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Behavior of the initially perfect f.c.c. crystal under homogeneous deformation

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Computer simulation of the process of generation, motion and annihilation of the dislocations in the initially perfect f.c.c. crystal which undergoes a plane homogeneous slowly increasing deformation was provided in the frame of quasi-three-dimensional crystal model. Range of deformation up to 8% was investigated. It was found that the appearance of the dislocations was preceded by the appearance of the stable sinusoidal displacements of atoms.

1. INTRODUCTION

It is well-known that different kinds of defects strongly affected the properties of crystal. Inelastic deformation of crystals is largely governed by the behavior of the dislocations. Measurements show the very large increase in dislocation density during a plastic deformation. There are many mechanisms of the generation of dislocations. The best known examples are Frank-Read source, formation of dislocations on a grain boundary, formation of dislocation loops by aggregation and collapse of vacancies and appearance of the prismatic loops near the hard, tiny particles of a second phase. All the above-listed mechanisms require the presence of a defect in the crystal. Possibility of generation of the dislocations in an ideal crystal under homogeneous deformation is of interest for dislocation theory.

A description of the defects formation process on the basis of the continuum theory meets with fundamental difficulties, which can be avoided by computer modeling at the atomic level. Some approaches and the results of the investigations in this area are reported in [1]. In the presented paper, the features of generation of the dislocations in a perfect f.c.c. crystal as a result of instability of a homogeneous deformation process is studied at the atomic level.

2. DESCRIPTION OF THE MODEL

Let us consider the f.c.c. crystal with lattice parameter a as a set of one-dimensional, infinite, undeformable arrays of atoms with orientation <211>. These arrays each have three degrees of freedom, one longitudinal and two transverse components of displacement vector. For description of interatomic interaction the Lennard-Jones (6,12) pair potential function with parameters for solid Ar was used. The OZ axis of the Cartesian coordinate system was directed along the rigid arrays and the OX axis was parallel to a closest-packed plane (111).

Undeformed pattern is shown in Fig. 1. The pattern contains 100x24 arrays along

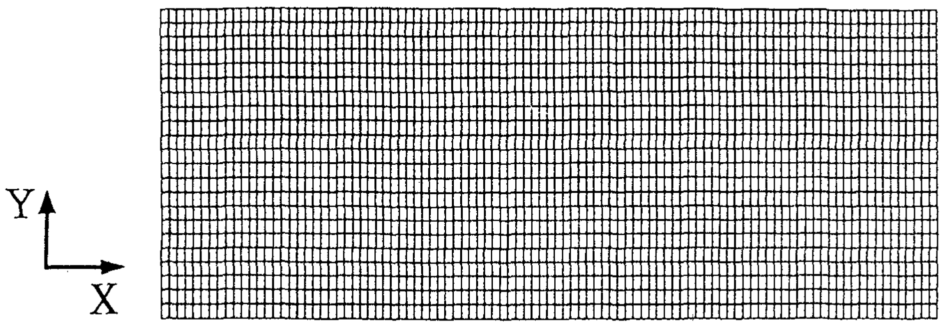

Figure 1. Undeformed crystal, ε=0%.

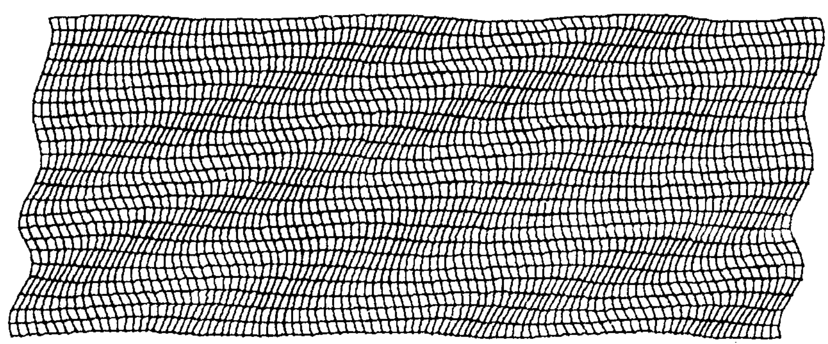

Figure 2. Crystal with the sinusoidal displacements of arrays, ε=4.25%. The displacements are shown on an significantly enlarged scale.

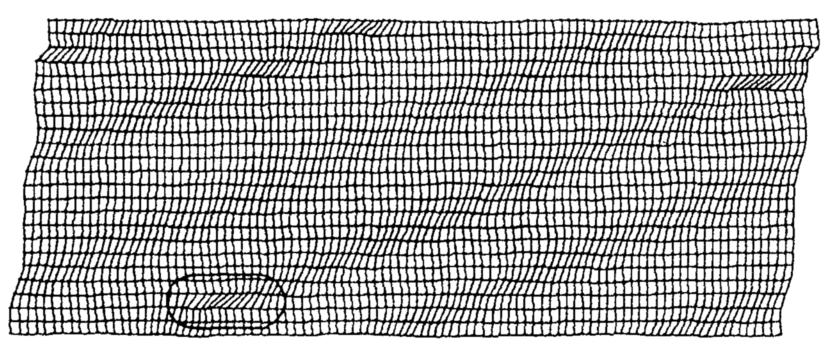

Figure 3. The early stage of the process of the dislocation loops formation. The displacements are doubled. The circled object is one of the forming loops. ε=4.3%.

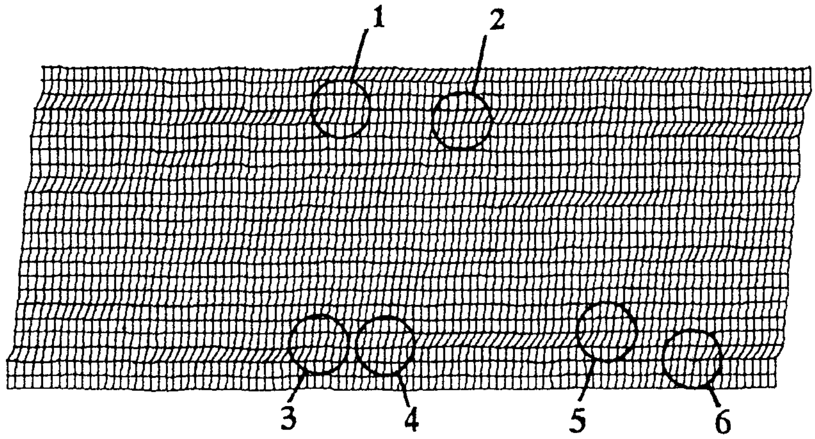

Figure 4. The interaction between moving dislocations. Dislocations 1,2 move in the same glide plane. Dislocations 3,4 and 5,6 move in two adjacent parallel glide planes. ε=4.3%.

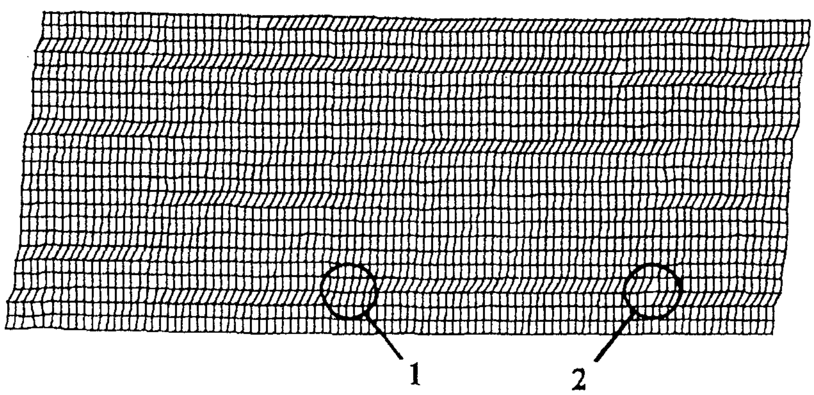

Figure 5. Equilibrium state of crystal at ε=4.3%. 1,2 - the results of annihilation of the dislocations 3,4 and 5,6 from Fig. 4 correspondingly.

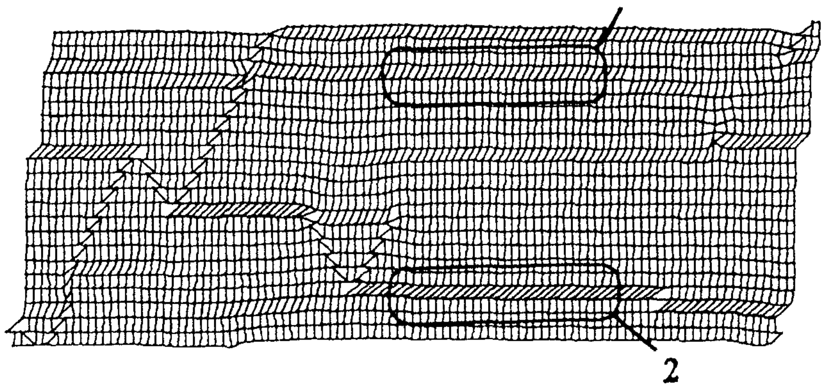

Figure 6. The equilibrium state of the pattern at ε=8%. Dislocations of the second slip system were formed. 1,2 - the regions with stacking fault and recovered structure respectively.

axes OX and OY respectively. The arrays go through the nodes of the rectangular mesh which is shown in Fig. 1. The periodic boundary conditions were assumed.

The pattern was subjected to shear in XY plane and compression along OY direction. The deformations ε_{xy} and ε_{yy} were increased slowly so that the condition $\varepsilon_{xy}=\varepsilon_{yy}=\varepsilon$ was fulfilled. After each small increment of ε the gradient method was used for quasi-static relaxation of positions of the arrays .

3. RESULTS AND DISCUSSIONS

It was founded that the homogeneous deformation of crystal was stable until the 4% level of the deformation was reached. If even a small perturbation of positions of arrays was made the arrays came back during the relaxation process.

At the 4% level of the deformation the picture of the deformation abruptly changed. The sinusoidal displacements of arrays with a small amplitude (about 10^{-6}a) and with the maximum allowable wavelength (one wave per whole pattern) were formed. Test by small perturbations showed the stability of such a displacements. Further increase of the ε led to fast growth of the displacement wave amplitude and in the certain moments the jumplike decreasing of the wavelength took place. In Fig. 2 the pattern with three wavelength per pattern is shown. The amplitude of displacements is about 10^{-3}a, therefore they are shown on a significantly enlarged scale. The crystal with sinusoidal displacement wave may be considered as an incommensurate phase [2].

When the 4.3% level of the deformation was reached the sinusoidal waves were destroyed and the dislocations of the main slip system were formed. The early stage of the process is shown in Fig. 3 where the displacements are doubled. The circled object in Fig. 3 is one of the forming dislocation loops. Such a loops expanded due to the motion of dislocations.

Next stage of the process is the interaction between moving dislocations. Different types of interactions were observed. Dislocations 1,2 of opposite signs moving towards each other are shown in Fig. 4. The result of their annihilation is shown in Fig. 5. Notice that from the Fig. 4 the displacements were not enlarged. Dislocations 3,4 and 5,6 in Fig. 4 give examples of annihilation in the case when they move in two adjacent parallel glide planes. The results of annihilations are shown in Fig. 5 by circles 1 and 2 respectively. In the first case one can see the appearance of the additional array, whereas in the second case the vacant node appears. These results are in agreement with the results, reported in [3].

In Figs. 3,4 nonequilibrium states of the crystal are presented. The motion of dislocations occurred even though the increasing of the deformation was stopped. Fig. 5 corresponds to the equilibrium state of crystal. One can see that not all the dislocations were annihilated. All the dislocations in Fig. 5 are the partial ones. They produce a stacking fault.

At 6% deformation the dislocations of the second slip system were formed. In Fig. 6 the equilibrium state of the pattern at 8% level of the deformation is shown. In some planes the second partial shear took place. In such a planes the f.c.c. structure of crystal was recovered. Figures 1 and 2 in Fig. 6 show the regions with stacking fault and recovered structure respectively.

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