Molecular dynamics simulations of intensive plastic deformation

L.S. Metlov

Donetsk Physico-Technical Institute, Ukrainian Academy of Sciences,
83114, R. Luxemburg str. 72, Donetsk, Ukraine

(Dated: October 6, 2001)

Kinetics of dislocations is studied by means of computer simulation during intensive plastic deformation. The dynamical effect in the form of soliton-like wave of sharply disrupted interparticle bonds is observed. Along with it, microbubbles similar to steam bubbles at water boiling are formed. After some deformation the solid takes an ideal structure again owing to "emission of the bubbles". The dislocations in this state (with microbubbles) can form a grain boundary in the case of nanostructural materials. The nanoscopic object of rotational nature is observed at uniaxial intensive deformation. Rotation of some volume of sample which realized with phase transition scenario was observed by intensive shear deformation.

PACS numbers: 62.20.Fe; 62.50.+p; 63.88.−r

Keywords: molecular dynamics, dislocation, intensive plastic deformation, soliton-like wave, phase transition

I. INTRODUCTION

A new methods of intensive plastic deformation for achievement of nanostructure in metals had been developed. It is common knowledge that the main vehicle of plastic deformation is dislocation. In recent papers new vehicle of plastic deformation had been investigated widely for metal glasses. It is so called shear transformation zone (STZ) and kinks in acoustic chains. The main property of these objects is spontaneous concentration energy in the large excitations at cost of suppress of weak ones. It is possible to assume that such concentration in three-dimensional case can lead to rearrangement of internal structure of solid during intensive deformation.

II. CONSTITUTIVE RELATIONS

For the check of mentioned above assumption numerical experiment on two-dimensional model was performed by means of MD-simulation. Model system of 18*18 particles with Lennard-Jones potential is used:

\[ U_{ijkl} = \frac{A}{6} \left( \frac{B}{r_{ijkl}} - \frac{1}{r_{ijkl}^6} \right), \]

where \( r_{ijkl} = \sqrt{(X_{ij} - X_{lk})^2 - (Y_{ij} - Y_{lk})^2} \) - is the distance between the particles numbered by \( i, j \) and \( l, k \) with Cartesian coordinates \( X_{ij}, Y_{ij} \) and \( X_{lk}, Y_{lk} \). Indexes \( i, l \) numerate atoms in the lattice along the \( Y \)-direction, \( j, k \) do the same along the \( X \)-direction. Let use a unit in which the constants are equal to \( A = 0.0025 J m^6 \), \( B = 1 m^6 \), where \( J_c \) and \( m_c \) are conventional units of energy and length respectively. We put the mass of a particle to be \( M = 0.01 kg \), where \( k_c \) is conventional unit of mass. The binding energy of pair interaction is found in which the constants are equal to \( A = 0.0025 J m^6 \), \( B = 1 m^6 \), where \( J_c \) and \( m_c \) are conventional units of energy and length respectively. We put the mass of a particle to be \( M = 0.01 kg \), where \( k_c \) is conventional unit of mass. The binding energy of pair interaction is found to be \( E_b = A/12 B = 0.00020833 J_c \) and equilibrium distance is \( r_0 = \sqrt{\frac{E_b}{J_c}} = 1 m_c \). In case of real material it is necessary to perform the re-computation with account of real values of \( E_b, r_0 \) and the mass \( M \). For example, in the case of copper \( E_b = 0.5493 \times 10^{-9} J_c \), \( r_0 = 2.66 \times 10^{-10} m_c \), \( M = 1.0541 \times 10^{-25} k_g \). Then, \( 1 m_c = 2.66 \times 10^{-10} m_c \), \( 1 k_g = 1.054 \times 10^{-23} k_g \), \( 1 s_c = 0.532 \times 10^{-13} s_c \). The time unit have the same order as the period of small vibrations \( T = 2\pi m_c / U''_{ijkl} \). Time step for simulation is chosen to be \( \Delta t = 0.18 s_c \).

III. UNIAXIAL LOADING

The first series of real time computer simulations is fulfilled for uniaxial loading of a crystallite sample. The system is placed on rigid platform constructed from the atoms identical with those in the sample (the lowermost line of atoms on the figures). The rigid atomic line (plane in a three-dimensional case) constructed from the same atoms moves downward with a constant velocity \( 2.778 \times 10^{-4} m_c / s_c \) (the uppermost line of atoms on fig. 1). Initial atom configuration is hexagonal lattice with interatomic distance \( r_0 = 1 m_c \).

In the first stage the usual uniaxial elastic deformation goes (Fig. 1a). Further, two microscopic defects occur almost simultaneously in the left upper corner of the lattice and in the right down one (Fig. 1b). Their Burgers vectors have identical direction (at a 120° angle with horizontal axis) and opposite signs. These defects are similar to usual dislocations. However each of them has two and only two inserted atomic lines. They can’t have one
FIG. 1: Evolution of crystallite structure at uniaxial loading: a - ideal crystal structure at time step 27007, b - birth of dislocation pair at 29253, c - full formed bidislocation pair at 35 35019, d - lightning-like breakthrough between bidislocations at 35923, e - turned bidislocation pair at 36042, f - pressing out of the bidislocations from the sample at 36117, h - graphics of total potential energy of the system and kinetic and full ones during the turn of the bidislocations. Average potential energy per atom is equal to $-0.00132 J_c$. Yellow circles present the atoms with potential energy $0.00002 J_c < U < 0.00004 J_c$, green circles - with $0.00004 J_c < U < 0.0001 J_c$, blue circles - with $0.0001 J_c < U < 0.00015 J_c$, red circles - $0.00015 J_c < U < 0.00038 J_c$. Potential energy of the particles on free lateral surfaces is equal $0.0006 J_c$. 
inserted atomic line since atomic configuration doesn’t permit it owing to very large energy of the defects. Two inserted lines and glide line are oriented at 60° angle each to another. Both of the inserted lines always lie on one and only one side of the glide line. It is pertinent to call a defect with two inserted atomic lines as bidislocation. Along with two-dimensional lattice, such defects may be observed in three-dimensional case on the planes of closely packed layers (planes \( \{1, 1, 1\} \)). In general case of hexagonal lattice six type of bidislocation having Burgers vectors with the angles \( 0, \pi, \pm \pi/3, \pm 2\pi/3 \) may take place. In complex plane these vectors are expressed as

\[
\pm a_0, a_0 \exp(\pm \frac{\pi}{3} i), a_0 \exp(\pm \frac{2\pi}{3} i),
\]

where \( a_0 \) - is equilibrium distance in the crystallite.

In these terms, arisen bidislocations have following Burgers vectors:

\[
a_0 \exp(-\frac{\pi}{3} i) \quad \text{and} \quad a_0 \exp(\frac{2\pi}{3} i).
\]

Under following loading the bidislocations move along their glide lines for as long as they reach the rigid lines of atoms (Fig. 1c). Then, the bidislocations stop for some time because the rigid lines play the role of obstacles for further moving. Owing to this retardation, the bidislocationions form the pair with zeroth total Burgers vector. In this case the rotation of the region between the bidislocations takes place. This region has approximately circle form. The bidislocations lie exactly on diametrically opposite sides of the circle boundary. In this nanoscopic region the orientation of atomic lines (planes) along Burgers vector changes continuously. Owing to this property, observed pair of bidislocations may be simplest two-dimensional model of displanaion \([10], [11]\). The displanations are known as defects of mesoscopic level. It is clear from presented experiment that simplest modification of the displanations has nanoscopic nature.

Stopping of the bidislocations creates difficulties for repairing of ideal crystal symmetry. As a consequence, local concentration of elastic energy around defects takes places. It is clear that for finishing of symmetry repairing gliding lines must turn to the direction along rigid lines of atoms. What scenario does the system choice for it?

At the time of 600 time steps flashover-like puncture of the region between the bidislocations occurs (Fig. 1d). After it both the bidislocations are turned (Fig. 1f) and pressed out from the lattice in the direction parallel to rigid lines (Fig. 1f). Thereafter, the sample takes ideal crystal structure. Then, with continuing of loading the processes are qualitatively repeated.

It is known that different transformations of dislocations can be regarded as chemical \([12]\) or, better still, as elementary particle reactions. From this standpoint, in the case of two-dimensional hexagonal lattice any bidislocation may be considered as an elementary particle with vector charge (2) or as three particles (like quarks) with different own polarization and with internal coordinate (as spin). Let us denote the set of "elementary particles" as

\[
\pi_1^\pm = \pm a_0, \quad \pi_2^\pm = \exp(\frac{2\pi}{3} i), a_0 \exp(-\frac{\pi}{3} i), \quad \pi_3^\pm = \exp(\frac{\pi}{3} i), a_0 \exp(-\frac{2\pi}{3} i).
\]

Then the transition with rotation of glide lines (fig. 1.d-f) can be written in the form of reaction:

\[
\pi_2^+ + \pi_2^- \rightarrow \pi_1^+ + \pi_1^-.
\]

Therewith, the law of conservation of charge is fulfilled:

\[
a_0 \exp(\frac{2\pi}{3} i) + a_0 \exp(-\frac{\pi}{3} i) = a_0 - a_0 = const. = 0.
\]

The law of conservation of charge momentum is fulfilled since the distances between glide lines pre and post-reaction are equal (7 lines between them on the fig. 1d). The law of conservation of energy is fulfilled since the system is Hamilton one. As own energy of each of two bidislocations pre and post-reaction doesn’t change (in consequence of their identical structure) accumulated elastic energy almost completely turns into kinetic energy (relaxation of stress).

Regarding all the pictures presented in the fig. one can note that bidislocation nucleus isn’t localized in the point, but it is continuously smeared along the glide line in the region of several atomic sizes. The discrepancy of crystalline atomic lines begins with the distortion of them at bidislocation edges and increases gradually toward center. Near a glide line the chain of atoms viewed from the side of more rarefied region of crystallite is stretched. Let call this atomic chain as "stretched" chain. The chain viewed from the opposite side of the glide line is termed as "compressed" chain. The atoms in the stretched chain are localized in energetically unfavorable positions to ones in the compressed chain. However, the atoms are fixed in these positions owing to effective interaction with those in their own chains and with nearest atoms of the rest lattice.

Let set as 1 equilibrium interparticle distance in the region far from the bidislocations. Then, in the com-
pressed chain interparticle distance is equal to 1.1 and to 0.95 in stretched chain. Moreover, all the simulations exhibit the next trend. In the chains parallel to compressed and stretched ones and viewed from the compressed chain interparticle distance takes its asymptotic value 1 rapidly, already in the first chain. Alternately, in parallel chains viewed from the stretched one several chains are markedly stretched. Thus, the region of compression is more localized then the region of rarefying. Owing to this, potential energy of any particle in the compressed chain is more large than one in asymptotic zone. This peculiarity is the main sign for structure defects of any nature and permits to separate bidislocations immediately during computer simulation. Moving colored bidislocations against the background of the rest atoms is very nice picture. Average potential energy per atom in the compressed chain consists of 60-70 percent of one on free surface of the sample. Potential energy of whole the system in initial state of lattice is chosen as zeroth level.

IV. "KNIFE" LOADING

More interesting result is obtained in the second series of computer simulation for cutting the sample by three-atom knife (fig. 2). Three atoms only are left from moving upper rigid line of atoms. Other parameters of the experiment remain as in the Sec. III.

In the first stage, in general, the picture qualitatively looks like to one obtained in the previous numerical experiments. Elastic stage of deformation isn’t so interest. Further, the pair of bidislocations is created in the upper left and right corners of the crystallite. Their glide lines are turned by 60° each to another. The bidislocations occur in the region under three-atom indentor and move downward. Then, the bidislocations turn and they are pressed out from the sample.

Interesting phenomenon is observed at such pressing out (Fig. 3). The defect displayed on the figure has two additional lines and Burgers vector as the bidislocation does, but its form sufficiently differs. The stretched chain has gap in the center of bidislocation nucleus. That is, binding among centered atoms is broken and micropore arises.

Owing to the micropore, the bidislocation becomes more local and more sharp. Atomic lines in the regions separated by the normal to glide line are inclined at a big angle each to other. One can regard the line which separates such regions as an element of a boundary between grains.

During numerical experiment new bidislocations with micropores arise and disappear again and again. Whole the picture is similar to formation of steam bubble at water boiling. Owing to this "emission of the bubbles", the solid take on ideal structure again after some deformation.

On the other hand, the movement of a such object through the lattice is similar to kink-like excitation in acoustic chain. Wave-like disruption and repairing of bonds between atoms give rapid pressing out of defects from a sample.

Thus, at intensive influence on metal it may release not only by well known shear deformation, but by wave-like (or excitation-like) bond disruption, which moves rapidly enough. One can assume that the micropore, namely, is the sign of new state of bidislocation, which arises just during intensive deformation. In three-dimensional case the micropores can be spherical or elliptic bubbles. After stopping of deformation they disappear through the "condensation" into usual dislocations. Probably, it is difficult to detect the bidislocations with micropores in experiment as separate objects. Usual X-ray diffraction analysis isn’t suitable for investigation of such states and structure re-arrangements for two reasons. By the first, such analysis is fulfilled much later after finish of intensive plastic deformation. By the second, the solid in such process can be in non-equilibrium amorphous state with large widening of X-ray spectrum line. For detection of such states and its changes, it is necessary to execute X-ray analysis just during intensive plastic deformation or, maybe, immediately after it.

V. SHEAR LOADING

A great amount of such objects occurs in the case of intensive deformation by shear scheme. This scheme is realized in the following way: the sample consisted from 28*28 particles is placed in rigid two-dimensional box constructed from atoms identical with those of sample. The box is deformed by horizontal movement of upper and down rigid lines with constant velocity.

The created dislocations with micropores form boundary separated regions with different orientation of crystalline atomic lines (Fig. 3b). Such boundary can play important role for forming of nano-structural state by means of the methods of large shear deformation.

At the beginning stage of deformation single bidislocation is borne in the left down corner of the sample (Fig. 3a). It has the charge \( a_0 \exp(-2\pi i/3) \) and moves along glide line toward the upper boundary. At the following stage, the second bidislocation with the charge \( a_0 \exp(-\pi i/3) \) comes into being and moves along glide line toward the upper boundary too (Fig. 3b). The glide lines of both bidislocations are crossed at the same point exactly on the upper boundary. With the lapse of time the first bidislocation takes the form of microcrack (Fig. 3c) and preserves this form for a time (Fig. 3d). In the following lapse the first bidislocation begin to take the form of sharp bend (Fig. 3e). Upon it, pair of bidislocations arises instead the first one. One of them has the charge \(-a_0\) and another has the charge \( a_0 \exp(-\pi i/3) \). Their total charge is equal to \( a_0 \exp(-2\pi i/3) \), i.e. it is equal to the charge of the initial first bidislocation. Such transformation can be written as decay reaction in the
FIG. 2: Evolution of crystallite structure at cutting by three atom knife: a - ideal crystal structure in beginning stage, b,c - formation of usual bidislocation, d, f-h - formation of bidislocation with micropore, e - renewal ideal crystal structure after first "bubble".
FIG. 3: Evolution of crystallite structure with shear deformation: a - birth of first bidislocation, b-d - moving of two defects, e - bidislocation decay with birth of two new bidislocation, f - system after bidislocation decay.
form:
\[ \pi_2^- + \text{energy} \rightarrow \pi_1^- + \pi_3^- . \]  
(7)

where the second term in the left part of equation is the energy of stress field which causes the birth of additional "particle". The rest of stress field energy transforms into thermal energy. As the result, almost full relaxation of elastic stress take place.

The dislocations with micropores form boundary separated regions with sharply different orientation of crystalline atomic lines (fig. 4). Such boundary can play important role for forming of nano-structural state by the methods of large shear deformation. Single, but very interesting result had been fixed in computer experiment when rotation of certain volume by scenario of phase transition takes place. At some deformation the boundary is formed as a chain of bidislocations with micropores. At following loading it moves steadily until escape from the sample. In this case the boundary separates phases of identical nature, but with different orientation of crystalline atomic lines only.

With my point of view, the defects described above have similar nature to them considered in ref. [2] - [5]. Our "STZs" differ from [2] - [3] ones because the former are observed in ideal crystallite, but no in amorphous metallic glass.

VI. SUMMARY

Thus, quark-like behavior of bidislocations is observed in different numerical experiments. It is established that the bidislocations may have at least two different structural states. The first of them has whole stretched chains, the second has micropores. The bidislocations with micropores, as a rule, have pentagon form. The states with crack-like form of bidislocations are possible too (Fig. 3b). The transient bent form of microcrack arises at the decay of dislocation (Fig. 3e). The superhigh-speed soliton-like movement of bidislocations with micropore is noted.

[1] E. G. Pashinskaya, L. S. Metlov, V. N. Varyukhin, and A. F. Morozov, Proceeding of the V International Conference Metallurgy, Refractories and Environment, Stara Lesna, High Tatras, Slovakia, May 13-16 (2002).
[2] S. F. Edwards and R. B. S. Oakeshott, Physica A 157, 1080 (1989).
[3] M. L. Falk and J. S. Langer, Physical Review E 57, 7192 (1998).
[4] M. L. Falk, Physical Review E 60, 7062 (1999).
[5] A. Lemaitre, http://arxiv.org/abs/cond-mat/0206417 (2002).
[6] T. Cretegny, T. Dauxois, S. Ruffo, and A. Toecini, Physica D 121, 109 (1998).
[7] L. S. Metlov, Phizika i Tekhnika visokikh davleniy 11, 121 (2001), see also http://arxiv.org/abs/physics/0101041 17 Apr 2002.
[8] L. S. Metlov and Y. V. Ereimechenkova, http://arxiv.org/abs/cond-mat/0200004 (2002).
[9] N. P. Bailey, J. P. Sethna, and C. R. Myers, http://arxiv.org/abs/cond-mat/0011097 (2000).
[10] T. E. Konstantinova, Meso-structure of Deformed Alloys (DonPhTI NAN of Ukraine, Donetsk, Ukraine, 1997), in Russian.
[11] T. E. Konstantinova, V. P. Primisler, and A. A. Dobrikov, Phizika i Tekhnika visokikh davleniy 2, 50 (1992), in Russian.
[12] K. Shizawa, K. Kikuchi, and H. M. Zbib, Materials Science and Engineering A 309-310, 416 (2001).
FIG. 4: Phase-like transition with moving boundary consisting from bubble-bidislocations having pentagon form.