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# The computer simulation of the plastic deformation of 2D Lennard–Jones crystals

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**Abstract**

The computer simulation of the processes proceeding under intensive mechanical action is carried out for two-dimensional Lennard–Jones crystals. The time and deformation dependencies of strain tensor, energy and quantity of structure disruptions is presented for different load intensities. It is shown that the energy absorbed by the crystal under macroscopic mechanical action is released in local regions that are several Angstrom-sized. The plastic flow occurs through dividing the initial structure into regions in which the atomic motion is to be correlated.

*Keywords:* Molecular dynamics; Plastic deformation; Mechanical treatment

## 1. Introduction

We present the results of computer modeling of plastic deformation of the model system composed of Lennard–Jones type particles. The problem of detailed knowledge of atomic motions under conditions of mechanical action arises from experimental data obtained in mechanical alloying, mechanical activation and other ways of mechanical treatment of solid [1,2].

The mechanical alloying proceeds at about 300 K and the main problem arising is an extremely fast atomic motion in the substance under action. Thus, the effective interdiffusion coefficient in the alloying metals is about $10^{-9}$–$10^{-11}$ $m^2$ $s^{-1}$ [3].

However, this kind of motion is different from thermally activated diffusion. If the diffusion causes full amorphisation of the substance, the atomic motions activated under mechanical treatment could leave the structure without any changes or cause formation of the new structures.

For example, the mechanical treatment of the materials with the simplest structure such as the close-packed metals or ionic salts (e.g. NaCl) leads to the formation of point and linear defects without any changes in common structure. But for the more complicated structures such as complex oxides (perovskites or spinels) mechanical treatment generates new types of structure; for example, in Ref. [4] was shown the formation of the metastable cubic phase $(Y_{0.33}Ba_{0.67})CuO_{3-x}$ during the treatment of the mixture of $Y_2O_3$, $BaO_2$, CuO oxides or $YBa_2Cu_3O_{7-x}$.

In this case the type of the main structural element defines the type of possible structure changes during the mechanical action. If one takes the close-packing anion sublattice with small cations in interstitial (ferrite-spinels) one can observe the formation of close-packing sublattice defects and changes in cation distributions between octa- and tetra- sites.

In the case of anion–cation close packing (for example perovskites) the mechanical action may lead to the full amorphisation of the material. Therewith the oxygen polyhedral forms random close packing (similar to Bernal's model) [5].

Thus, the mechanical activation causes the intensive remixing of a substance on the atomic level. It seems that deformation mixing is common for all mechanochemical processes, but their effects are defined by initial structure and chemical bond type. The result of mechanical treatment is not defined by the intensity of the action alone. The other important factor controlling this process is the possibility of the starting material stabilizing the structural disruptions caused by reconstruction of several immediate coordination spheres.

The time and space scales ($10^{-6}$–$10^{-8}$ s, 100–2000 Å) of mechanical activation processes strongly hamper


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their direct experimental study. Therefore, the possibility of modeling the behavior of atomic ensembles under mechanical action using the molecular dynamic method is very promising.

Butjagin and co-workers [6] have made preliminary attempts to carry out such a simulation. It was shown that during the intensive plastic deformation the initial substance degrades into small clusters about 10 interatomic distances in diameter. These clusters conserve the initial structure inside the clusters, being fully amorphized on the boundaries. But the quantitative characteristics of processes under study in this and other works devoted to computer modeling are quite lacking. We concentrate our attention on revealing the macroscopic characteristics for the simplest model to compare them later with available experimental results.

## 2. Computation model

The classical equations of motion 1600 ($40 \times 40$) particles under periodic boundary conditions were integrated in the conventional manner using the second-order Euler algorithm.

As parameters of the pair potential

$$\Phi_{ij} = 4\varepsilon((\sigma/r_{ij})^{-12} - (\sigma/r_{ij})^{-6}) \quad (1)$$

we have chosen the values: $\sigma = 3.405$ Å; $\varepsilon = 119.6$ K, particle mass $m = 6.24 \times 10^{-26}$ kg, which correspond to potential parameters and the atomic mass of liquid argon. Potential was set at $r = 2.25\ \sigma$.

Hereafter the following arbitrary units shall be used: time $(m\sigma^2/\varepsilon)^{1/2} = 2.09 \times 10^{-12}$ s, velocity $v = \sigma/t = 156$ m s$^{-1}$, pressure $p = \varepsilon/\sigma^3 = 4.18 \times 10^7$ N m$^{-2}$; distance and energy are expressed in corresponding parameters of potential.

The time step $\Delta t = 0.008$ has been chosen as sufficiently good; the total energy error was typically less then 0.1%. The value of the average period of atomic oscillations (obtained from the velocity autocorrelation function) is equal to $t_0 = 0.4$ ($8 \times 10^{-13}$ s).

The deformation procedure was simulated as follows.

The periodically copied computation unit consisting of 1600 close-packed particles covers the two-dimensional space by uniform blocks. In this virtual system one can produce a shear deformation by shear flow-like displacement of computation unit copies as rigid bricks in the $X$ direction. We set the velocity, $V_s$ of the relative displacement of the blocks constant. In this mode of deformation the distortions inside the computational unit are caused by movement of neighboring blocks.

In the process of computations the atom is free to leave the computation unit through the border. In conventional periodic boundary conditions at this moment the atom coordinates change from $X_i$, $Y_i$ to $X_i \pm (L_x,0)$ (if the atom crosses the $Y$ boundary) and $Y_i = \pm(0,L_y)$ (if the atom crosses the $Y$ boundary). In our case the conditions of jump along $X$ are the same but the vector determining the atom jump along the $Y$ axis is taken as $\pm(V_s t,L_y)$. In such a method the sequence of checking of the atoms' movement through the border is of importance: at first we need to analyze the boundary conditions $P_0$ along the $Y$ axis.

The $Y$ dimension of the computational unit was taken as constant. We provided isobaric conditions for pressure $P_0$ along the $X$ axis.

This procedure allows the modeling of dynamic processes of shear deformation progress in a "surfaceless" sample, that is to remove the surface influence as a possible source of structure defects (dislocations). But in periodic conditions the system is closed upon itself. This condition cuts the upper value of the dislocation's lifetime. For example, two dislocations of opposite charge appear in one plane (in one line in two dimensions), move apart, cross the corresponding boundaries, return in unit from the opposite sides, move together in one plane, meet and annihilate.

All the deformation experiments were conducted under isothermal conditions. The velocity of all particles lying in the layer $3\sigma$ wide near the Y border was renormalized at every time step to provide an energy of particle motion equal to $E = 0.15$ arb.u. The melting temperature of our system obtained from melting modeling is equal to 0.51 arb.u with $P_0 = 1.0$.

With the parameter $P_0 = 1.0$ shear velocity $V_s$ lies in the interval from 3 m s$^{-1}$ to 45 m s$^{-1}$, which allows a deformation velocity in the range from $0.21 \times 10^8$ to $3.19 \times 10^8$ s$^{-1}$. At first moment the system axially stressed along the $Y$ axis by 0–3%. Thus we have conditions of axial stress and shear.

To make the data more representative the modeling results were accumulated and averaged over 10 runs.

From the axial deformation experiments the elastic characteristics of the system were determined: stress modulus equal to $K = 30.4 \pm 0.5$ arb.units, shear modulus $\mu = 17.0 \pm 0.5$ arb.units. The velocities of the elastic wave's propagation (sound velocity) were calculated from the elastic characteristics: $C_l = 7.55$ arb.u. (1177 m s$^{-1}$), $C_t = 4.12$ arb.u. (643 m s$^{-1}$).

## 3. The process of deformation

One could describe the qualitative picture of modeling process as shown in Fig. 1 and Fig. 2 as a dependence of the system's total energy and pressure tensor components

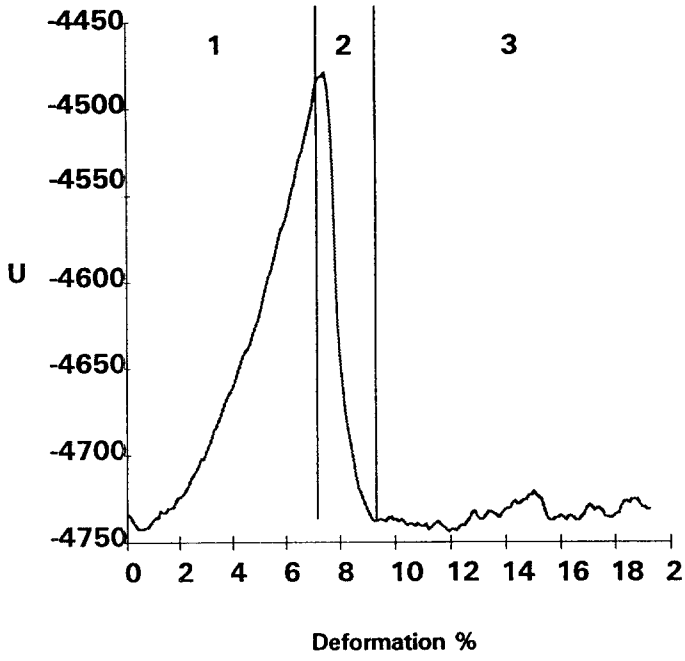


Fig. 1. Total system energy as a function of deformation.

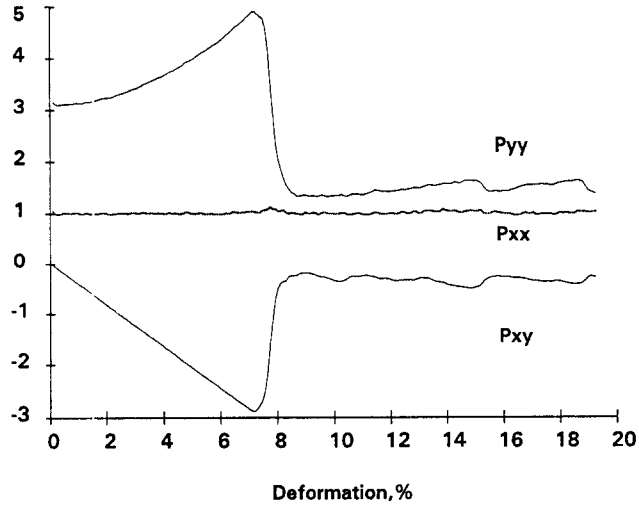


Fig. 2. The strain tensor components as a function of deformation.

$$P_{\alpha\beta} = 1/V \cdot \left( \sum_i v_i^{\alpha} v_i^{\beta} + \frac{1}{2} \sum_{i \neq j} + r_{ij}^{\alpha} (\delta \Phi_{ij} / \delta r_{ij}^{\alpha}) \right) \quad (2)$$

on shear deformation $\varepsilon = L_{yx}/L_y$. Preliminarily we have squeezed the model by 3% along the $Y$ axis from the equilibrium state (with isotropic external pressure $P = 1.0$ arb.units). Shear velocity $V_s$ was determined as $V_s = 0.02$ arb.units (about 3 m $s^{-1}$) causing the deformation rate $d\varepsilon/dt = 0.21 \times 10^8$ $s^{-1}$.

Commonly the process proceeds through three main stages. At first (1 on Fig. 1), the deformation is maintained in an elastic manner, the energy stored in the system in the form of particle interaction energy. When the deformation value approaches 7–10%, the homogenous birth of dislocation pairs occurs (2), dislocations start the very fast (with velocity about that of sound) motion and discharge the inner system stresses after about $10^{-10}$ s. After this the system transfers to the quasistationary state of plastic flow (3). The shear stress value of homogenous dislocation birth is equal to $P_{cr} = 3$ arb.u. $\approx \mu/6$, which corresponds to the theoretical limit of strength.

Depending on the action intensity in the model (defined in our case by shear velocity $V_s$ ) the number of structure disruptions and dislocations appearing may be different. In order to quantitatively describe the amount of dislocations we calculate at every time step the number of nearest neighbour atoms for each particle as the number of particles lying in a circle with radius

$$R = 1/2(R_1 + R_2) \quad (3)$$

where $R_1$ and $R_2$ are the radiuses of first and second coordinate spheres. As shown in Ref. [9], that number statistically matches the number of nearest neighbours defined by Voronoi polyhedra analysis.

In Fig. 3 the number of particles in perfect crystalline surroundings (six nearest neighbors) is presented for different deformation rates (a) and different initial axial stress (b). As would be expected the more intensive the mechanical action is the greater the amount of structure disruptions. One could see that the typical disruption's value is about several percent. One could take the number of dislocations at stage (3) as the number of particles in imperfect sites divided by two: every dislocation typically contains two atoms with five-fold surrounding. The maximum number obtained is equal to $10^{16}$ dislocations per square meter.

The structural disruptions have a dynamic nature: after relatively large structure disordering at stage (2) the imperfection's value relaxes to equilibrium at stage (3). This is an equilibrium between outer disordered action defined by shear velocity in our case and inner relaxation controlled by the initial structures' capacity for movement of their basic building elements.

In order to obtain quantitative characteristics of this kind of relaxation we have performed the following experiment. We have cooled our system from the melted phase to a temperature about 0.15 arb.units (the temperature of the main deformation experiments). In this cooled system we observe the number of particles in perfect crystalline site as a function of time. When this number is less than about 10% of the total particle amount then the structural imperfections' relaxation is described well as

$$C = 1 - \exp(-t/\tau) \quad (4)$$

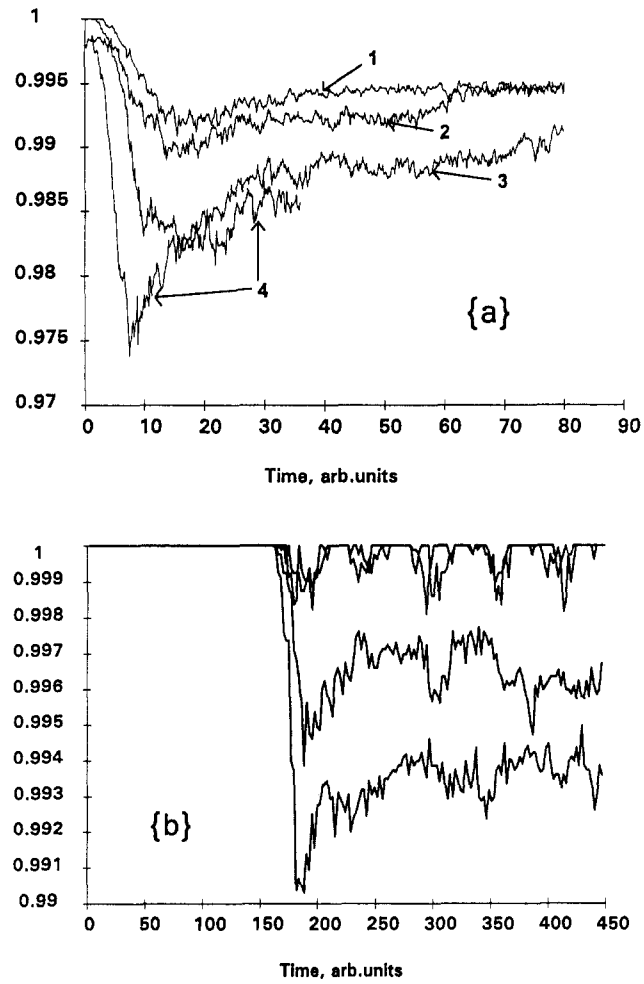


Fig. 3. (a) The concentration of atoms with perfect neighbour for different deformation rates 0.21 (1), 0.42 (2,) 1.59 (3) and $3.19 \times 10^8$ (4) $s^{-1}$. (b) The concentration of atoms with perfect neighbour for different preliminary axial stresses: 0, 1, 2, 3 percent, deformation rate $0.21 \times 10^8$ $s^{-1}$.

where $C$ is the concentration of particles in perfect crystalline site, $\tau$ is relaxation time, $\tau = 2.02 \times 10^{-10}$ s. This very small time value means that all structural disruptions have relaxed before one could observe them by any experimental method.

One could compare this behavior of the model system with the plastic deformation of thin copper monocrystals ("whiskers") described, for example, in Refs. [7,8]. They show the same (peak-like) character of deformation development that one could see in our model. After the initiation of fast homogenous dislocations at a stress value close to the theoretical limit of strength, the thin whiskers flow plastically. From the inner friction data one could observe the relaxation of the large amount of dislocation which appeared at first to be the equilibrium value.

We must note that in Figs. 1 and 2 we have shown "the best" case of the process maintenance. This plato-like character of the time evolution ensured that the dislocations arising have the possibility of moving in different planes of sliding. In other cases with different starting conditions (preliminary squeezing along the $Y$ axis, for example) the stress field in the model is insufficient for this kind of dislocation motion. As described above we have a "closed model" which enables the dislocations to disappear in a short time and one could see at stage 3 many less intensive peaks as at stage 2 (Fig. 3(b)). We suggest that at low stress intensities the model designed does not describe real processes properly.

The microscopic picture of atomic motion at the stage of plastic flow could be described as follows.

In the substance under action at every moment one could see the regions with which the atoms' movement correlated (Fig. 4). These regions are involved in the relative displacements and rotations. The dividing of the inner volume of the model into these regions has a temporal character: one cluster with about 100 atoms has a lifetime of about 10 atomic oscillations ($10^{-12}$ s). In spite of the whirl-like picture of atomic displacements at every moment, the particles as a whole move in an orderly fashion which causes uniform shear deformation. This indicates that the microdisplacements and microrotations of small regions of the substance develop in time in a mutual relationship.

On deformation development the energy loaded into the system is transformed to heat. The main source of heat generated in our case is dislocations in movement. The observed dislocation's velocity may be very high: about the velocity of sound. In order to determine the details of heat dissipation by this kind of dislocation we performed the following calculations.

We created a single dislocation in periodic boundary conditions along the $X$ direction. After this we loaded the system. Then we calculated the average kinetic energy of particles around the moved dislocation in a system of coordinates of the dislocation core. The core was determined as the arithmetic average of coordinates of atoms having five or seven nearest neigh-

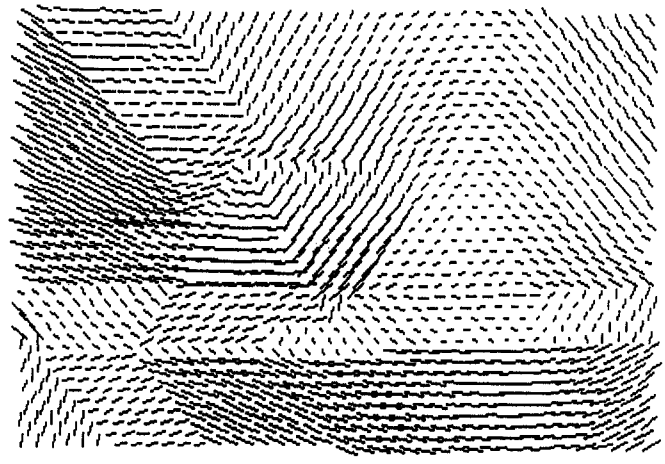

Fig. 4. Particle displacement traces averaged over $10^{-11}$ s.

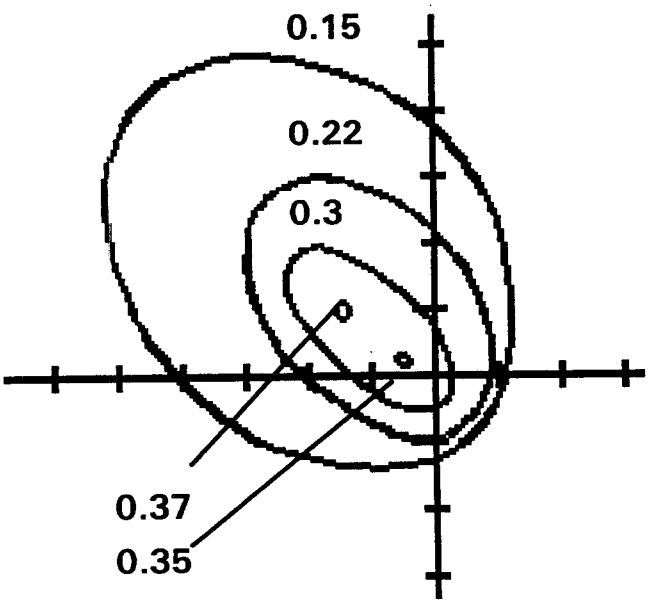


Fig. 5. Outline of the mean kinetic energy of the particle field. The core of dislocation is placed at the zero point of the coordinate system. The dislocation moves from left to right. Each point on the axis corresponds to one interatomic distance.

bours. At the $Y$ boundaries the temperature $T = 0.1$ arb.units was established. The schema of the obtained average kinetic energy fields is plotted in Fig. 5. The dislocation is placed in the zero point of the coordinate's system and moves from the left to the right. The two peaks with the value of 0.37 and 0.35 arb.units correspond to two nearest (to core) atoms in the atomic plane that move to the region of low density. The heat track follows the dislocation movement and is spread about to six interatomic distances. We must note that this track is turned from the line of dislocation movement by an angle about 30–40° to the lower density direction. This may be caused by lowering the elastic wave propagation rate in regions with lower density and as a result decreasing the heat conductivity.

## 4. Conclusion

We have performed a quantitative investigation of model system behavior in shear and axial pressure conditions. The microscopic picture of plastic flow in our system could be described as proceeding through decomposition of perfect structure on clusters in dimensions about 10–20 interatomic distances. The clusters move and rotate, which provides the stress field relaxation and causes the structure disruption.

The plastic deformation carrier, i.e. the dislocations, acts as point heat sources in the energy dissipation processes.

Thus the macroscopic internal action is transformed into local microscopic energy release processes through (i) the defect generation and (ii) local heat dissipation by the generated and moving imperfections.

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