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"Severe Plastic Deformation" of 2D Crystallites

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Abstract The kinetics of dislocations is studied by means of computer simulation at different severe loadings. It is found that the dislocations can have a few (at least, two) different structural states. The localized dislocations with core shape as "micropore" play important role in formation of large curved grain boundaries, and, as a consequence, in formation of fine grains. Saltatory alternation of elastic and non-elastic stages of deformation is revealed too. At shear loading in view of special kinetics the system would have to accumulate whole set of localized dislocations leading to formation of new boundaries and fine grains.

Keywords Molecular Dynamics Simulation, Dislocations, Dislocation Reactions, Structural Defects

1 Introduction

The greatest progress of modern technologies is connected with production of nanomaterials. The most promise methods of reception of bulk metal samples with homogeneous properties on all section are processing of them by the severe plastic deformations (SPD) [1]. During SPD a usual metal sample with coarse grains about several tens micrometers gets fine grain structure with the sizes of grains about hundred nanometers. The mechanisms of formation of fine grains and homogeneous properties on all section of sample till now are not yet clear up to the end. Ones consider, that grain boundaries and diffusion along of them [2-4] or slipping on them with elements of superplasticity [5] are crucial for formation of such structure. Others try to explain their formation from positions of dislocation dynamics into bulk of grains [6-11].

The deformation of polycrystalline solids at the large loadings is complex multilevel p combining elements of elastic and no elastic behavior. The elastic deformation proceeds without change of internal structure of a solid, while the not elastic one is necessarily accompanied by realignment of its structure. The rebulding of internal structure of a solid is carried out with involving of their internal degrees of freedom in the form of structure defects - vacancies, interstitial atoms, dislocations, disclinations, the twin zones etc. Most widespread defects of a solid crucial for plastic deformation are dislocations. The theory of dislocations qualitatively, and in some cases quantitatively, describes behavior of solids under the large loadings. Now this theory has reached a high level of formalization [6-9,12,13]. Behavior both separate dislocations and dislocation ensembles, including processes of their self-organizing, is described with its help. Large massive of investigations is devoted to studying of problem with help of molecular dynamics simulation [14-18].

In too time the processes of birth, annihilation or mutual transformation of dislocations are still insufficiently investigated and are unclear. The questions connected to structural states of dislocation cores in fields of external pressure, the questions of stability of non-equilibrium boundaries are poorly investigated. In three-dimensional space these processes are difficult enough, therefore is of interest to consider them in simplified two-dimensional variant. The dislocation dynamics in 2D systems under different deformation loading has been the subject of a large number of theoretical investigations [19-23]. Thus such researches do not put by the purpose to exact modeling of any particular materials, and only task to understand qualitative features of dislocation behavior at an atomic level.

In [19] the passage through a potential barrier of an atom in the core of a moved single dislocation is investigated at its displacement on one intersite distance under external deformation or stress. The height of the barrier was defined on a difference of potential energy in a saddle point and its minimal value after freezing system. Let's pay attention to a configuration of atoms in initial and final states of the dislocation core outlined by a circle in fig. 1 of [19]. It has the form of an almost correct pentagon as against vacancy, for which the hexagonal form of environmental atoms counter is typical. It is properly one of structural dislocation core states, about what there will be discussed below in more detail.

In [22] the single and pair dislocations, which were entered into system by withdrawal of atomic lines and subsequent relaxation of system through an intermediate stage with partial dislocations, were investigated. The pressure acting on the dislocations, were created owing to lattice mismatch. Thus the authors presented remarkable on the beauty and deep on sense a sequence of dislocation reactions. In an initial state a pair of dislocations was entered by "hands" with planes of sliding parallel to boundary on some distance from boundary in

a substrate, while energetically more favorable accommodation of such dislocations is directly on boundary (see fig. 3.5 of [22]). Relaxation of system at the expense of direct moving of the dislocations to boundary is impossible owing to the given special orientation of their sliding planes. Therefore in the beginning the system provokes reaction between pair of dislocations accompanying with turn of planes of sliding, and only then one of them goes to boundary. After that, they once enter in reaction again, restoring orientation of sliding planes to parallel boundary. Certainly, such simple and beautiful reaction has appeared possible owing to a successful choice of initial conditions of problem - dislocations in pair are separated on necessary distance, pressure of lattice mismatch has appeared enough for initiation of these reactions etc.

The authors of [22] do not analyze the features of structural states of the dislocation cores during movement and reactions, but as follows from the presented there figures they are in other structural state, than similar dislocation cores in [19]. Namely, the core of the dislocation is not located in the form of a pentagon, and is in regular intervals allocated along a plane of sliding. The reasons of occurrence of various structural states, some features and regularities connected with it, and also possible consequences for physics of materials are a subject of research of the presented paper.

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

$$U_{ijlk} = E_b((\frac{r_0}{r_{ijlk}})^{12} - 2(\frac{r_0}{r_{ijlk}})^6), \qquad (1)$$

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 pair numbering of particles is convenient for definition of an initial state of a two-dimensional lattice and further control of its change. The indexes i, l numerates atoms in the lattice along the Y-direction, j, k does 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 constants of the potential (1) and mass of particles in certain conditional system of units are chosen $E_b = 0.20833mJ_c$, $r_0 = 1m_c$, and $m = 0.01kg_c$, and the time step is chosen $t = 0.18s_c$. 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 $5.12s_c, 3.63s_c$ and $2.55s_c$, respectively. The velocities of sound waves in the low-frequency limit in both the last cases are $1.22m_c/s_c$ and $1.5m_c/s_c$, respectively.

Loading regimes used here in numerical experiments are typical for equalcannel torsion methods [24,25] and for formation of nanostructures under friction [26]. Besides, it is found, that nanostructures are formed in the near-surface layer of rails during their expluatation. Really, the surfaces of a rail and a wheel represent some set of roughness' of different scales. During "rolling" the roughness on the wheel uniformly or non-uniformly is placed over the roughness on the rail. In result each roughness undergoes uniform or non-uniform uniaxial deformation. Besides, the tractive forces developed at movement of a rolling-stock creates shear efforts on the roughness. Qualitatively the same picture is present during formation of nanostructures with friction under pressure [26].

2 Uniaxial compression of sample under rigid boundary conditions

The rigid boundary conditions can take place into a material when a soft microscopic inclusion is surrounded with more rigid matrix. The rigid boundary conditions are idealistic, but they can be useful at study of structural relaxation in small particles. 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 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 by means of soft boundary conditions also are considered in section 3.

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 atomic layer goes rigidly from the top down with the constant velocity $2.77810^4 m_c/s_c$ (the uppermost atomic layer). The lateral sides of the sample are free. The initial atomic configuration is presented by the hexagonal lattice with interparticles distance $r_0 = 1m_c$. The initial configuration of the rigid boundaries and the system as a whole is shown in the insert in the fig.1a. In the initial configuration between the rigid top of atomic line and the sample there is a small gap.

In the basic experiment 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 were executed in the beginning and through everyone 29900 time steps. Such cooling liquidates heat excess arising because of higher strain rate, than it takes place in a real experiment. The additional details in description of the basic experiment may be found in [27]. Here for comparison the computer experiments distinguished from the basic one a) by absence of periodic cooling of the sample through 29900 time steps (cooling only on the initial stage) b) without cooling at all are presented also.

Time change of different kinds of energy during the initial stage is given in the fig.1. At the expense of attraction to the rigid boundary separated from the sample by the small gap the sample in the beginning is slightly stretched, and own to it low-frequency oscillations covering all system are arisen (Fig.1b). The period of the low-frequency oscillations is approximately $21s_c$. The small change of the total internal energy is negative. It testifies that at this stage the system itself performs work at the moving rigid boundary. In due course, the low-frequency oscillations are dissipated, and their

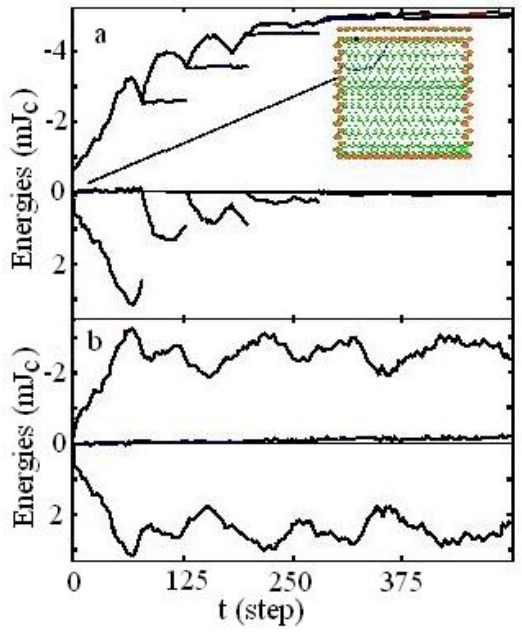

Figure 1. Changes of the total potential, kinetic and internal energy of system on the initial stage: a - base experiment, b - experiment without cooling.

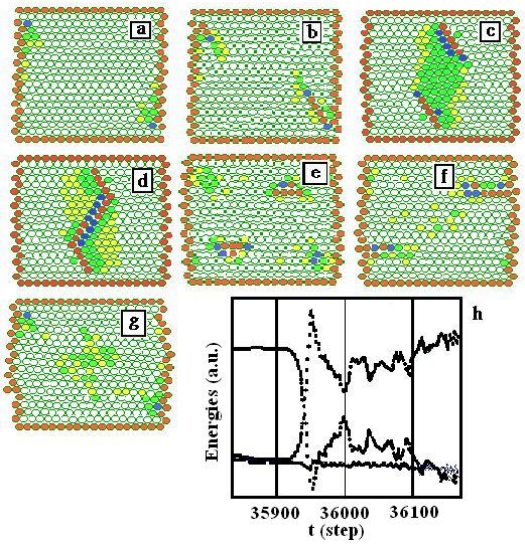

Figure 2. Evolution of crystallite structure at uniaxial loading in the base case: a - ideal crystal structure at time step 27007, b - birth of dislocation pair at 29253, c - full formed dislocation pair at 35 35019, d - lightning-like breakthrough between dislocations at 35923, e - turned dislocation pair at 36042, f - pressing out of the dislocations from the sample at 36117, h - graphics of total potential energy of the system and kinetic and full ones during the turn of the dislocations. Average potential energy per atom is $-0.00132J_c$. Yellow circles present the atoms with potential energy $0.00002J_c < U < 0.00004J_c$, green circles - with $0.00004J_c < U < 0.0001J_c$, blue circles - with $0.0001J_c < U < 0.00015J_c$, red circles - $0.00015J_c < U < 0.00038J_c$,. Potential energy of the particles on free lateral surfaces is $0.0006J_c$.

energy completely transforms in 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 [28]. The energy removal at cooling reduces its total potential and internal energy (Fig.1a). In both considered cases the potential energy decreases in comparison with its initial value, however, in the experiment with cooling it decreases on larger magnitude $(4,838mJ_c)$.

In the regarded cases the overall picture of crystallite deformation at the uniaxial compression is similar. In the first stage the usual uniaxial elastic deformation goes (Fig.2a). Further, two 2D dislocations occur almost simultaneously in the left upper corner of the lattice and in the right down one (Fig.2b). Their Burgers vectors have identical direction (at a 120° angle with horizontal axis) and opposite signs. These dislocations are similar to ones in [19]. However each of them has two and only two inserted atomic lines. They can't have one inserted atomic line since atomic configuration doesn't permit it owing to very large energy of the defects in this case. 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. Along with 2D lattice, such defects may be observed in 3D case on the planes of closely packed layers (planes $\{1,1,1\}$). In a general case for hexagonal lattice six type of dislocations 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

$$\pm a_0, a_0 \exp(\pm\frac{\pi}{3}i), a_0 \exp(\pm\frac{2\pi}{3}i), \qquad (2)$$

where a_0 - is equilibrium interatomic distance in the crystallite.

In these terms arisen in fig. 2b dislocations have following Burgers vectors:

$$a_0 exp(-\frac{\pi}{3}i) \quad and \quad a_0 exp(\frac{2\pi}{3}i). \qquad (3)$$

During later loading the dislocations move along their glide lines for as long as they reach the rigid lines of atoms (Fig. 2c). Then, the dislocations stop for some time as the rigid lines play the role of obstacles for further moving. Owing to this retardation, this two dislocations form a pair with zero total Burgers vector. Stopping of the dislocations creates difficulties for restoring of ideal crystal symmetry. As a consequence, local concentration of elastic energy around the defects takes places.

At the 600 time step a flashover-like puncture of the region between the dislocations occurs (Fig. 2d). After this the both dislocations are turned (Fig. 2e) and pressed out from the lattice in the direction parallel to rigid lines (Fig. 2f). Thereafter, the sample takes an ideal crystal structure. In spite of beginning state (Fig. 2a) achieved state (Fig. 2g)is distinctive in that: one horizontal atomic layer is absent, and kinetic energy of sample is more almost on the work of external forces. Further, with continuing of loading the processes are qualitatively repeated.

It is known that different transformations of dislocations can be regarded as chemical [29] or, better still, as elementary particle reactions. From this standpoint, in the case of 2D hexagonal lattice any dislocation can 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

$$\begin{aligned} \pi_1^{\pm} &= \pm a_0, \\ \pi_2^{\pm} &= \langle a_0 \exp(\frac{2\pi}{3}i), a_0 \exp(-\frac{\pi}{3}i)\rangle, \\ \pi_3^{\pm} &= \langle a_0 \exp(\frac{\pi}{3}i), a_0 \exp(-\frac{2\pi}{3}i)\rangle. \end{aligned} \qquad (4)$$

Then the transition with rotation of glide lines (fig. 2.d-f) may be written in the form of reaction:

$$\pi_2^+ + \pi_2^- \rightarrow \pi_1^+ + \pi_1^-. \quad (5)$$

Therewith, the law of conservation of charge is fulfilled:

$$a_0 \exp(\frac{2\pi}{3}i) + a_0 \exp(-\frac{\pi}{3}i) = a_0 - a_0 = const = 0. \quad (6)$$

The law of conservation of charge momentum is fulfilled too since the distances between glide lines pre and post-reaction are 7 lines between them in fig. 2d,f). The law of conservation of energy is fulfilled too since the system is Hamilton one. As own energy of each of two dislocations pre and post-reaction doesn't change in consequence of their identic structure) accumulated elastic energy almost completely turns into kinetic energy (relaxation of stress).

Regarding all the pictures presented in fig. 2, one may note that dislocation cores isn't localized in a point, but it is continuously destributed along the glide line in a region of several atomic distances. The discrepancy of crystalline atomic lines begins with the distortion of them at dislocation 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 us 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 placed 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 us take equilibrium interparticle distance in the region far from the dislocations as 1. Then, in the compressed chain interparticle distance is 1.1 and 0.95 in stretched chain. Moreover, all the simulations exhibit the next trend. In the next 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 next 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, the potential energy of a particle into the compressed or stretched chains is more large than one in asymptotic zone. This peculiarity is the main sign for structure defects of any nature and permits to view separate dislocations immediately during computer simulation. Average potential energy per atom in the compressed chain consists of 60-70 percent of one on free surface of the sample. Total potential energy of the system in the initial state is chosen as zero.

At different stages of system evolution features of energy transformations is presented of the special interest. In the experiments with initial cooling only the kinetic energy is close to zero at the beginning time, and the potential and internal energies are approximately equal among themselves down to a instant of birth of a dislocation pair (Fig.3).

The dislocation pair birth on a background of slow growth of the total internal energy at the expense of

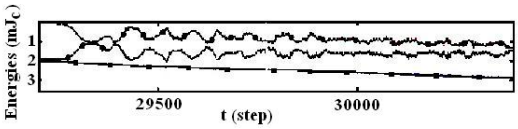

Figure 3. Elastic vibrations of nanobulk at stripping of the first dislocations and their change during transformation into the thermal fluctuations (cooling only on the initial stage)

work by 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 [17] of the resonant character, which frequency gradually grows in due course, and the amplitude falls. During about a two tens periods of the low-frequency vibrations the lasts-named calm down, and completely pass into the thermal motion. On record of the transition the potential energy decreases on magnitude $1.164mJ_c$.

Without the prior cooling the described process gets some other character (Fig.4).

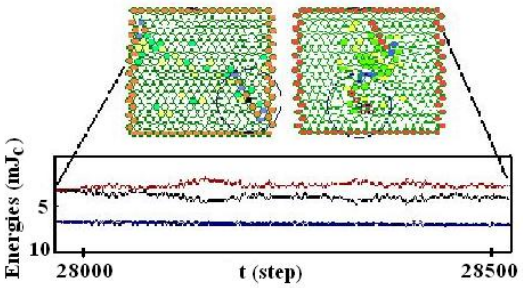

Figure 4. Elastic vibrations of nanobulk at stripping of first dislocations and their change during transformation into the thermal fluctuations (the cooling is absent at all). On inserts the Yellow circles present the atoms with potential energy $0.02mJ_c < U < 0.04mJ_c$, green circles - with $0.04mJ_c < U < 0.1mJ_c$, 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 $0.6mJ_c$.

Higher initial value of the internal energy leads to more earlier birth of dislocation pair, approximately, on 1000 time steps. "Premature birth" results that the dislocations are languid and inactive, as the overall store of the elastic energy setting them in motion, is not so great yet. The dislocations enough slowly during $300 - 350$ time steps advance in the rigid boundaries directions. The jump of the potential energy during the transition is $0.537mJ_c$, that it is much less, than with cooling.

At turn of dislocations similar transformations of energy take place too. In these cases the jumps of the potential energy are $1.041mJ_c$ with the cooling and $2.608mJ_c$ without the cooling, respectively.

Example of potential energy distribution around a dislocation is presented on fig.5.

The atoms of largest energy are placed on the "compressed" chain. Next series of atoms ranged with energy is placed behind "compressed" chain, and only next series - on the "stretched" chain.

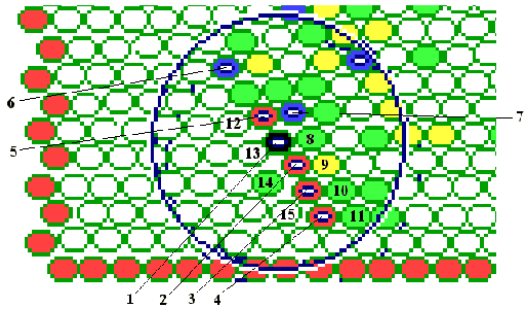

Figure 5. Values of the potential energy of particles in a vicinity of the dislocation core (in mJc): 1 - 0.429; 2 - 0.403; 3 - 0.268; 4 - 0.202; 5 - 0.19; 6 - 0.129; 7 - 0.101; 8 - 0.058; 9 - 0.025, 10 - 0.063, 11 - 0.067, 12 - 0.019; 13 - 0.012; 14 - 0.041; 15 - 0.002. For a zero level the average potential energy on one particle in the sample is accepted.

3 Uniaxial compression of sample under soft boundary conditions

The rigid boundary conditions as though completely, both in thermodynamic and in the mechanical sense, isolate allocated bulk from other part of a crystal. If it is possible to allow 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 far-action of the 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 is a question, whether - will be and as far as to differ character of dislocation behavior from one under the rigid boundary conditions?

Deformation 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 $E_b = 0.2083mJ_c$ occur on the 46839-th time step. According to the accepted definition they are dislocations of a type π_3^-, π_2^-, π_3^+, π_2^+. In the given series of experiments the dislocations arise not at edges of up and/or down boundaries, as in the case of the rigid loading, and at the central parts of free lateral sides of the sample (Fig.6). They move in the directions of the horizontal boundaries and pass through them (Fig.6b). 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. In result they meet at the centre of the sample (Fig.6c). 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.6d). At last that, on 47240-th time step a part of dislocations come out on the free lateral surfaces, derivating roughnesses of its relief, the others annihilate among themselves, derivating 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 deformation (46800 time steps). Furthermore the system calms down for a long time, and during 36000 time steps in it dislocations are

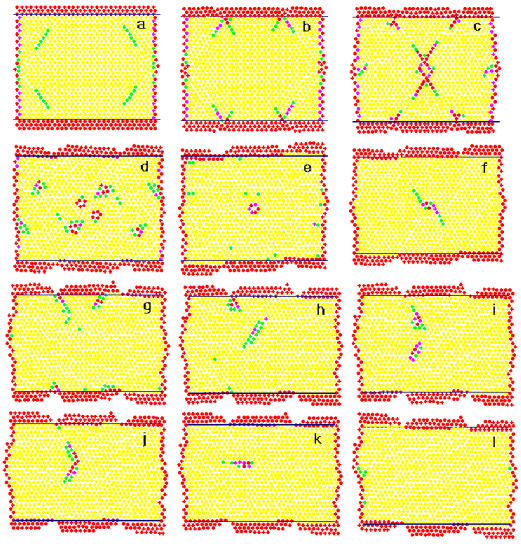

Figure 6. Evolution of structure of crystallite at soft deformation. The images correspond to the following time steps: a - 46840, b - 46850, c - 46880, d - 46990, e - 47240, f - 83152, g - 83630, h - 83715, i - 83816, j - 84005, k - 84040, l - 117000; a-e - first cycle of not elastic deformation, f-k - second cycle of not elastic deformation, l - beginning of the third cycle of not elastic deformation.

absent at all. During this time the deformation again proceeds in the elastic manner. On the 83152-th time step the vacancy at the centre of the sample breaks up to the pair of dislocations π_3^+ and π_2^- (Fig.6f), which move in different directions (Fig.6g). The whole series of births and annihilations of dislocations begins with this decay which completely on the fig.6 is not given. From this series the fragments, illustrating merge two of dislocations and birth of thirds (Fig.6) are given only. On the 83630-th time step from the top boundary begin to move dislocations π_2^- and π_3^+. At first the dislocation π_3^+ outstrips the dislocation π_2^-, crossing the sliding plane of the last-named before arrival of one to this point (Fig.6i, j). At that instant, when the dislocation π_2^- reaches the point of crossing of the sliding planes (Fig.6i), it begins to attract the first one. As a result of this attraction the first dislocation comes back along the own sliding plane (Fig.6j), both dislocations merge and form new one (Fig.6l). The last is pressed out from the sample in parallel to it horizontal boundaries. In result in the system perfect crystal structure, already without vacancy again is restored. The following stage of not elastic deformation begins approximately through 28000 time steps (Fig.6m). Thus, it is possible to ascertain, that the general feature, - cyclic change elastic and non-elastic stages of deformation, marked at pressing by the rigid boundaries, is kept in the case of the soft boundaries too.

4 Cutting sample by three-atom knife

More interesting result is obtained in the second series of computer simulation for cutting the sample by three-atom knife (fig. 7).

Three atoms only are left from moving upper rigid line of atoms. Other parameters of the experiment remain

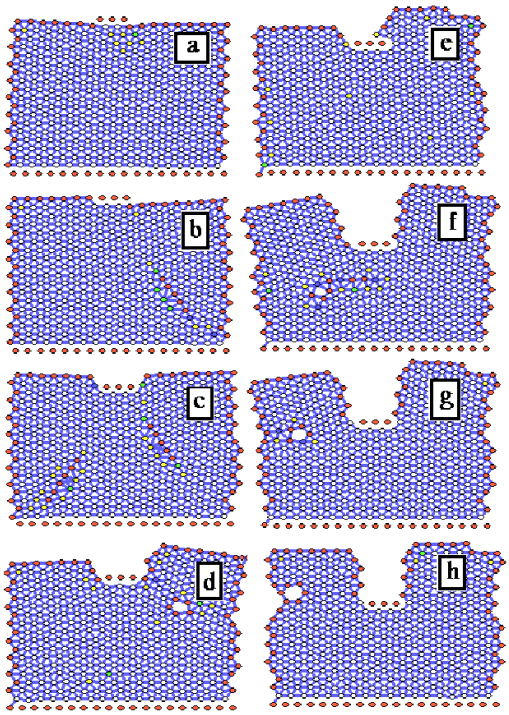

Figure 7. Evolution of crystallite structure at cutting by three atom knife: a - ideal crystal structure in beginning stage, b,c - formation of usual dislocation, d,f,g - formation of located dislocation, e,h - renewal ideal crystal structure after "bubbles".

as in the Sec. II.

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 dislocations is created in the upper left and right corners of the crystallite (Fig. 7b,c). Their glide lines are turned by 60^o each to another. The dislocations occur in the region under three-atom indentor and move downward. Then, the dislocations turn and they are pressed out from the sample.

Interesting phenomenon is observed at such pressing out (Fig. 7d,f,g). The defect displayed on the figure has two additional lines and Burgers vector as usual dislocation does, but its form sufficiently differs. The stretched chain has gap in the center of dislocation nucleus. That is, binding among centered atoms is broken and micropore arises. Owing to micropore a dislocation to become more located, than in the usual allocated state.

The atomic planes in area divided with normal to a plane of sliding, diverge under more larger corners than in the previous example (compare directions of upper sides on the (Fig. 7b,c) and (Fig. 7d,f,g)). Such dislocation can be considered, as a possible element of great-corner grain boundaries, which at small quantity of these elements can result in formation of curved boundaries and, as a consequence, to formation of a fine grain.

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

Thus, in the previous series of experiments is shown, that dislocations, having the same Burger's vector, can be, at least, in two structure modifications or states, - in allocated (basic) states and located ones. A distinctive attribute of a located state is the presence on the lattice images of typical pentagons. It is characteristic, that a "located state" occurs at non-uniform or severe loading more preferably. Except for the mentioned above the two structure modifications there are also others [27], which can have the large impotent means in dynamics of SPD.

5 Shear strain of sample by rigid shell

The plenty of dislocations arises at strain of a sample under the shear loading (Fig. 8,9).

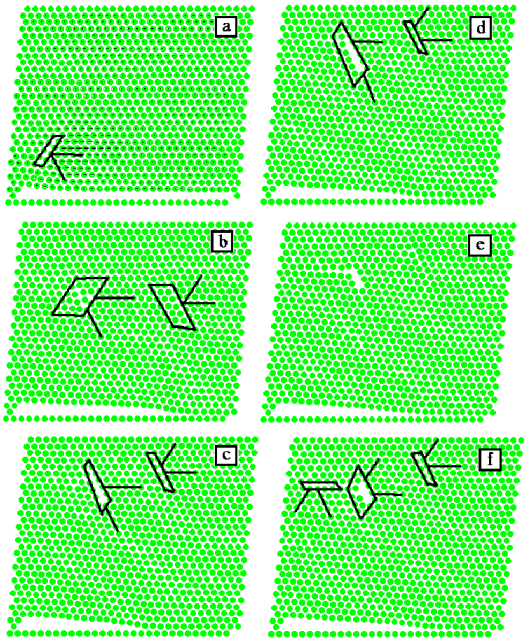

Figure 8. Evolution of crystallite structure with shear deformation: a - birth of first dislocation, b-d - moving of two defects, e - dislocation decay with birth of two new dislocation, f - system after dislocation decay.

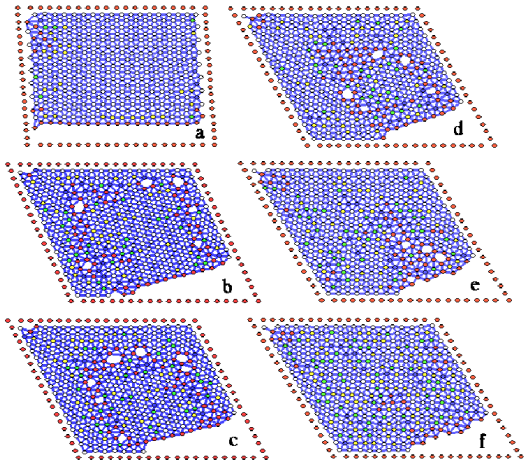

Figure 9. Phase-like transition with moving boundary consisting from bubble-dislocations having pentagon form.

This loading is realized as follows: the sample from 28*28 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 horizontal movement of the top and bottom sides of the shell to mutually opposite direction with constant velocity.

At an initial stage of deformation dislocations π_3^- and π_2^- are born. Then first of them decays on two new dislocations according to the equation of reaction:

$$\pi_3^- + energy \rightarrow \pi_1^- + \pi_2^- . \qquad (7)$$

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.

Deformation under the uniaxial loading leads to repeated recurrence of the same common script of system behavior, - birth of dislocations, them turning out, restoration of perfect crystal structure etc. At deformation of a sample under the shear loading the system evolution proceeds under essentially other script. In view of special kinematics of such deformation the restoration of perfect structure is possible only after turn some "macroscopic" bulk as whole on a finite discrete corner being an element of crystal symmetry (this reminds alternation of fragmentation and recrystalization during SPD [30] or effect stick-slip in lubricant sliding [31]). For two-dimensional problem it is the corner 60°. For realization of such turn it is impossible to make 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 deformatoin 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", about what the typical pentagon fragments on the images of a lattice testify. Owing to "pentagons" the strongly bent boundaries of fine grains are formed.

The developed in this paper approach can be usefull for analysis of other low-dimensional systems [32,33].

6 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 firsts of them have whole stretched chains, the seconds have "micropores". The located dislocations, as a rule, have pentagon form. Owing to "micropore" a dislocation to become more located, than in the usual allocated state. The atomic lines (planes) in area divided with normal to a plane of sliding, diverge under more larger corners. Such dislocation can be considered, as a possible element of great-corner fine grain boundaries, which at small quantity of these elements can result in formation of curved boundaries and, as a consequence, to formation of a fine grain.

Deformation under the uniaxial or "knife" loadings lead to repeated recurrence of the same common script of system behavior, - birth of dislocations, them turning out, restoration of perfect crystal structure etc. Alternation in time of elastic and non-elastic deformation stages leads one to 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 deformation of a sample under the shear loading the system evolution proceeds under essentially other script. In view of special kinematics of such deformation the restoration of perfect structure is possible only after turn some "macroscopic" bulk as whole on a finite discrete corner being an element of crystal symmetry. For realization of such turn it is impossible to make 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 deformation as the effective tool of material structure transformation.

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