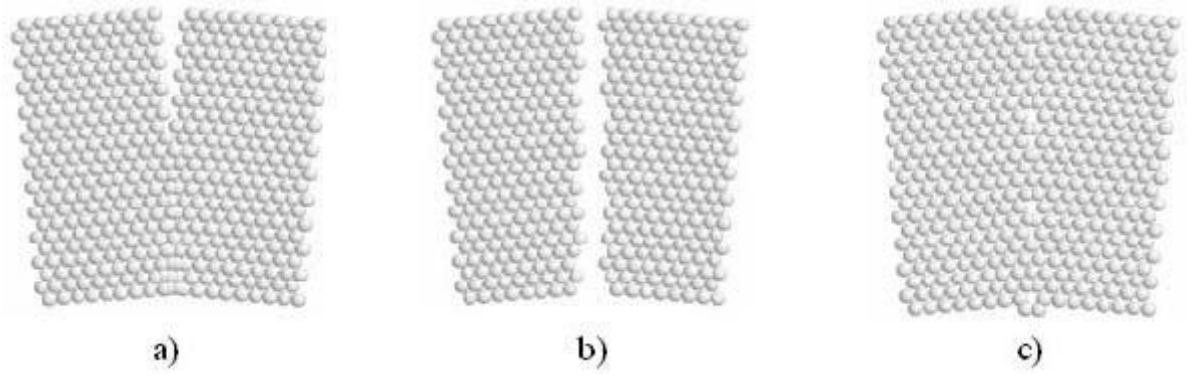

Fig. 1. The process of creating a model of symmetrical tilt grain boundaries: (a) rotation of grains, (b) pruning, (c) shift.

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.

Table 1. The specific energy y of the tilt grain boundary for different models depending on the misorientation angle θ. Model I: the boundary without a relative grain shift; Model II: the boundary with a relative grain shift.

θ	Model I	Model II
4º	0.539	0.461
6º	0.593	0.502
8º	0.596	0.536
10º	0.600	0.569

As can be seen from Table 1 the values of γ increases with θ. Furthermore, when using a two-stage relaxation ("hard" and "atomic") lower boundary energy can be achieved. The specific energy of the tilt grain boundary for gold was obtained experimentally as 0.364…0.406 J/m^2 [24], which is somewhat less than the energy values determined by the computer simulation. But, in our view, this difference is not critical and the models considered are well suited for future research.

Let us consider the simplest case: the vacancy void of a spherical shape located on the border of the two tilt grain boundaries. The tilt grain boundaries are usually represented as the wall of edge dislocations. Obviously, in this case, the relative position of the void and the grain boundary dislocation must affect the energy of grain boundaries. Thus, Figure 2 shows the variation of the specific energy γ of the grain boundary when the void is shifted along the *Y* direction by a distance ΔS from the edge of the considered block.

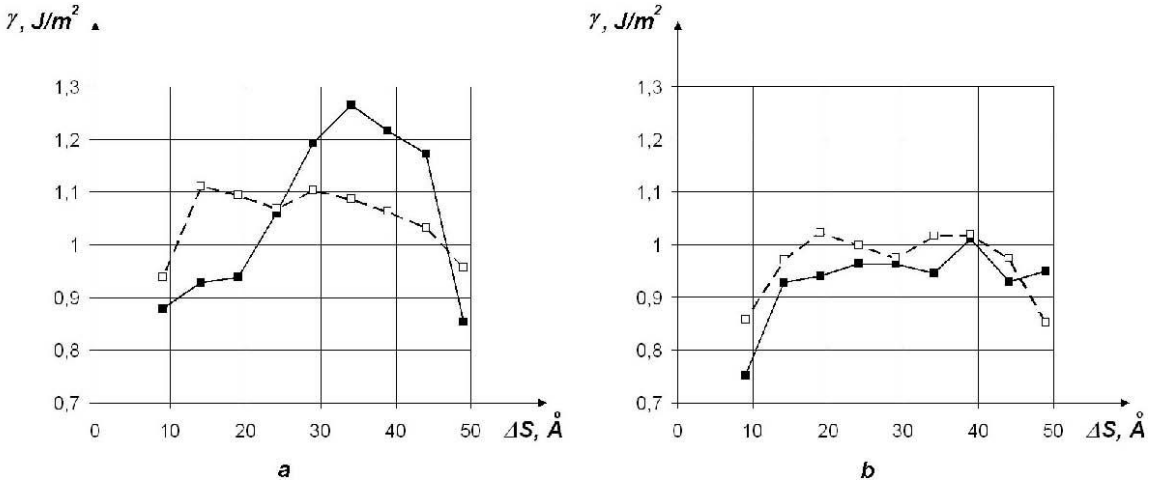

Fig. 2. The specific energy of the tilt grain boundary vs the distance between the center of the void and the considered block edge (a) without the grain shift and (b) with the shift. Solid line represents the misorientation angle 4º, dashed line 10º.

It must be noted that the sharp gradients at the beginning and end of the curves are due to the fact that the void partially crosses the boundaries of the domain for which the energy is calculated.

As can be seen from the figure, for a model with a relative shift of the grains, the change of the location of the void on the boundary does not affect much the value of the energy. For the model, which does not incorporate the grain shift, the void location has a profound effect on the energy only for a small misorientation angle. The reason for this is as follows. At a small misorientation angle a sequential shift of the vacancy void leads to the fact that it can occupy a place between the two cores of the grain boundary dislocations. Such a location of the void corresponds to a local maximum in the curve (see Fig. 2a). A local

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).

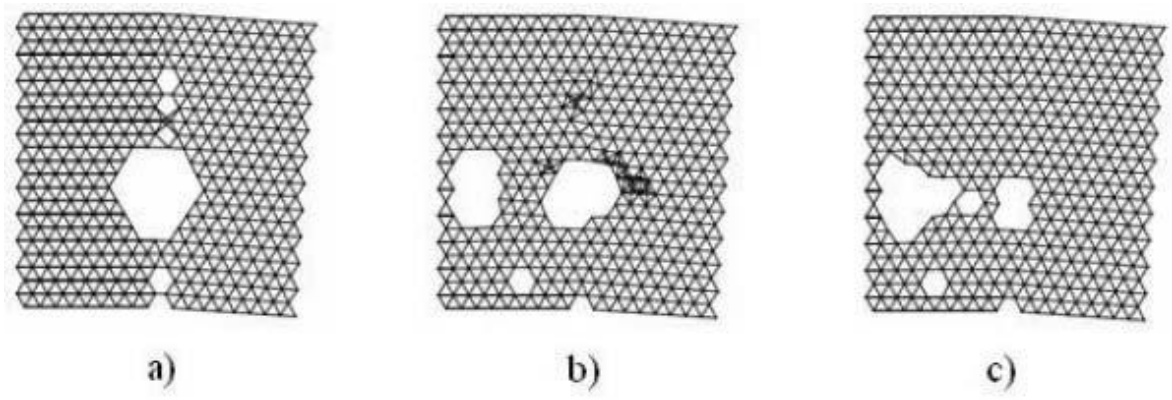

Fig. 3. (a) A detail of plane <111> of the considered block with the void located between the cores of grain boundary dislocations at the beginning of the experiment,
(b) after passing of the six shock waves at a speed of 4000, and (c) 7000 m/sec.
The waves propagate from left to right relative to the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

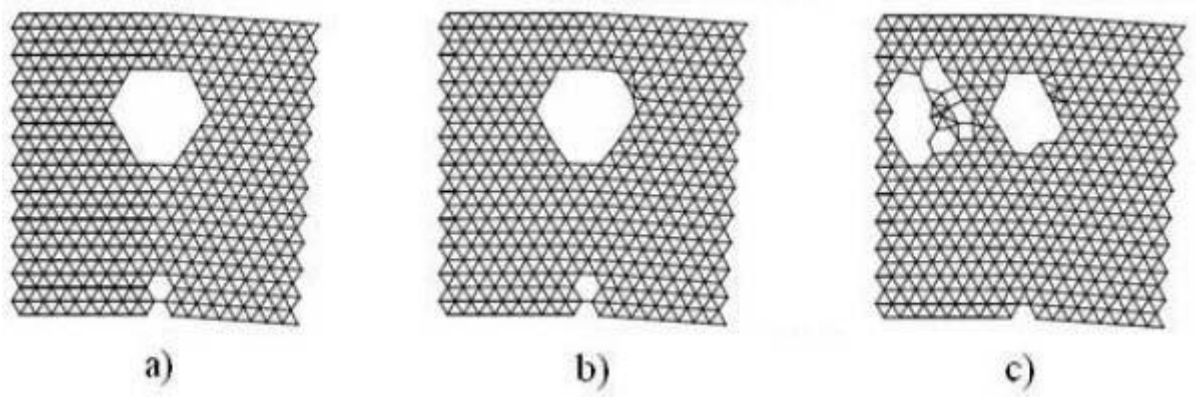

Fig. 4. (a) A detail of plane <111> of the calculated block with a void, whose center is aligned with the core of the grain boundary dislocation at the beginning of the experiment,
(b) after passing the six shock waves at a speed of 4000, and (c) 7000 m/sec.
The waves propagate from left to right relative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

The considered block in the experiment described above has the misorientation grain angle of four degrees. For larger angles the conclusions made remain valid, but in this case the dislocation density of the grain boundaries increases, and as a result, the considered void is in contact with them in most of the experiments.

When considering the voids of smaller dimensions, it is possible that the void is completely displaced from the border. The mechanism of the void displacement is described in detail in [15]. Here we mention only that the boundary atoms can be thrown to the opposite side of the void if the wave passes through it. When this happens, the void is shifted by one interatomic distance toward the source of the waves. Thus, the implementation of this mechanism requires a certain combination of wave velocity and void size.

As follows from Fig. 2b, when using a model with a relative shift of the grains, the void location at the border does not play a singficant role. This can explain the fact that in this case it was not possible to detect the effect illustrated in Figs. 3 and 4, and described above for the model without shifting.

Now consider the void, located in one of the grains. In the experiments the void remained stable and the diffusion drift of individual vacancies to the grain boundary was not observed. In [25, 26] also noted that the vacancies interact relatively weakly with the boundaries as compared with interstitial atoms. The drift of vacancies is observed at temperatures close to the melting point, when the void starts to rapidly evaporate the vacancies. Thus, as described above, the vacancy void breaks into two parts under the influence of shock waves. These parts can be treated independently of each other as at low temperatures, they are stable and do not merge into a single entity.

Next we study the possibility of the influence of the shock wave on the structural transformation of the vacancy void, if it is separated from the source of the waves by the tilt grain boundary. Note that the border is not an insurmountable obstacle to the waves. For example, it was shown in [26] that at the intersection of grain boundaries of a special type $\sum 7$ only about 20 % of the single wave energy is dissipated in the grain boundary domain.

For our models we define the loss of the wave velocity at the border. To do this, we select in the considered block a chain of sixteen atoms in such a way that the border would divide it in half. Assigning the initial atom the velocity in the direction of X, we obtain the maximum speed of each atom in a given direction.

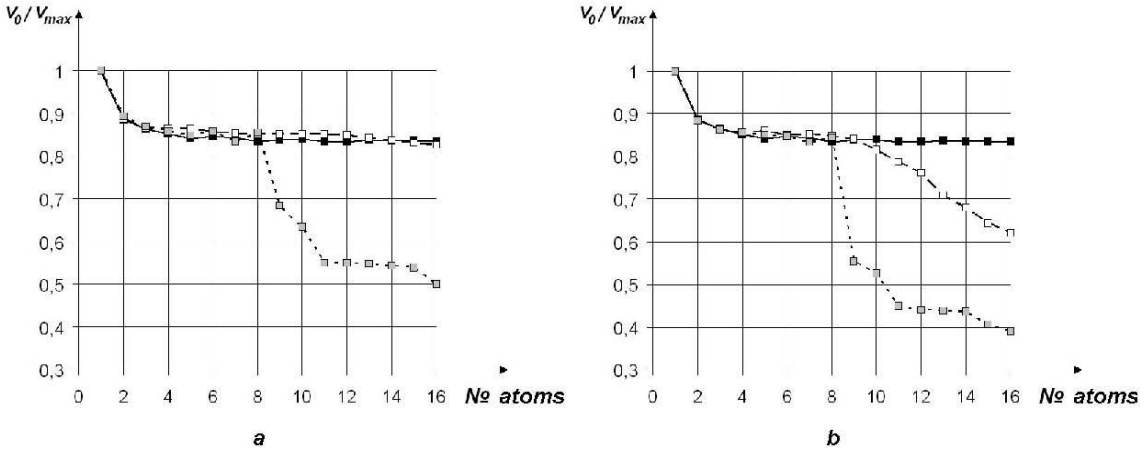

Fig. 5. Change in the initial velocity in the chain of atoms at the misorientation angles of the grains equal to (a) 4º and (b) 10º. The models are considered (a) without the shift of the grains and (b) with the shift. For comparison, the results are given for a single crystal. The initial velocity v_0 is equal to 5000 m/sec.

Figure 5 shows the results of the experiment for the chains of atoms located in the considered

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.

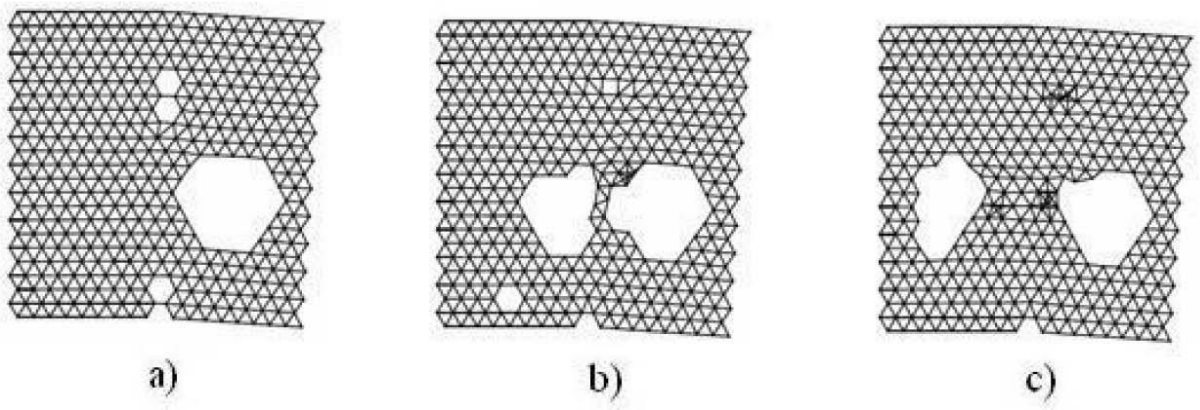

Fig. 6. (a) A detail of plane <111> of the considered block with the void located in one of the grains at the beginning of the experiment, and also after the shock wave passes (b) five times and (c) nine times at a velocity of 7000 m/sec.
The waves propagate from left to right relative to the figure.

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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