Evolution of Metal Structure at Intense Plastic Strains: Molecular Dynamics Simulation

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(Dated: February 7, 2020)

The kinetics of dislocations is studied with computer simulation at loadings of different intensity. It is established that the dislocations have a few different structural states. The dislocations “with the micropore” play important role in the formation of large curved boundaries, and, as a consequence, in the formation of fine grains. Alternation of elastic and inelastic strain stages is established too. At shear loading, in view of special kinetics, the system would have to accumulate the whole set of dislocations leading to the formation of new boundaries and fine grains.

PACS numbers: 62.20.Fe; 62.50.+p; 63
Keywords: molecular dynamics, dislocation, intense plastic strain, uniaxial compression, equilibrium state

I. INTRODUCTION

Processing of materials by using the intense plastic strains (IPS) to obtain the grains with the size of about tens and hundreds nanometers is a promising direction of modern technologies [1]. During the IPS the processes with high strain rate take places. As a consequence, there is not enough time to establish the equilibrium state in the systems, and the process has essentially the non-equilibrium character. From the thermodynamic point of view, fast strain of a metal sample is similar to the process of quenching with the difference, that the transition is realised not by a change in temperature, but with a change of pressure. Owing to this, at the IPS the energy pumping into the sample occurs through the creation of structural non-equilibrium objects, such as fine grains, additional non-equilibrium strongly curved boundaries, etc. It is possible to obtain many qualitative results about features of the IPS with the molecular dynamics simulation on rather small systems of about 1000 atoms and less.

The computer experiments, the results of which are discussed below, are carried out using the pair Lennard-Jones potential of interparticle interaction in the form:

\[ U_{ijlk} = E_b\left((\frac{r_0}{r_{ijlk}})^{12} - 2(\frac{r_0}{r_{ijlk}})^6\right), \]  

(1)

where \( r_{ijlk} = \sqrt{(X_{ij} - X_{lk})^2 - (Y_{ij} - Y_{lk})^2} \) - is the distance between the particles numbered \( i,j \) and \( l,k \) with Cartesian coordinates \( X_{ij}, Y_{ij} \) and \( X_{lk}, Y_{lk} \). The indices \( i, l \) numerate atoms in the lattice along the \( Y \)-direction, \( j, k \) do the same along the \( X \)-direction. \( E_b, r_0 \) - are the binding energy and equilibrium interparticle distance in the two atomic system, respectively.

The regimes of loading the samples, used below in the numerical experiments, are typical of methods of equalchannel torsion [1], [2], and for formation of nanostructures through friction [3]. Besides, it is established that nanostructures are formed in the near-surface layer of rails during their operation. Really, the surfaces of a rail and a wheel represent some set of roughness of different scale. In the process of "rolling", a roughness of a wheel uniformly or non-uniformly is superimposed over a roughness of a rail. As a result, each roughness undergoes uniform or non-uniform uniaxial strain. Besides, the tractive forces developed at movement of a rolling-stock, create shear forces on the roughness. Qualitatively the same picture is present during the formation of nanostructures through friction under pressure [2].

II. UNIAXIAL COMPRESSION OF SAMPLE UNDER RIGID BOUNDARY CONDITIONS

The rigid boundary conditions can occur in a material when a soft microscopic inclusion is surrounded with a more rigid matrix. The rigid boundary conditions are idealistic, but they can be useful at study of structural relaxation in a small bulk. It is known that in a small bulk the equilibrium state is established much faster without the special influence of the other bulk. Therefore for the time of the establishment of the equilibrium state it is possible to isolate the investigated microbulk from the other bulk through the rigid boundary conditions. The influence of the other part of the bulk through the soft boundary conditions will also be taken into account in section III.

The uniaxial loading of a perfect crystallite under the rigid boundary conditions can be realised, for example, at the central contact of roughnesses at rolling of a rail by wheels of a rolling-stock. The constants of the potential (1) and mass of particles in certain conditional system of units are chosen to be equal, \( E_b = 0.20833mJ/c, \) \( r_0 = 1nm, \) and \( m = 0.01kg/c, \) and the time step is \( t = 0.188c. \) The period of small vibrations of particles is calculated.
with the formula $T = 2\pi\sqrt{m/U_{ij}}$, where $U_{ij}$ is the total potential energy of $i,j$-particle in the field of the other particles. In the cases of a) two molecular system, b) non-linear chain and c) vibration of crystalline "planes" in a two-dimensional crystal, the periods of vibrations are equal to $5.12s_c$, $3.63s_c$ and $2.55s_c$, respectively. The velocities of sound waves in the low-frequency limit in the both last cases are equal to $1.22m_c/s_c$ and $1.5m_c/s_c$, respectively.

The crystallite was placed on a rigid motionless platform consisting of atoms of the same sort, as the sample (the lowermost atomic layer). The same rigid atomic layer goes from above downwards with the constant velocity of $2.77810^4m_c/s_c$ (the uppermost atomic layer). The lateral sides of the sample are free. The initial atomic configuration is presented by the hexagonal lattice with the interparticle distance $r_0 = 1m_c$. The initial configuration of the rigid boundaries and the system as a whole is shown on the insert in fig.1. In the initial configuration between the rigid top side and the sample there is a small gap.

In the base experiment, in the beginning and through every 29900 time steps were executed the deep cooling of the sample by five-multiple zeroing of kinetic energy of the atoms on 80, 130, 200, 280 and 284-th time steps. Such cooling liquidates surplus of heat arising because of higher strain rate, than in a real experiment. The additional details of the description of the base experiment may be found in ref. [4]. Here for comparison the computer experiments were distinguished from the base one a) by the absence of periodic cooling of the sample through 29900 time steps (cooling only at the initial stage) b) the absence of cooling.

Change of different kinds of energy during the initial stage of strain is given in the fig.1. At the expense of attraction to the rigid boundary separated from the sample by a small gap the sample in the beginning is slightly stretched, thus, in a consequence of this, the low-frequency oscillations covering all the system are arisen (Fig.1). The period of the low-frequency oscillations equals approximately $21s_c$. The small change of the internal energy is negative. It testifies that at this stage the system itself performs work on the moving of the rigid boundary. In due course, the low-frequency oscillations are dissipated, and their energy completely transforms to heat. In this limit, the double average kinetic energy per one degree of freedom, to within Boltzmann’s constant, is a measure of temperature of a sample $\mathcal{E}$. The energy removal at cooling reduces its total potential and internal energies (Fig.1). In the both cases under consideration the potential energy decreases in comparison with its initial value, however, in the experiment with cooling it decreases by a larger magnitude ($4,838m_Jc$).

In the regarded cases the overall picture of crystallite strain at the uniaxial compression is similar. After the stage of elastic strain in the left top and right bottom corners of the sample two dislocations are almost simultaneously formed. According to the introduced in [4] definitions, they can be considered as "elementary particles" of a kind $\pi^+_{ij}$ and $\pi^-_{ij}$. At further strain the dislocations move along their own planes of sliding up to those, do not achieve the rigid boundaries, where are stopped. The stop of the dislocations results in an additional elastic energy concentration around them. At some time the puncture of material between the dislocations similarly to a lightning stroke or electrical discharge occurs. The regrouping of atoms owing to the puncture results in turning the both dislocations by $60^\circ$ and their planes of sliding proved to be parallel to the rigid boundaries. The last circumstance promotes their further pressing out of the sample. As a result, the sample completely restores its perfect crystal structure. With growth of the strain the picture qualitatively repeats more then once with the same script, - birth of dislocations, their movement, turning out and leaving the sample, and complete renewal of the crystal structure.

The irreversibility of the process is expressed by a change of the lateral surfaces relief of the sample after each exit of the dislocations, and with reduction of number of the layers in the vertical direction just one. In the end, the work of external forces is spent for increasing the bulk elastic energy, the potential energy of the curved lateral surfaces, and for increasing the energy of the thermal movement. Actually in this picture dislocations are an intermediate link of transformation (relaxation) of energy or an intermediate state. With temperature increase the birth of dislocations is facilitated, the interval between cycles is reduced and, at last, they merge in one continuous process.

At different stages of system evolution features of energy transformations are of special interest. In the experiments with initial cooling, the kinetic energy is close to zero, and the potential and internal energies are approximately the same down to the moment of birth of a dislocation pair (Fig.2). The dislocation pair birth on a background of slow growth of the internal energy of the system at the expense of work of the rigid boundaries is accompanied by conversion of a part of the potential energy (elastic pressure) into the kinetic energy. The transition is accompanied by excitation of elastic low-frequency vibrations of the resonant character, with frequency gradually growing in due course, and the amplitude falling. During about a two tens periods of the low-frequency vibrations the latter calm down, and completely pass into the thermal fluctuations. On record of the transition the potential energy decreases by $1.164m_Jc$.

Without the prior cooling the described process gets some other character (Fig.3). Higher initial value of the internal energy leads to a more earlier birth of dislocation pair, approximately, by 1000 time steps. "Premature birth" results in the fact that the dislocations are languid and inactive, as the overall store of the elastic energy for setting them in motion, is not so great yet. The dislocations slowly enough during 300 − 350 time steps advance in directions of the rigid boundaries. The jump of the potential energy during the transition is equal to $0.537m_Jc$. 
that it is much less, than with cooling.

At turn of the dislocations, similar transformations of energy are taking place too. In these cases the jumps of the potential energy are equal, accordingly, to 1.041mJc with the cooling (see fig.1 in ref. [4]) and 2.608mJc with no cooling.

Example of potential energy distribution around a dislocation is presented in fig.4. The atoms of the largest energy are placed on the “compressed” chain. Next series of atoms ranged in energy is placed behind the “compressed” chain, and only the next series - on the “stretched” chain.

III. UNIAXIAL COMPRESSION OF SAMPLE UNDER SOFT BOUNDARY CONDITIONS

The rigid boundary conditions as though completely, both in thermodynamic and in mechanical sense, isolate the allocated bulk from other part of a crystal. If this is possible to assume from the point of view of thermodynamic isolation, as the heat equilibrium before all is established in a small bulk, from the point of view of far-acting mechanical fields it is not always justified. The soft boundary conditions are reached at the expense of introduction of the periodic boundary conditions along the loading axis. In this connection there arises a question, whether - will be and as far as to differ character of dislocation behaviour from one under the rigid boundary conditions?

Strain is given by change of the periodicity size with the same velocity, as movement of the rigid boundary in the previous experiments. First dislocations in system consisting of 30*30 particles with binding energy $E_b = 0.2083mJc$ occur at the 46839-th time step. According to the accepted definition (4) in ref. [4] they are dislocations of a type $\pi_1^+$, $\pi_2^-$, $\pi_4^-$, $\pi_2^+$. In the given series of experiments the dislocations arise not at edges of up and down boundaries, as in the case of the rigid loading, but at the central parts of free lateral sides of the sample (Fig.5). They move in the directions of the horizontal boundaries and pass through them (Fig.5). As in such system the stoppers for movement of dislocations, playing the important role in the previous example, are absent, the dislocations continue to move at achievement of the horizontal boundaries. As a result, they meet at the centre of the sample (Fig.5). Further the picture becomes complicated and in the sample 5, 6 dislocations are observed simultaneously, and, they transit into the structural state ”with micropore” (Fig.5). At 47240-th time step a part of dislocations come out on the free lateral surfaces, deriving roughnesses of its relief, the others annihilate among themselves, deriving to the vacancy at the centre of the sample, and in the system the perfect crystal structure is restored. The described events occur during 400 time steps, that is in current the short interval of time in comparison with the previous phase of elastic strain (46800 time steps). Furthermore, the system calms down for a long time, and during 36000 time steps the dislocations are absent at all. During this time the strain again proceeds in the elastic manner.

At the 83152-th time step the vacancy at the centre of the sample breaks up to the pair of dislocations $\pi_1^+$ and $\pi_2^-$ (Fig.5), which move in different directions (Fig.5). The whole series of births and annihilations of dislocations begins with this decay which is not given completely in the fig.5. From this series the fragments, illustrating the merge of two dislocations and the birth of third ones (Fig.5) are only given. At the 83630-th time step from the top boundary begin to move dislocations $\pi_2^-$ and $\pi_4^+$. At first the dislocation $\pi_4^+$ outstrips the dislocation $\pi_2^-$, crossing the sliding plane of the last-mentioned before arrival of one to this point (Fig.5 j). At that instant, when the dislocation $\pi_4^+$ reaches the point of crossing the sliding planes (Fig.5), it begins to attract the first one. As a result of this attraction the first dislocation comes back along its own sliding plane (Fig.5), both dislocations merge and form a new one (Fig.5). The latter is pressed out from the sample in parallel to its horizontal boundaries. As a result, in the system perfect crystal structure, already without vacancy is again restored. The following stage of inelastic strain begins approximately through 28000 time steps (Fig.5).

Thus, it is possible to ascertain, that the general feature, - the cyclic change of elastic and inelastic stages of strain, marked at pressing by the rigid boundaries, is kept in the case of the soft boundaries too.

IV. CUTTING SAMPLE BY THREE-NUCLEAR KNIFE

In the previous experiments on a nanoscopic level an analogue of a homogeneous and non-hydrostatic state was realised. The influence of a non-uniform loading on character of generation and behaviour of dislocations is of large interest too. This problem was investigated in the next series of computer experiments simulating the cutting of the same sample by a rigid three-atomic knife [4]. In the moving downwards rigid top boundary the three central atoms are only left. The binding energy of particles in these experiments is accepted to be equal to 0.0416mJc, other parameters are same, as in section 1.

The initial elastic stage of strain ends, when in the region of three-nuclear indentor first pair of dislocations is born, the sliding planes of which form an angle of 60°. Then they move to the bottom rigid boundary, are turned and leave the sample. However they leave the sample not with parallel rigid side as in a case of uniaxial compression, but mainly at an angle of 60° to it, being directed to the left or right top corners of the sample (see fig. 2 in the ref. [4]).

However at general similarity of the script the character of dislocations is different, - they pass in some new structure modification with micropore at the dislocation nucleus [4]. Owing to micropore a dislocation becomes...
more localized, than in the usual allocated state. The atomic planes in area divided by a normal to the plane of sliding, diverge at a more larger angles than in the previous example. Such dislocation can be considered as a possible element of large-angle grain boundaries, which at small quantity of these elements can result in the formation of curved boundaries and, as a consequence, in the formation of a fine grain.

Thus, in the previous series of experiments has been shown that dislocations, having the same Burgers vector, can be, at least, in two structure modifications or states, - in allocated (basic) states and ones with a micropore. A distinctive attribute of a state with micropore is the presence on the lattice images of typical pentagons. It is characteristic, that a "state with micropore" occurs at non-uniform or intense loading more preferably. Except for the mentioned above two structure modifications there are also others [4], which can have the large importance in dynamics of IPD.

V. SHEAR STRAIN OF SAMPLE BY RIGID SHELL

A plenty of dislocations arises at straining a sample under the shear loading. This loading is realised as follows: the sample from 28x28 particles with binding energy of $0.0416mJ_c$ is placed in the rigid two-dimensional shell consisting of atoms of the same type, as the sample. The shell is deformed through movement of the top and bottom sides of the shell to itself with constant velocity in mutually opposite directions.

At an initial stage of strain, dislocations $\pi^-_3$ and $\pi^-_2$ are born (see classification and fig. 3 in ref. [4]). Then the first of them decays on two new dislocations according to the equation of reaction:

$$\pi^-_3 + \text{energy} \rightarrow \pi^-_1 + \pi^-_2. \quad (2)$$

(In formula (7) of ref. [4] in recording of this reaction there was an annoying misprint).

Strain under the uniaxial loading leads to a repeated recurrence of the same common script of system behaviour, - birth of dislocations, them turning out, restoration of perfect crystal structure etc. At straining a sample under the shear loading the system evolution proceeds under essentially different script. In view of special kinematics of such strain the restoration of perfect structure is possible only after a turn of some "macroscopic" bulk as whole through a finite discrete angle being an element of crystal symmetry. For two-dimensional problem it is the angle of $60^\circ$. For realization of such a turn it is impossible to do with a sequence of births and annihilations of one or two dislocations only. The system would have to accumulate set of dislocations, and, as a consequence to form new boundaries and fine grains to restore the symmetry even if in a local region. This feature determines the shear loading of strain as the effective tool of material structure transformation. And in most cases dislocations are not in the basic structural state, and in a "state with micropore", which is testified by the typical pentagon fragments on the images of a lattice. Owing to "pentagons" the strongly bent boundaries of fine grains are formed.

VI. SUMMARY

Thus, the kinetics of dislocations is observed in different numerical experiments. It is established that the dislocations may have at least two different structural states. The first of them has whole stretched chains, the second has micropores. The dislocations with micropores, as a rule, are of pentagon form. Owing to micropore a dislocation becomes more localised, than in the usual allocated state. The atomic planes in area divided by a normal to the plane of sliding, diverge at more larger angles. Such dislocation can be considered as a possible element of large-angle grain boundaries, which at small quantity of these elements can result in the formation of curved boundaries and, as a consequence, in the formation of a fine grain. Strain under the uniaxial or "knife" loadings lead to repeated recurrence of the same common script of system behaviour, - birth of dislocations, their turning out, restoration of perfect crystal structure etc. Alternation of elastic and inelastic strain stages leads one to the assumption that the studied sample can be alternatively as elastic or non-elastic element of more complex bodies such as Foit or Maxwell ones.

At straining a sample under the shear loading the system evolution proceeds under essentially other script. In view of special kinematics of such strain the restoration of perfect structure is possible only after turning some "macroscopic" bulk as whole through a finite discrete angle being an element of crystal symmetry. For realization of such turn it is impossible to do with sequence of births and annihilations of one or two dislocations only. The system would have to accumulate set of dislocations, and, as a consequence to form new boundaries and fine grains to restore the symmetry even if in a local region. This feature determines the shear loading of strain as an effective tool of material structure transformation.

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FIG. 1: Changes of the general potential, kinetic and internal energy of system on the initial stage: a - base experiment, b - experiment without cooling.
FIG. 2: Elastic vibrations of nanobulk at stripping of the first dislocations and their change during transformation into the thermal fluctuations (cooling only on the initial stage)
FIG. 3: Elastic vibrations of nanobulk at stripping of first dislocations and their change during transformation into the thermal fluctuations (the cooling is absent at all). On inserts the Yellow circles present the atoms with potential energy $0.02mJ_c < U < 0.04mJ_c$, green circles - with $0.04mJ_c < U < 0.1mJ_c$, blue circles - with $0.1mJ_c < U < 0.15mJ_c$, red circles - $0.15mJ_c < U < 0.38mJ_c$. Potential energy of the particles on free lateral surfaces is equal $0.6mJ_c$. 
FIG. 4: Values of the potential energy of particles in a vicinity of the nucleus of dislocations (in mJc): 1 - 0.429; 2 - 0.403; 3 - 0.268; 4 - 0.202; 5 - 0.19; 6 - 0.129; 7 - 0.101; 8 - 0.058; 9 - 0.025; 10 - 0.063, 11 - 0.067, 12 - 0.019; 13 - 0.012; 14 - 0.041; 15 - 0.002. For a zero level the average potential energy on one particle in the sample is accepted.
FIG. 5: Evolution of structure of crystallite at soft strain.
The images correspond to the following time steps: a - 46840, b - 46850, c - 46880, d - 46990, e - 47240, f - 83152, g - 83630, h - 83715, i - 83816, j - 84005, k - 84040, l - 117000; a-e - first cycle of not elastic strain, f-k - second cycle of not elastic strain, l - beginning of the third cycle of not elastic strain.