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Simulation of atomic structure evolution solid argon under impulsive loading

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In present communication we investigate the mechanisms of crystal relaxation under an impulsive preassure deformation. It's investigate wave generation, wave confluence, wave transformations, defect structure generation, dislocations annihilation.

1. INTRODUCTION

The quasi-three-dimensional and quasi-static approach within a periodic boundary conditions is used to perform a computer experiment for research of transformation mechanisms of homogeneous deformed crystal from nondefect state to defect state.

It often a study of dislocation properties consists in bring into crystal by definition atoms displacements in response to exact solutions of ellasticity theory and following relaxation for the refirement atoms dispositions in dislocation nucleus field. Such approach was used by Y. Kogure, T. Tsuchiya, Y. Hiki who in the Ar and Xe F.C.C. crystal atomic configurations are obtained in the Burgers dislocation nucleus. In present communication aim to run down all chain transformations of crystal state under the increasing deformation was pursued starting to nondefect state from the dislocation generation.

It was used an interatomic interaction Lennard-Jones potential with parameters for solid argon. The interatomic potential was tabulated. The table has two dimensions because an interatomic interaction is depended as on distance from each toother as on their relative axis shift. The interaction cut radius was disposed between 9-th and 10-th coordinate spheres, that is the each atom was interacted with 164 neightbours. In fact the Lennard-Jones potential is more short-range. However introducing long-range is justified because crystal structure transformation leads to big atomic chain comparative moves, and as the result a chains on long distance in nondeformed crystal may become enought near from each to other.

The calculating area had have parallelepiped view with one endless rib along $[1\bar{2}1]$ direction and sides (111) and (101) oriented. The area dimension is 24 interatomic distances (111) and 100 interatomic distances $(\bar{1}01)$. The periodical boundary conditions were used. The certain coordinate system OZ axis was directed along the endless rib, OX axis was orthogonal to planes $\bar{\quad}$, OY axis was orthogonal to planes (111).

The crystal block has been undergo a combination of homogeneous deformations, compression in direction of OY axis (the deformation is Ey negative) and shear (the deformation Exy positive). The absolute deformation values both Ey and Exy was equal. The third component of plane deformation tensor - the deformation in direction along was supposed zero. The deformation has been araised with the step 0.05%. After each deformation raise the quasi-static relaxation of crystal was performed up to reach the equilibrium crystal state. The equilibrium state criteria is based on the calculation of the maximal by a magnitude power, effected on the chains. If this power didn't exceed some small value then the equilibrium state was being counted reaching, else the relaxation was being continued. In this way the crystal was carried out through series stable states, meeting to raising value of deformation.

2.THE EXPERIMENT RESULTS

The computer experiment was carried out by the next way.

1) The crystal was undergo a certain level preassure deformation, then deformation level was fixed.

2) For the speed up of the transformation the small dinamic disturbance according non-zero degrees of Kelvin temperature was introduced to the crystal.

3) Then a crystal relaxation process was performed.

The next results were obtained.

1) Under the deformation level 5% the crystal safes it stable state. The graphic for non-relaxed crystal practicaly have no differences from realxed crystal graphic. It is shown on the potential energy from deformation level dependence graphic (fig.1.) Curve marked by digit "1" is correspond to nonrelaxed elastic deformed crystal. The graphic looks alike square parabola. The curve marked by digit "2" correspond to relaxed crystal potential energy. The bifurcation points are marked by letters A, B, C, D,E.

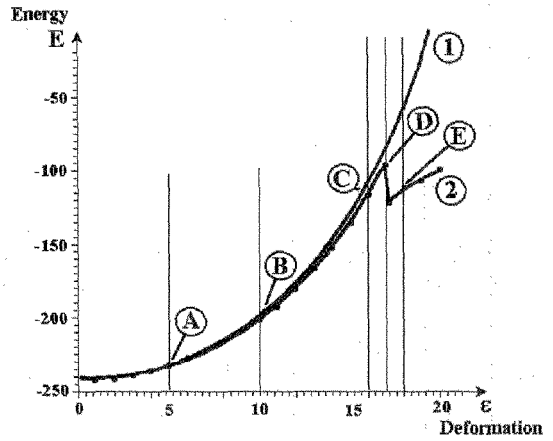

Fig.1 The energy on deformation dependence graphic

2) The deformation level 5% is correspond to the process first bifurcation point. This point is marked by A. The static atom displacement waves have been appeared. There are one wave in direction of preasure and one wave in perpendicular direction have been appeared under the the deformation level 5% - vertical and horizontal waves for simple. Waves amplitudes are very small and for they observe the atom displacements are inreased 10^8 times. The crystal view under 5% deformation level is shown at the fig. 2.

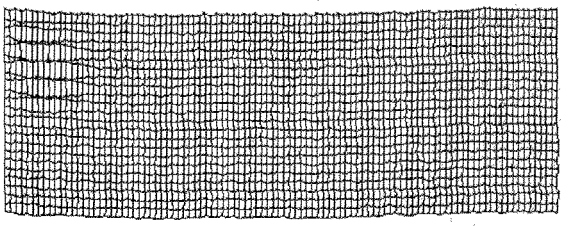

Fig.2 The crystal view under 5% deformation level.

3) The deformation level 10% (point B) is correspond to the process second bifurcation point. With the deformation increase a horizontal waves amount also have been increased. The vertical waves have been disappear. There are three horizontal waves under the deformation level 10%. And there are six horizontal waves in crystal under the deformation level 15%. The crystal view under the deformation level 10% is shown at the fig.3.

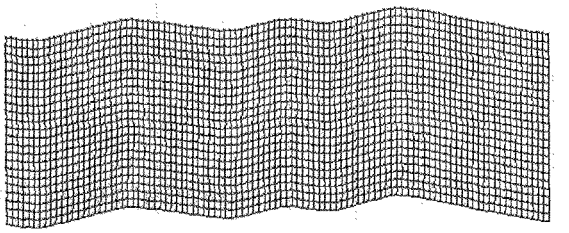

Fig.3. The crystal view under the deformation level 10%.

4) The deformation level 16% (point C) is correspond to the third bifurcation point of process. The atom movements waves become nonstable. There are 15 waves at the begin. During the relaxation process three pairs of them have been conflued and the wave amplitudes have been increased. There are twelve horizontal waves now. Then this state become nonstable, too. Two wave pairs are conflued. The final stable state is reached with 10 horizontal waves of atom displacements. The atom displacements configuration under the deformation level 17% are shown at the fig.4, 5

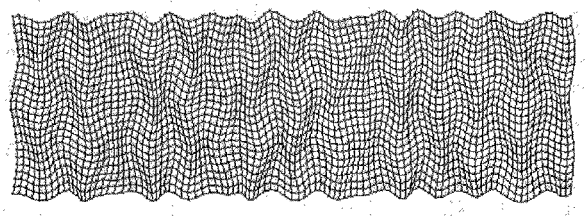

Fig.4. Atom displacements waves generation

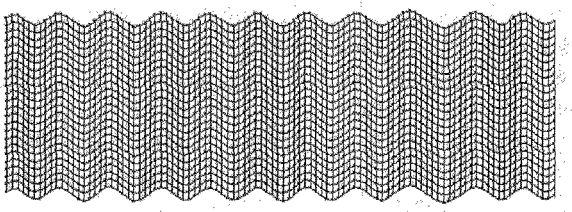

Fig.5. Final atom displacements configuration

5) The deformation level 17,1% (point D) is correspond to the fourth bifurcation point of process. Horizontal waves become nonstable and three diagonal waves appeared. Three diagonal waves become nonstable and the next relaxation step is a defect structures appearence. The dislocations amount under the deformation level 17,1% is two - different by sign dislocation pair. The dislocations moving inside the crystal, making a structure transformations. The dislocations slip direction may be appear in two alternative by direction planes. The dislocations of this type appearence direction is

random value and only dependent on the relaxation results of dinamic disturbance. The next step of deformation level increasing the dislocations amount is increased too. They slip directions are always the same. There are four dislocations in the crystal under the deformation level 17,2% - two pairs of different sign dislocations (fig.7). The atom displace-ments configurations under the deformation level 17,2% are shown at the fig.6,7,8,9.

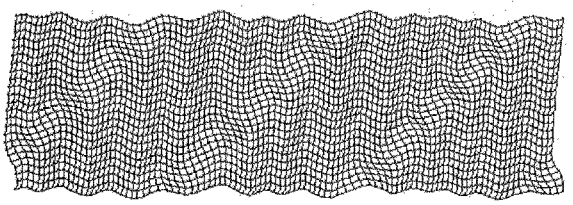

Fig.6. Diagonal waves generation

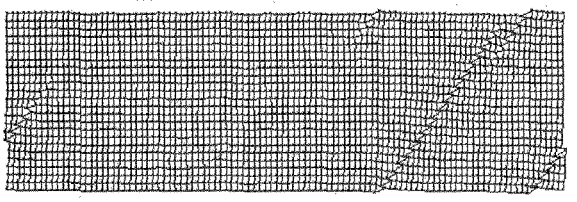

Fig.7. The two pairs different by sign dislocation generation

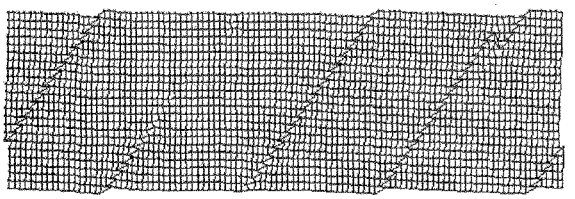

Fig .8. Dislocation movement and annihilation

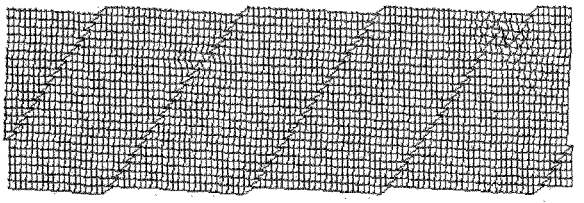

Fig. 9. The result of crystal relaxation

6) The deformation level 18% (point E) is correspond to the fifth bifurcation point of process. Under this deformation level the dislocations of both slip directions have been appeared simultaneously.

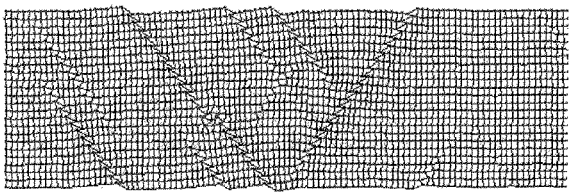

Fig.10. Dislocations of both slip directions.

Besides this classification type the process may b separate on three main phases which are illustrate by using atoms radial distribution function:

1) 0-5% - stable phase or else elastic relaxatio phase. At picture this phase is lasted from zero t point A. At the fig.11 corresponding to the defo mation level 5% clear-cut peaks are observed;

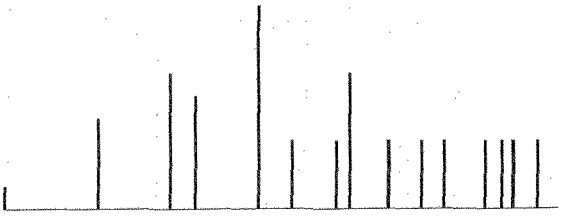

Fig.11. Radial distribution function

2) 5-17% - relaxation with elastic displacemen waves formation. The situation is changed. Aton displacements peaks are splited. Splited spheres vie shown at the fig.12.. Spheres spliting correspond to crystal amorphization. At the picture interval A-D correspond to this phase.;

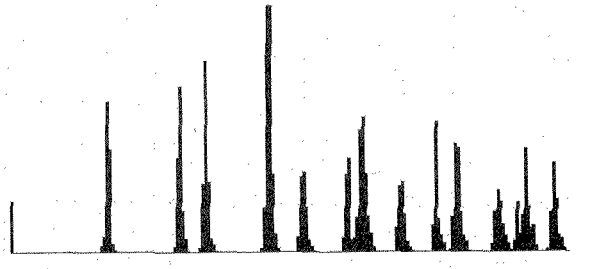

Fig.12. View of splitted spheres

3) 17,1% - relaxation with appearence of defe structures - a dislocations. At picture this phase st at point D. Fig.13 is correspond to deforma-tion le 17,2%. Crystal amorphization is increa-sed.

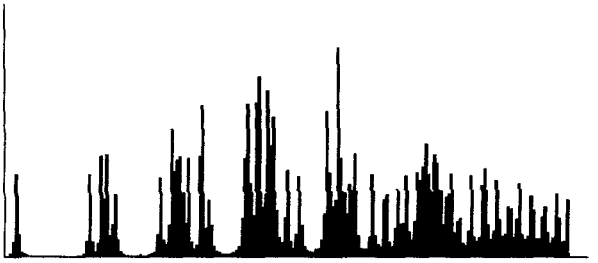

Fig.13. Next step of spheres splitting. Crystal amorphization

At the fig.14 the maximum displacement (1) and maximum forces (2) dependencies from time are shown.

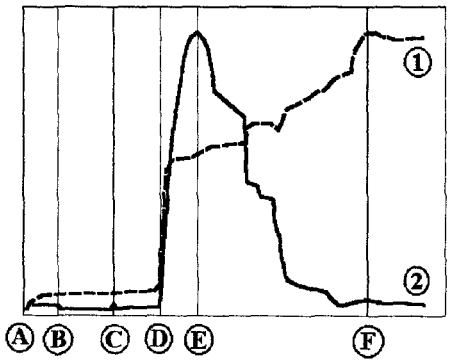

Fig.14. A maximum movement (1) and maximum power (2) from time dependence graphic

The relaxation process may be also separated on five stages.

1) Interval A-B is the generation of atoms displacements wave stage. Fifteen horizontal waves of atoms displacements are formed in the investigated crystal.

2) Interval B-C is the waves relaxation stage. Depending on deformation level the equilibrium waves number is settle at. At first 15-18 waves are formed. Then waves loss their stability and conflue pairwise. Confluence take place either to equilibrium state achievement or loss stability of this type waves. Stage is finished with 12-15 horizontal waves depending on relaxation rate.

3) Interval C-D is next waves stability loss. Diagonal displacements waves are formed. This interval corresponds to subcritical crystal state.

4) Interval D-E corresponds to stability loss and dislocations generation. Diagonal displacements waves are formed inside them. Dislocation slip direction agree with waves orientation.

5) Move and annihilation of dislocation take place in interval E-F. Dislocations are moved in their slip planes in crystal and annihilated. Depending on distance between slip planes annihilation may be of three types:

a) Total annihilation if dislocations slip in one plane;

b) Annihilation with dislocations overcrawl (intersitial chains formation) if they slip in parallel planes;

c) Annihilation with intersitial formation if dislocations slip in alternative planes.

3. CONCLUSION.

As the result of conducted experiment it was obtained that the relaxation process of stressed crystal has five bifurcation points corresponding with fifth varies on character types of intercrystal reconstructions.

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