Atomic Mechanisms of Structural Reconstruction of FCC Metallic Nanowires in the Process of Tension Deformation

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1. 1 Introduction

In recent years there has been growing interest in the study of materials whose physical and mechanical properties are formed at nanometer scale and even at the scale of molecules and atoms. Such materials are called nanostructures or nanomaterials [1, 2]. It is accepted by many researchers that structural units of nanomaterials have characteristic size of less than 100 nm but sometimes this limit is extended up to 400 nm. Experimental study of structural changes taking place in nanomaterials under intensive external impacts and severe plastic deformation is a challenge. Atomistic computer simulations can be effectively used in parallel with theory and real experiment when deformation of nanomaterials takes place at a very high strain rate.

The main computational methods used in simulations at microscale and nanoscale levels are the molecular dynamics (MD), quasistatic relaxation, and Monte-Carlo methods [3]. These methods find many applications in the study of the peculiarities of deformation and fracture processes in nanomaterials. In particular, the processes of structural reconstruction of an ideal nanocrystal of solid Ar under homogeneous strain condition have been studied in details by the method of quasistatic relaxation in quasi three-dimensional approximation [4, 5]. Mechanical properties and mechanisms of plastic deformations of nanowires have been extensively studied in the recent past [6-9].

It was found [10, 11] that the crystalline material undergoes up to 12 stages of structural changes being deformed at the temperatures close to 0 K. The stage of elastic deformation ends, as a rule, by the appearance of the waves of statistic atomic displacements at a bifurcation point. Dislocation nucleation is then observed in the zones of crossing of the waves. The sharp jump-like decrease of energy appears on the parabolic branch of the energy density vs strain curve. Similar catastrophic events can be noticed at higher levels of strain and they are related to the activation of the secondary slip system, appearance of micropores, and fracture [12]. In [13-15], the atomic structure and peculiarities of deformation and failure near different types of grain boundaries in metals and in ordered alloys have been studied by the method of quasistatic relaxation.

In the works [16, 17], the diffusion mechanisms and atomic mechanisms of fracture have been studied by the method of molecular dynamics for several metals and for Ni_3Al intermetallide at different temperatures during tensile strain up to fracture.

In the present work we report on the results of molecular dynamics simulation of behavior of Ni, Al, and Ni_3Al nanoclusters in the form of rectangular parallelepipeds under uniaxial tensile strain.

1.2 Model

First of all, the simulation block (nanowire) was made. The simulation block had the form of rectangular parallelepiped having [001] faces of FCC lattice with the longest dimension oriented along <001> direction. Mixed boundary conditions were applied to the boundaries of the simulation block: free faces along <100> and <010> directions and contact with rigid continuation of the crystal in <001> direction. The number of atoms in the simulation block was 24x24x36 = 20736. The interatomic interactions between atoms of sorts K and L were given by the Morse pair potentias

$$\varphi_{KL}(r_{ij}) = D_{KL}\left(e^{-2\alpha_{KL}(r_{ij}^{KL}-r_0^{KL})} - 2e^{-\alpha_{KL}(r_{ij}^{KL}-r_0^{KL})}\right) \tag{1}$$

where r_{ij} is the distance between the chosen pair of atoms and D_{KL} , α_{KL} , r_0^{KL} are the potential parameters. The parameters D_{KL} , α_{KL} , r_0^{KL} were fitted using the well-known experimental data: sublimation energy, equilibrium lattice parameter, bulk elastic modules for pure metals Ni and Al. The interatomic potentials of Ni_3Al intermetallide describing the Ni-Ni and Al-Al bonds were the same as in pure metals. The potential parameters corresponded to the interaction of atomic pairs Ni-Al were fit to experimental values of energies of the following antiphase boundaries ½ <110> {100}, ½ <110> {110}, ½ <110> {111} [18]. The cut-off radius of the interaction between atoms was chosen at the distance between the third and the fourth coordination spheres. The use of simple pairwise potentials was dictated by the necessity to decrease the computation time. At the same time, in the simulation of a high-speed deformation of materials (which is the subject of the present work) the most important experimental parameters are the force characteristics of interatomic interactions defined by the elastic properties of a material with a high precision. Comparison of the simulations result obtained with the use of ab-initio fitted potentials and simple pairwise potentials have been done in the work [19] and no significant influence of the type of the potential was noticed.

The study was made using the method of molecular dynamics [20] where one solves the equations of motions for a set of atoms inside a computational cell. The equations of motion can be presented as follows:

$$m_i \frac{d\upsilon_i}{dt} = F_i , \frac{dr_i}{dt} = \upsilon_i ; \; i = 1,2,...., N \tag{2}$$

where m_i, r_i , and υ_i are the mass, the radius-vector, and the velocity of i-th atom, respectively, t is time, F_i is the force acting on i-th atom from all other atoms within the cutoff radius, N is total number of atoms in the computation cell.

The Euler's method with the semistep was used for integration of the equations of motion. The absolute value of initial velocities of atoms in an ideal crystal was calculated as follows:

$$|v_i| = \sqrt{\frac{2k_bT}{m_i}}\ , \qquad (3)$$

where k_b in the Boltzman's constant, T is the desired temperature.

The directions of the atomic velocities were set in a way to have zero total momentum of the computational cell. The uniaxial tensile strain was applied to the nanowire by moving the atoms at one of the two ends along <001> axis with the velocity of 20 m/s. This value of the velocity corresponded to a high-speed impact loading of the nanowire. Similar or even higher velocities are often used in molecular dynamics simulations [21] because of limitations on the duration of computer experiments. We consider the temperature of 300 K and the temperature close to the melting pont and use the Nose-Hoover thermostat to control the temperature every 10^{-13} s.

1.3 Results and discussion

The work done by the external force that straines the nanowire was transformed into the form of potential energy of the nanowire that included the energy of elastic strain and the energy of defects and also the increase of kinetic energy of the atoms (heat). The last energy was removed from the crystal by keeping constant temperature.

Figure 1 shows the energy density per one atom as the functions of time for Ni, Al, and Ni_3Al (indicated in each panel) nanowires strained at 300 K. Four main stages of deformation can be observed for all materials: (i) quasielastic deformation of perfect crystal (potential energy of the crystal increases quadratically with strain and thus with time); (ii) plastic flow with work-hardening that saturates at certain value of strain; (iii) steady flow at constant energy density; (iv) fracture. At the last stage, the level of potential energy density was almost constant until the fracture of the last interatomic bond in the neck. The stage of plastic flow ends by the formation and of the neck. The energy density vs time curves presented in Fig. 1 have revealed some differences in behavior of the three considered materials, namely, in the peak values of energy density. At the end of stage (i), Al appeared to have a higher energy in comparison with the stage of plastic flow. Contrary to that, Ni and Ni_3Al showed the highest energy densities at the end of the stage of plastic flow.

It can be noted that the first stage for all materials finishes somewhere near the first 50 ps of the time of materials deformation. It can be explained by high velocity of materials deformation. At the same time, the intervals of the development of three following stages were different.

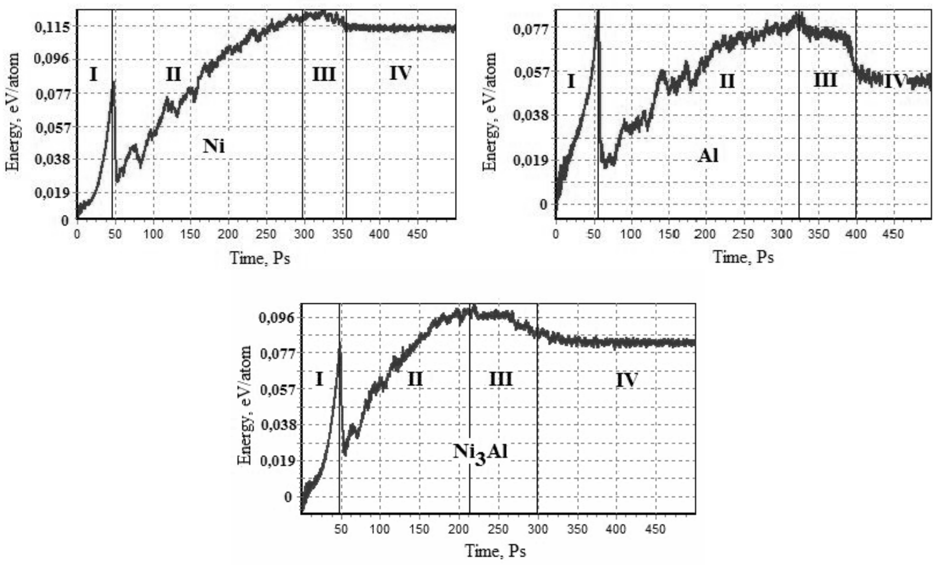
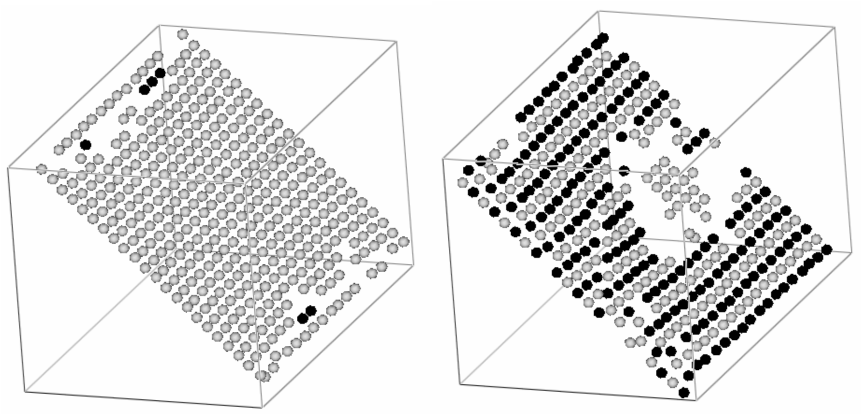


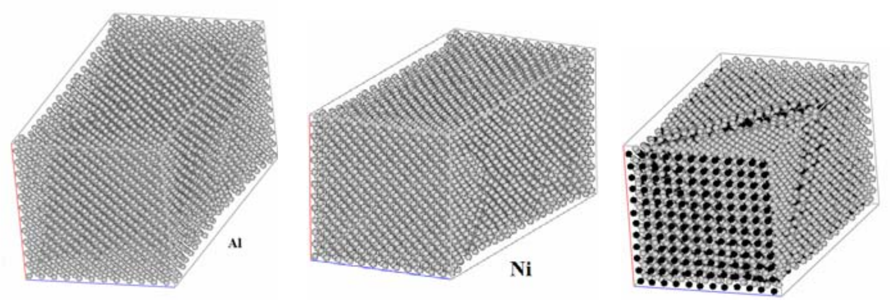
Fig. 1. Energy density per one atom as the functions of time for Ni, Al, and Ni_3Al (indicated in each panel) nanowires strained at 300 K.

The first stage was completed close to *t*=50 ps of the process of material deformation (for all materials). This can be explained by high strain rate used in our simulations. The time span of the development of three following stages appeared to be different. Maximum potential energy of at the end of the first stage is close for all three materials and lies within 0.084-0.090 eV/atom, as it can be seen in Fig. 1. If one tries to relate this energy to the energy of formation of Frenkel’s pairs (a vacancy and a interstitial atom) (5-6 eV per a pair) [22], then the concentration of point defects in the crystal would reach up to 10^{-1}- 10^{-3}. It is worth noting that similar estimation for the concentration of point defects can be made for the crystal near the melting point. Fig. 2 (a) shows the example of the accumulation of point defects in Ni_3Al alloy at the end of the first deformation stage. First, vacancies and interstitial atoms were formed, vacancy knots of Ni atoms were displaced by Al atoms. Point defects were united into the complexes (Fig. 2, (a)), the complexes formed dislocation loops (Fig. 2, (b)). The structural order was broken in the structure of pure metals, superstructural order – in intermetallides. The process completed by the slipping of the part of deformed material along the planes {111}, fig. 3 (a, b, c). The least considerable effect of slipping was observed in Al. It is explained by the biggest value of formation energy of fault defect in the material in comparison with Ni and Ni_3Al.



a) b)

Fig. 2. Atomic structure of a) initially monoatomic plane [110] at *t*=40 ps and b) initially biatomic plane at *t*=50 ps.



a) b) c)

Fig. 3. The structure of (a) Al, (b) Ni, and (c) Ni_3Al nanowires just after the completion of the first (quasielastic) stage of deformation.

Figs. 4 and 5 show the pictures of the change of the structures of deformed nanostructures Ni_3Al and Al at the stages of flowing and fracture. As it follows from the comparison of the figures, pure metal is characterized by the break of structural order in the process of deformation; the area of amorphisation is observed in the neck. The deformed alloy Ni_3Al is characterized by the break of structural and superstructural order. The strips of shear corresponding to the passage of full and super partial are clearly seen dislocations. The amorphisation is less expressed in the neck in comparison with pure Al. Similar properties were noticed in pure Ni in the area of fracture. The following experiments were made at the temperatures 780 K for Al and 1300 K for Ni and Ni_3Al intermetallide (Fig. 6).

The pictures of the distribution of the deformation stored energy for all materials suffer considerable changes. The first stage has less duration. The extreme energy of quisielastic deformation stage is less – in the limits of 0.52 eV/atom. It means that less energy is required for the formation of Frenkel pairs at such temperatures. Their concentration increases not only at the expense of deformation energy but also on the processes of thermoactivation.

The jump of energy at the end of the first stage is relatively big for Al. It is connected with relatively high value of energy of FD formation in the metal. The increase of energy expenses in due course at the stage of plastic deformation is typical for all materials. The jumps on the boundaries at the given stage can be interpreted by the accumulation of new point defects, their clapping into dislocation disks which cause the strips of shear in the material. In a whole, all materials behave as plastic materials up to the stage of fracture.

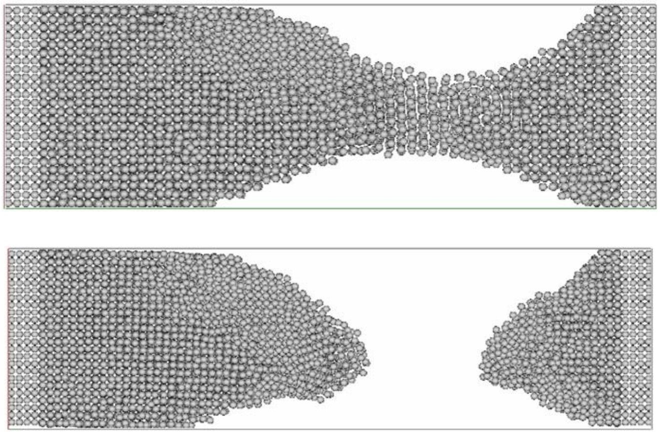


Fig. 4. Structural changes in Al nanowire at the stages of steady plastic flow (290 ps) and fracture (400 ps).

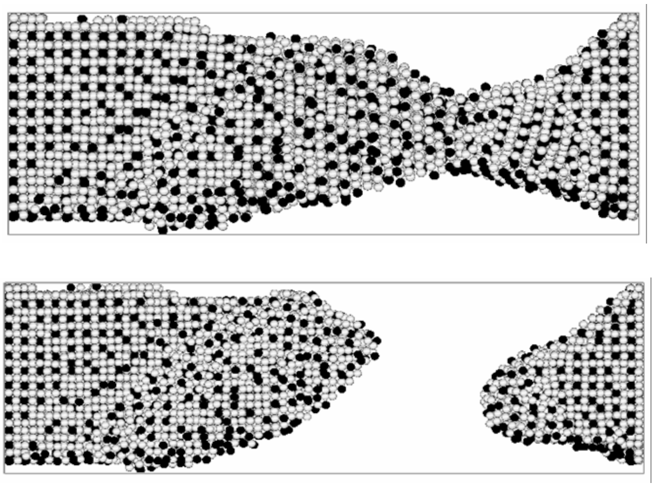


Fig. 5. Structural changes in the Ni_3Al nanowire at the stages of steady plastic flow (290 ps) and fracture (400 ps).

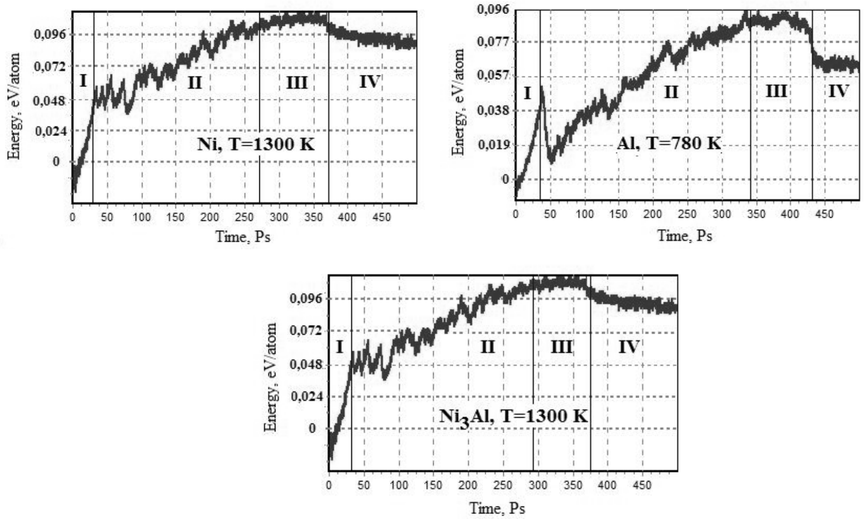


Fig. 6. Same as in Fig. 1 but for temperature close to the melting point.

1.4 Conclusion

Main mechanisms of atomic reconstruction in metallic nanowires (Ni, Al, and Ni_3Al) subjected to uniaxial tension were identified using the molecular dynamics technique. Analysis of the potential energy per atom vs time curves has revealed that the deformation of the initially perfect nanowires until their fracture includes four main stages: quasielastic, plastic flow with work-hardening, steady plastic flow, and fracture. Reduction of the long and short order in the Ni_3Al superstructure was observed during plastic flow stages. Similar stages of structural reconstruction have been identified earlier in our simulations for the bulk materials.

1.5 References

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