Materials Physics and Mechanics 18 (2013) 53-62 Received: October 6, 2013

EFFECT OF VOLUME ON THE MECHANICAL PROPERTIES OF NICKEL NANOWIRE

M.M. Aish[1,2*], M.D. Starostenkov[2]

[1]Physics department, Faculty of Science, Menoufia University, Egypt

[2]I.I. Polzunov Altai State Technical University, Barnaul, Russia,

*e-mail: mohamedeash2@yahoo.com

Abstract. Molecular Dynamics (MD) simulations have been carried out on pure nickel (Ni) crystal with face-centered cubic (FCC) lattice upon application of uniaxial tension at nanolevel with a speed of 20 m/s. Morse potential was employed to carry out three dimensional molecular dynamics simulations. MD simulation was used to investigate the effect of volume of Ni nanowire on the nature of deformation and fracture. The engineering stress–time diagrams obtained by the MD simulations of the tensile specimens of these Ni nanowires show a rapid increase in stress up to a maximum followed by a gradual drop to zero when the specimen fails by ductile fracture. The feature of deformation energy can be divided into four regions: quasi-elastic, plastic, flow and failure. The nature of deformation, slipping, twinning and necking was studied. Stress decreased with increasing volume and the breaking position increases.

1. Introduction

Figure1 shows MD simulation model of Ni nanowires generated from a bulk fcc Ni crystal with the lattice parameter of 3.52 Å. Let x, y, and z coordinate axes represent the [100], [010] and [001] crystallographic directions, respectively. The initial lengths of the MD models are denoted by Lx, Ly, and Lz, respectively, with z denoting the length direction of the Ni nanowires. Seven nanowires of different volume are considered at the temperatures corresponding to 300 K and 1000 K.

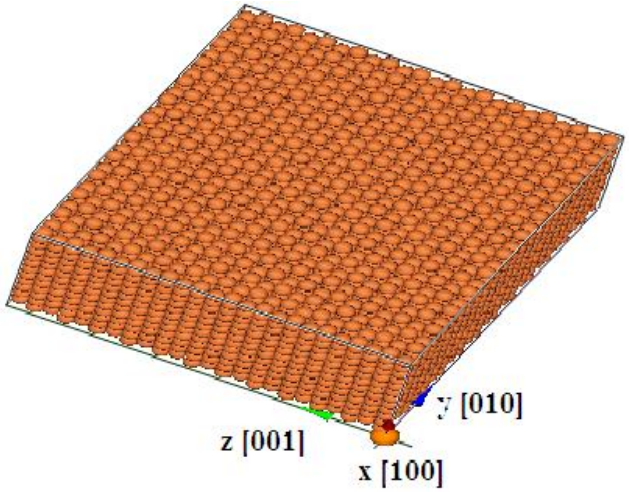

Fig. 1. MD simulation model of 24x24x24 Ni nanowire.

All of them have free surfaces in the length direction. In the MD simulation, the periodic boundary conditions are applied in both x and y directions. The deformation corresponds to the direction <001>. To the calculated block of crystal - free boundary conditions are applied in the directions <100>, <010>.

2. Potential model and simulation methods

In this paper for calculating the dynamics of the atomic structure of the method of molecular dynamics using paired Morse potential function [1-4], suitable in terms of their computing time and quality of results.

Morse pair potential is written as:

$$\varphi_{KL}(r) = D_{KL}\beta_{KL}e^{-\alpha_{KL}r}\left[\beta_{KL}e^{-\alpha_{KL}r} - 2\right], \quad (1)$$

where α_{KL}, β_{KL}, D_{KL} are parameters defining the interaction of pairs of atoms of type K and L; r is the distance between the atoms.

The initial velocities of particles are a Maxwell – Boltzmann distribution corresponding to a given temperature. They are given by

$$\frac{N(v)}{N} = \sqrt{\frac{m}{2\Pi kT}}\exp(-\frac{mv^2}{2kT}), \quad (2)$$

where N(v) denotes the number of particles which have velocity v; k is Boltzmann's constant, and T is temperature. To keep the system temperature, the following correction is required:

$$v_i^{final} = v_i\sqrt{\frac{T_d}{T_a}}, \quad (3)$$

where v_i^{final} is the velocity of the particle i after correction; T_d and T_a are the desired temperature and actual temperature of system, respectively. The initial configuration of the molecular dynamics simulation is shown in Fig. 1. In the atomistic simulations the stress on *m* plane and in *n*-direction σ_{mn} is calculated by [5-7]:

$$\sigma_{mn} = \frac{1}{N_s}\sum_i[\frac{m_i v_i^m v_i^n}{V_i} - \frac{1}{2V_i}\sum_j\frac{\partial\phi(r_{ij}^m)}{\partial r_{ij}}\frac{r_{ij}^m r_{ij}^n}{r_{ij}}], \quad (4)$$

where N_s is the number of particles contained in the region S and S is defined as the region of atomic interaction; r_{ij}^m and r_{ij}^n are two components of the vector from atom *i* to *j*; V_i is the volume assigned to atom i and given by

$$V_i = \frac{4\pi a_i^3}{3}, \quad (5)$$

where

$$a_i = \frac{\sum r_{ij}^{-1}}{2\sum r_{ij}^{-2}}. \quad (6)$$

The form expressed in Eq. (4) contains two terms on the m right hand side. The first is a kinetic part and caused by atomic motions and the second is a potential part and affected by

the interactive forces of atoms

The strain in the z-direction is calculated by:

$$\varepsilon = \frac{l - l_0}{l_0}, \quad (7)$$

where l is the stretching length in the z-direction and l_0 is its initial length.

Using Eqs. (4) and (7), the stress – strain curve can be yielded; and then the elastic modulus of the material can be obtained from the curve. Generally, the mechanical properties are dependent on the loading condition, volume of the nanowires and temperature.

The object of investigation is taken different nanowires of Ni alloy. Alloy structure is presented in the form of a face-centered cubic cell. We study the effect of volume on the mechanical properties of simulation nanowires at a temperatures corresponding to 300 K and 1000 K. The estimated size of the crystal unit was for various experiments of 63 atoms (5 atoms along the edges at the bottom and 5 - in height) to 32000 atoms (40 atoms along the edges at the bottom and 40 - in height).

3. Results and discussion

Since the breaking and the yielding of Ni nanowires are of main interest in this work (Table 1 and 2), it seems to be reasonable to adopt small L_x, L_y and L_z for the simulations. To save the computing time, the dimensions of the MD models used in the following simulations are set to be Lx=Ly=Lz and Lz changes from 5 to 40. The nature of deformation, slipping, twinning and necking were studied.

Table. 1. The typical MD results of different system at 300 K including the time required to attain atomic break, the number of atoms, initial length, breaking length, yielding time, yielding stress and yielding strain and the calculated final breaking position.

	System	N	l_0	Breaking			Yielding point			
				t	l_b, nm	Position	σ, GPa	t, ps	$l_{z1.}$ nm	ε
1	5x5x5	63	2.3	66	5.8	2.6	28	9	2.4	0.043
2	10x10x10	500	4.5	110	9.9	5.7	24	15	5.4	0.2
3	20x20x20	4000	9.1	245	22.8	13	22	27	10.5	0.153
4	24x24x24	6912	10.1	270	23.1	10.6	21	32	11.7	0.158
5	30x30x30	13500	14.2	-	-	-	19	35	16.2	0.135
6	36x36x36	23328	16.7	463	40.7	16.7	19	40	18.8	0.126
7	40x40x40	32000	19	-	-	-	18	42	21	0.1579

3.1. Four stages of deformation. The experiments were obtained plots of the stored energy of deformation of the time, reflecting the processes in the nanowire during deformation. There are four stages of deformation: the quasi-elastic deformation (I), plastic deformation (II), the breaking (flow) (III), and failure (IV). At all volumes, in the first stage there was almost linear increase in stress. The initial stage quasi-elastic area there is only relative displacement of atoms and there are no defects. Therefore, in this region the energy stored varies periodically. This stage is completed in 15 ps for 10x10x10 Ni nanowire and 40 ps for 36x36x36. The sharp fall takes place only at the point of transition from the first to second stages of deformation (Fig. 2 a and 2 c). Experiments have shown that when the volume increases the first stage of deformation was widened, and also the second stage was widened.

Table. 2. The typical MD results of different system at 1000 K including the time required to attain atomic break, the number of atoms, initial length, breaking length, yielding time, yielding stress and yielding strain and the calculated final breaking position.

	System	N	l_{z0}	breaking			Yielding point			
				t	$l_{b,}$ nm	Position	σ, GPa	t, ps	$l_{z1.}$ nm	Ɛ
1	5x5x5	63	2.3	54	5.2	2.5	25	9	2.4	0.043
2	10x10x10	500	4.5	105	10.8	4.8	16	15	5.5	0.222
3	20x20x20	4000	9.1	301	25.2	8	15	17	10.3	0.119
4	24x24x24	6912	10.1	243	24	7	14	20	12.3	0.218
5	30x30x30	13500	14.2	500	41.3	8.3	14	25	14.4	0.014
6	36x36x36	23328	16.7	-	-	-	13	28	18.3	0.095
7	40x40x40	32000	19	-	-	-	13	32	20.5	0.079

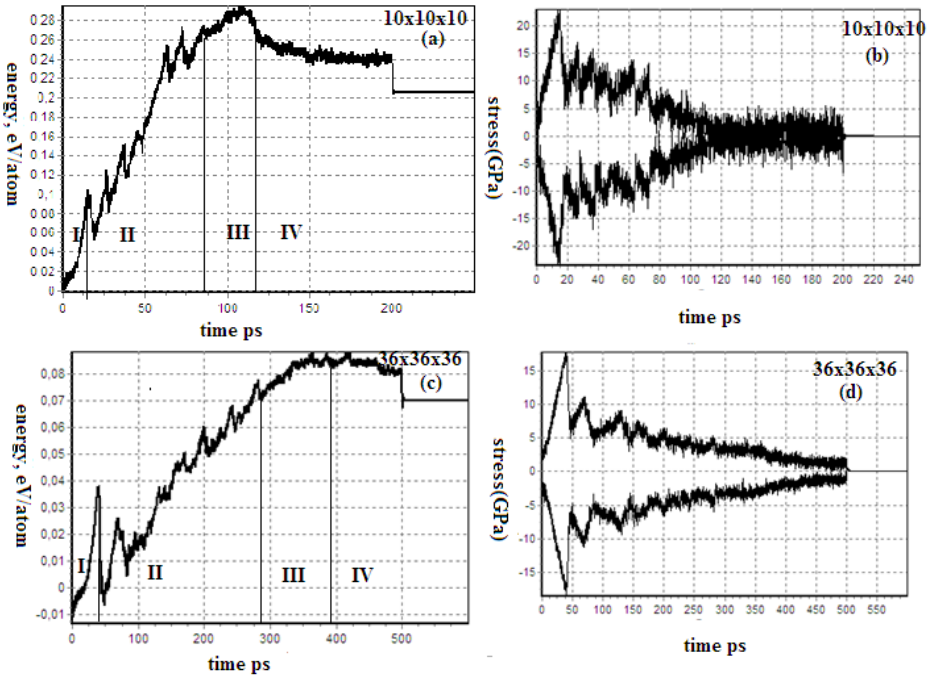

Fig. 2. the dependence of the stored energy of deformation of the experiment at 300 K for nickel-10 x 10x 10 (a), the relation of stress with time at temperatures 300 K for nickel-10 x 10 x 10 (b), the dependence of the stored energy of deformation of the experiment at 300 K for nickel-36 x 36x 36 (c) and the relation of stress with time at temperatures 300 K for nickel-36 x 36x 36 (d).

3.2. Volume effect on stress. Figure 3 shows the stress– length relations obtained from the simulations for temperature at 300 K as listed in Table 1. As it can be seen from the figure, the simulated stress decreased with increasing volume. However, further analysis for high temperature at 1000 K (Table 2) shows that the stress– length results exhibit a large oscillation about a mean curve (Fig. 3); however, the magnitudes of the oscillation can be reduced with increasing number of atoms. Figure 3 shows a decrease in strength with increasing nanowire volume at the strain rate of 2×108 s^{-1} for all temperatures. This is a "smaller is softer" effect. The effect of "smaller is softer" occurs for the nanowires with

smaller volume and the self-similar hardening effect occurs for those nanowires with high volume.

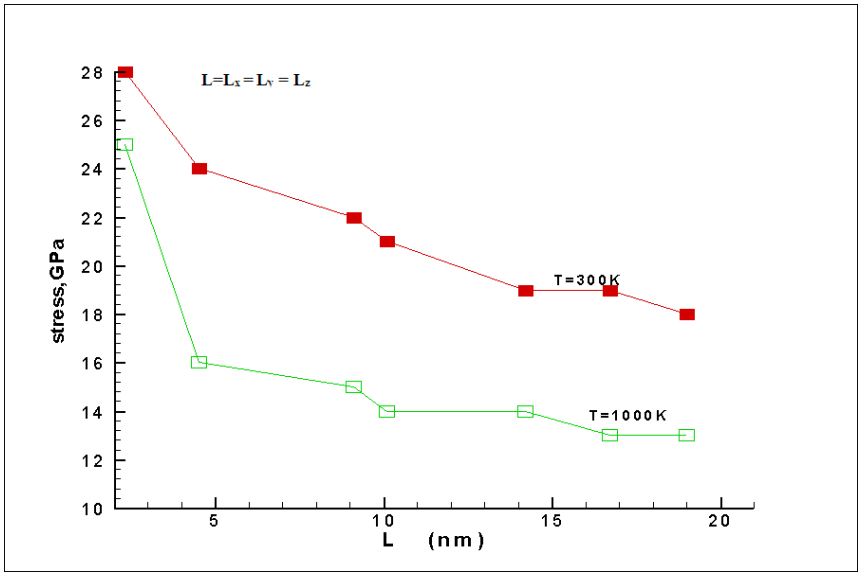

Fig. 3. The simulated ultimate strength of ultrathin Ni nanowires as a function of nanowire length for different temperatures.

The neck of the nanowire forms after the slips happened, and the deformations have been carried mainly through the elongation of the neck. Beyond the neck region, atomic structures have no significant changes. The atomic rearrangements in the neck region induce the zigzag increase–de-crease in stress as the strain is increased. The atoms, close to the narrowest region of the neck, are highly disordered. At the point of breaking, we observe a one-atom thick. With further pulling of the nanowire, the bond between the two atoms lying in the one-atom breaks and then the rupture happens.

3.3. Plastic deformation. We now discuss the plastic deformation simulations of the Ni nanowire. Beyond the elastic limit, the nanowires are not able to retain the structure and the plastic deformation starts to take place in order to accommodate the applied compressive uniaxial loading. In order to study the plastic deformation process of Ni nanowires that arises beyond the elastic limit.

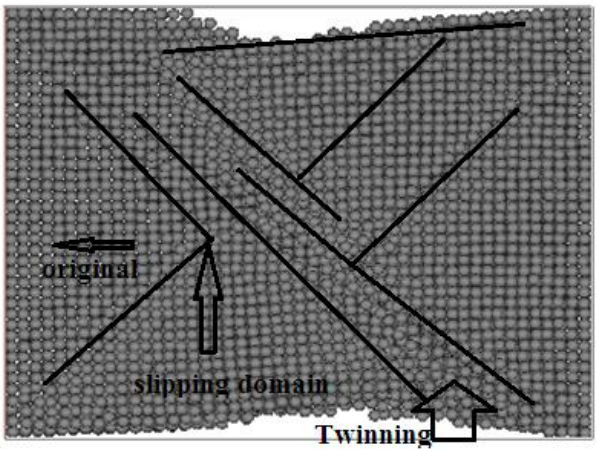

Fig. 4. Deformation of 40x40x40 Ni nanowire under tension. Plastic deformation of dislocation slips, slipping domain and twins at time 100 ps.

With the volume increasing furthermore, we find that sliding happens (see Fig. 4 and 5), and many atoms rearrange in the neck region. Significant necking occurs at small volume. Through further analysis, we find that after the formation of the neck, the plastic deformations have been carried mainly through the reconstruction and rearrangement of the neck region. Beyond this region, the nanowire keeps ordered structure and have no significant change.

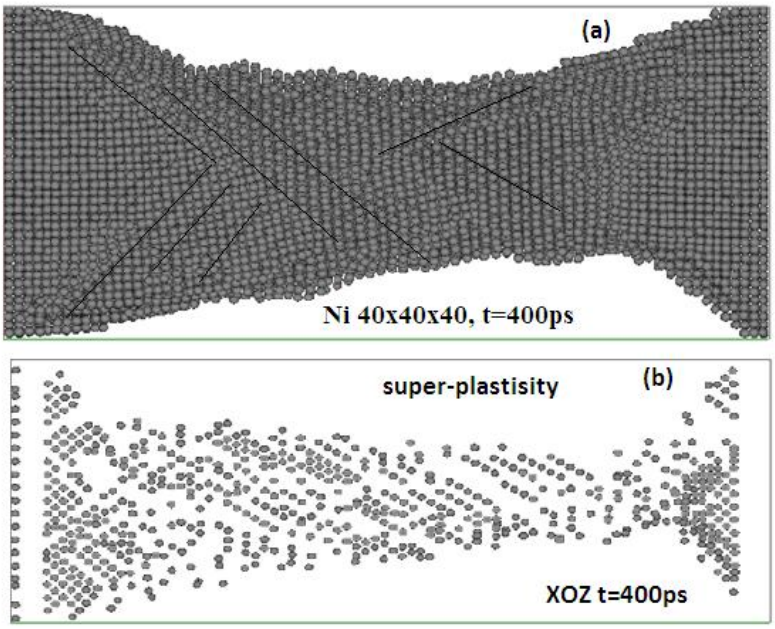

Fig. 5. Deformation of 40x40x40 Ni nanowire under tension super-plasticity deformation of dislocation slips, slipping domain and twins (a) at time 400 ps, (b) 5th XOZ plane at time 400 ps.

Figure 6 a shows the cluster produced on 5th XOY plane at time 600 ps for 40 x 40 x 40 nanowire under tension. Figure 6 b shows the gamma for deformation of 40 x 40 x 40 Ni nanowire under tension 5th XOY plane at time 600 ps.

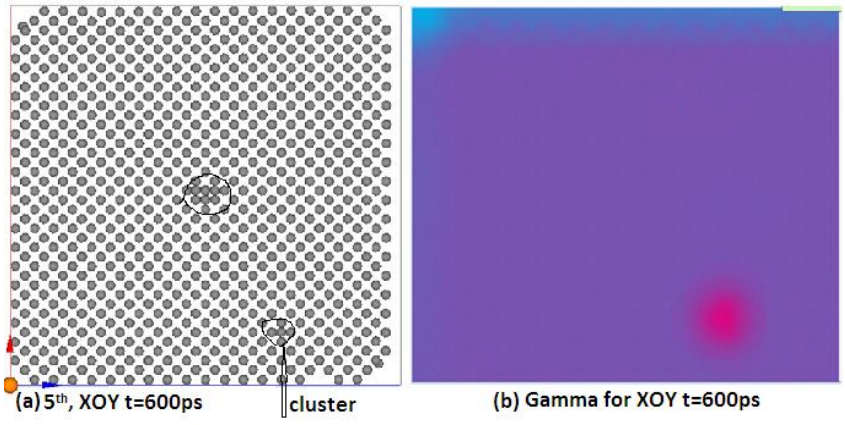

Fig. 6. Deformation of 40x40x40 Ni nanowire under tension 5th XOY plane at time 600 ps (a) with clusters, (b) Gamma for (a).

3.4. Breaking. Figure 7 and 8 presents the breaking position for Ni nanowires. Unlike the stress, the breaking position increases with increasing volume. Figure 4 and 5 shows the variation of breaking position with the Volume (indicated by the side length) of the cross-section. Surface atoms play an important role in the mechanical behaviors of nano structures,

and the volume effect commonly found in small-scale systems is the surface effect. The results showed that breaking position depended on the nanowire length. If the breaking position is predictable, the nanowire can be strengthened near the breaking position to avoid failure. Although the single breaking case is not predictable, many breaking cases show a statistic feature.

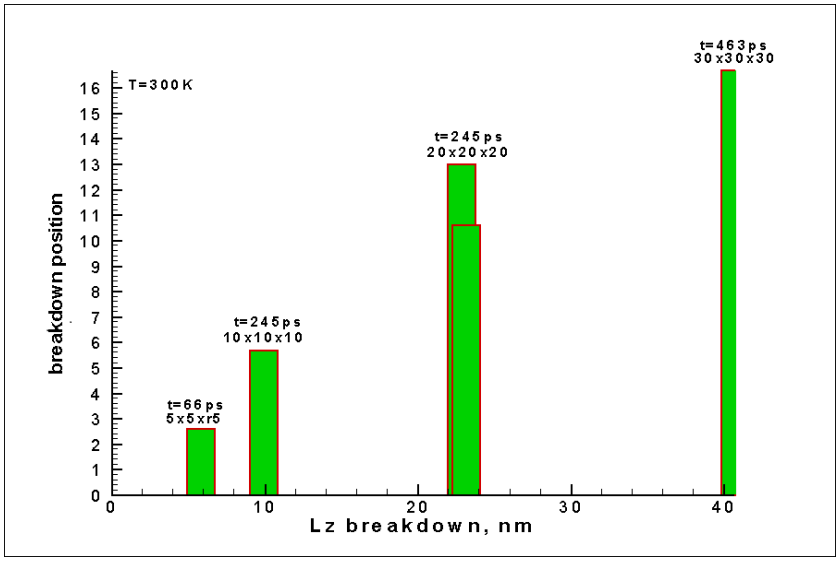

Fig.7. Histograms of the breaking position with breaking length L_z measured in units of Ni at T=300 K.

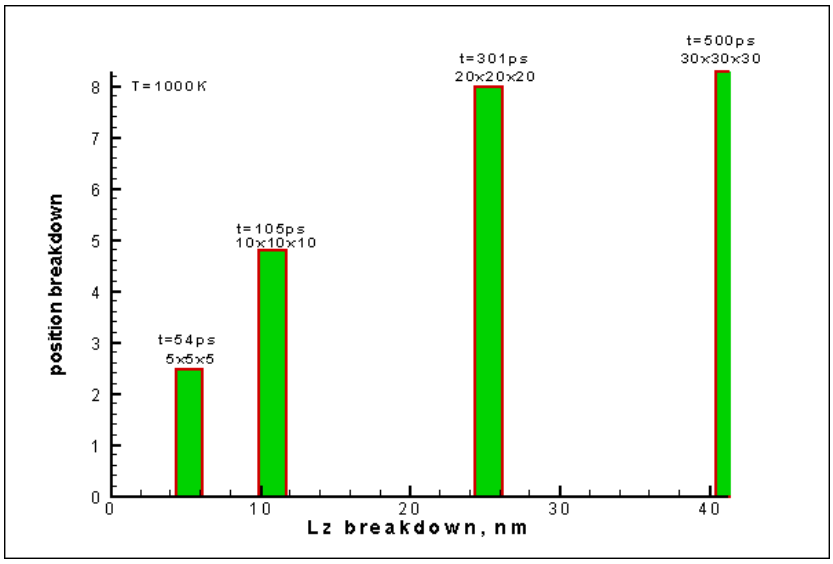

Fig. 8. Histograms of the breaking position with breaking length L_z measured in units of Ni at T=1000 K.

Figure 9 presents the representative snapshots of Ni nanowires with different Volume at the breaking moment. In most cases, the final breaking position occurs at the central part of the nanowire when it is short, as the nanowire length increases the breaking position gradually shifts to the ends.

3.5. Simulation for one atom long (z direction). Figures 10 and 11 present the representative snapshots of 70 x 70 x 1 Ni nanowires at 300 K different amount of time. Pores produced at 30 ps, number and size of these pores increases. Failure occurs quickly as the breaking time for this simulation is 53 ps.

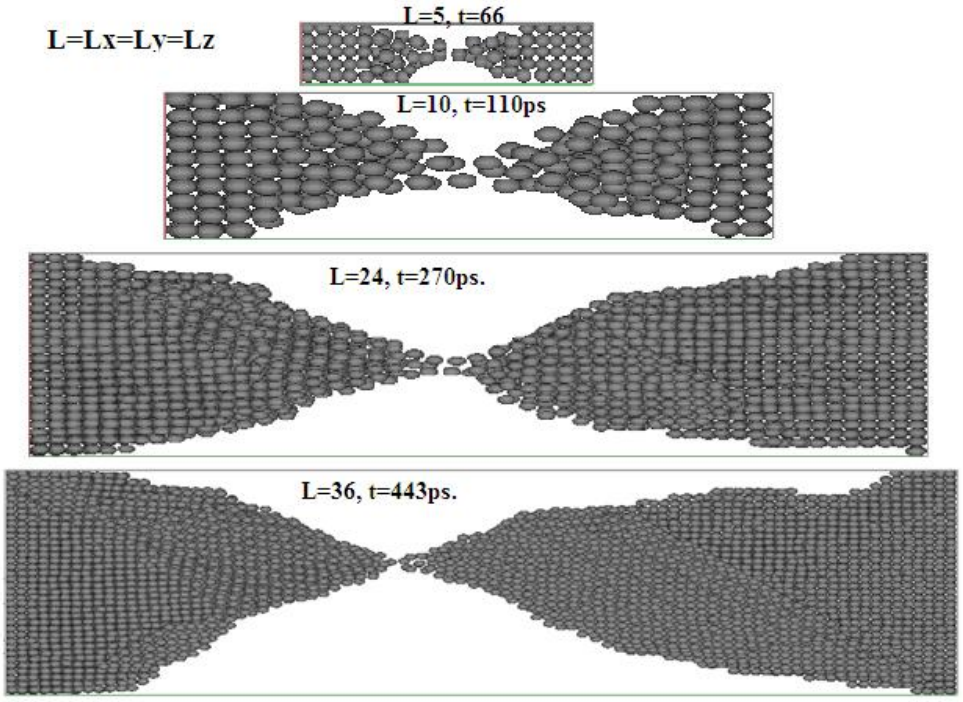

Fig. 9. Snapshots of Ni nanowires with different volume at the breaking moment at T =1000 K.

The experiments were obtained plots of the stored energy of deformation of the time, reflecting the processes in the nanowire during deformation (Fig. 12 a). There are two stages of deformation: the quasi-elastic deformation (I), the breaking (flow) (II). The initial stage quasi-elastic area there is only relative displacement of atoms and there are no defects. Therefore, in this region the energy stored varies periodically but completely different from Fig. 2. This stage is completed in 18 ps for 70 x70 x 1 Ni nanowire.

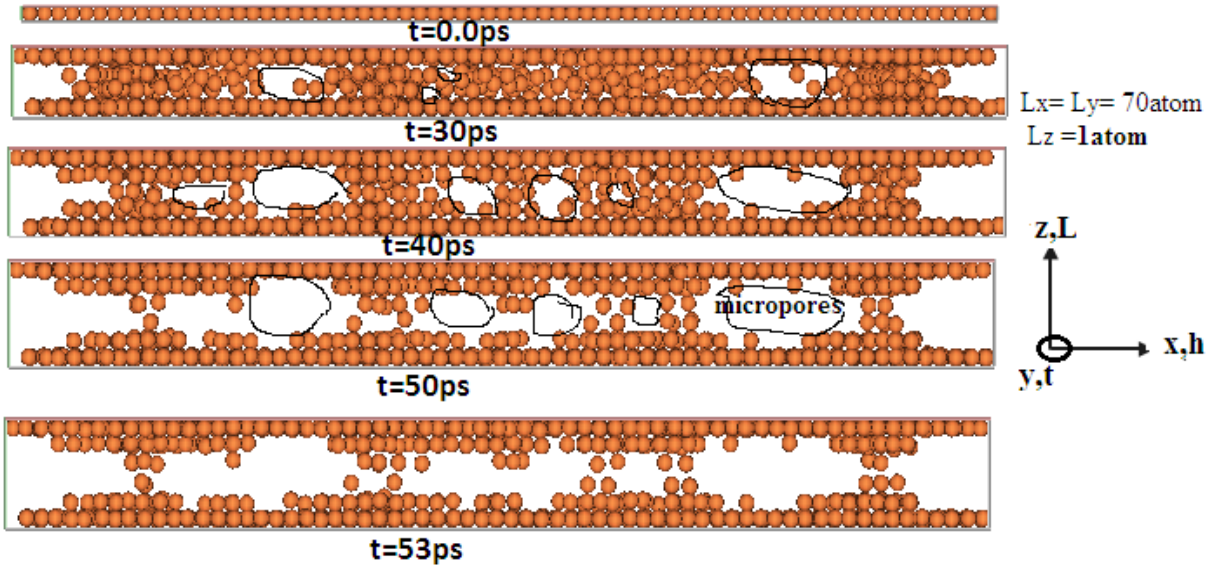

Fig. 10. Snapshots of the atomic configuration rearrangement of 70 x 70 x1 Ni nanowire at 300 K. The configurations presented correspond to the following times: 0 ps, 30 ps, 40 ps, 50 ps and 53 ps.

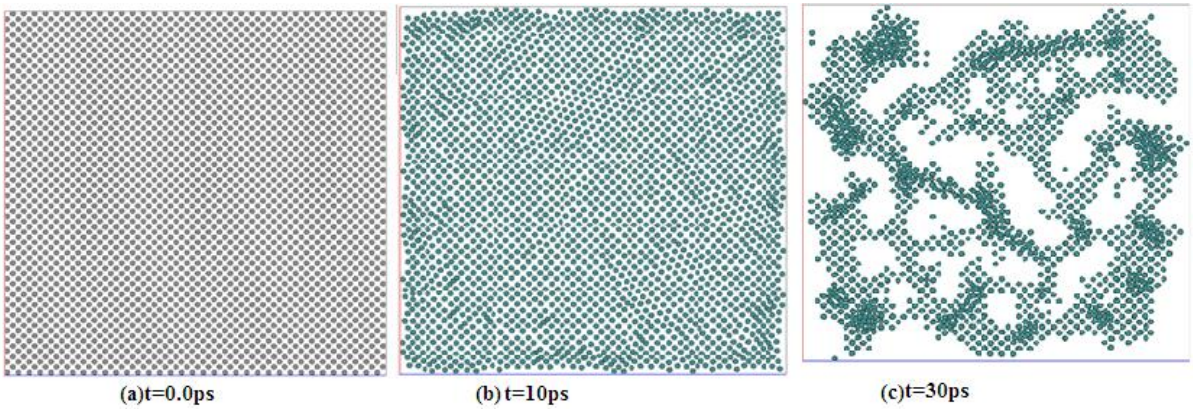

Fig. 11. Snapshots of the XOY rearrangement of 70 x70 x1 Ni nanowire at a temperature of 300 K. The configurations presented correspond to the following times: (a) 0 ps, (b) 10 ps, (c) 30 ps.

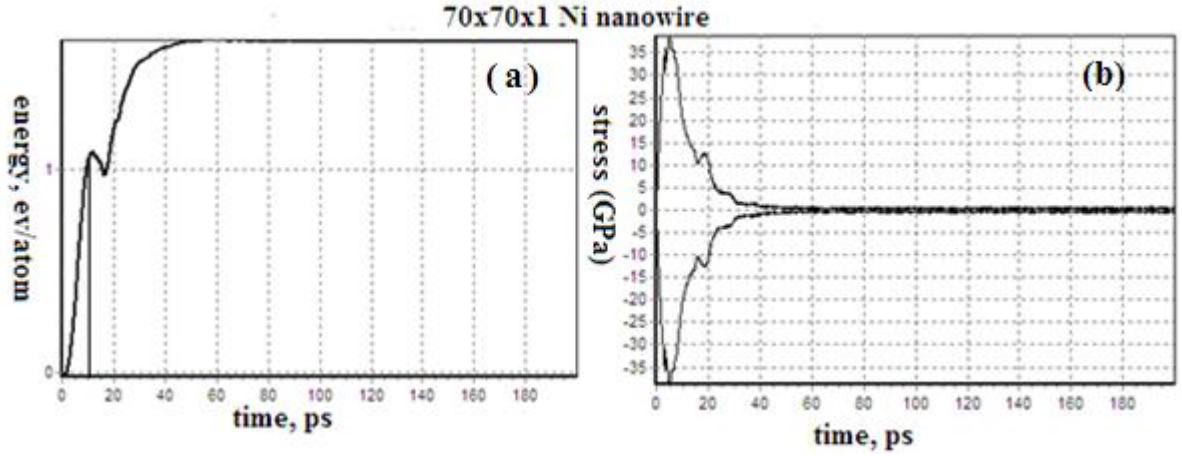

Fig. 12. The dependence of the stored energy of deformation of the experiment at 300 K for nickel-70 x 70x 1 (a), the relation of stress with time at temperatures 300 K for nickel-70 x 70 x 1 (b).

4. Conclusions

Molecular dynamics simulation results about Ni nanowire at 300 K and 1000 K temperatures are presented. The mechanical properties of Ni nanowire for these temperatures are different. The stress–time and stress length curves for nanowires are simulated. The breaking and yield stress of nanowires are dependent on the volume and temperature. The necking, plastic deformation, slipping domain, twining, clusters, microspores and break-up phenomena of nanowire are demonstrated. Stress decreases with increasing nanowire volume and temperature. The final breaking position occurs at the central part of the nanowire when it is short, as the nanowire length increases the breaking position gradually shifts to the ends.

Reference:

[1] E.V. Kozlov, L.E. Popov, M.D. Starostenkov // *Russian Physics Journal* **15 (3)** (1972) 395.
[2] L.A. Girifalco, V.G. Weizer // *Physical Review* **114** (1959) 687.
[3] S.V. Dmitriev, A.A. Ovcharov, M.D. Starostenkov, É.V. Kozlov // *Physics of the Solid State* **38 (6)** (1996) 996.
[4] G.M. Poletaev, *Atomic mechanisms of diffusion in metallic systems with fcc lattice*, D. Sc.

Thesis (I.I. Polzunov Altai State Technical University, Barnaul, 2006).
[5] X. Yang, L. Liu, P. Zhai, Q. Zhang // *Computational Materials Science* **44** (2009) 1390.
[6] Potekaev A.I., Dudnik E.A., Popova L.A., Starostenkov M.D. // *Russian Physics Journal* **51 (10)** (2008) 1053.
[7] M.D. Starostenkov, B.F. Demyanov, S.L. Kustov, E.G. Sverdlova, E.L. Grakhov // *Computational Materials Science* **14** (1999) 146.