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MODELING AND SIMULATION OF Ni NANOFILM USING MORSE PAIR POTENTIAL

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Abstract. Morse potentials were employed to carry out three-dimensional molecular dynamics simulations. A computer experiment was performed at the temperature corresponding to 300 K and 1000 K. MD simulation was used to investigate the effect of cross-sectional area of Ni nanofilm on the nature of deformation and fracture. The engineering stress–time diagrams obtained by the MD simulations of the tensile specimens of these Ni nanofilms showed a rapid increase in stress up to a maximum followed by a gradual drop to zero when the specimen was failed by ductile fracture. The feature of deformation energy can be divided into four regions: quasi-elastic, plastic, flow, and failure. The results shows that breaking position depends on the nanofilm cross-sectional area.

1. Introduction:

Figure 1 shows the MD simulation model of Ni nanofilms 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 nanofilms.

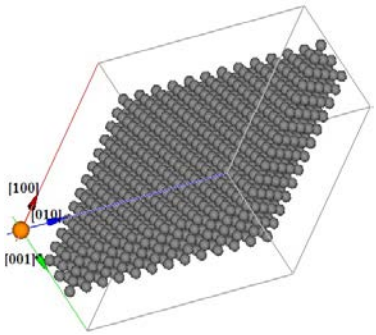

Fig. 1. MD simulation model of Ni nanofilm
(25 atoms along the edges at the bottom and 5 - in length).

Different nanofilms of different cross-sectional area are considered at the temperatures corresponding to 300 K and 1000 K. 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. Aish et al. [1-7] have studied the mechanical properties of Ni nanowires where they concluded that the mechanical properties of Ni nanowires are highly dependent on the size, shape as well as the atomic vacancies in the nanowire.

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 [8, 9, 12], 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} - 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. Td and Ta are the desired temperature and actual temperature of system, respectively. The initial configuration of the molecular dynamics simulation is shown in Fig. 1. The stress calculation in the atomistic simulations σ_{mn}. On m plane and in n-direction σ_{mn} is calculated by [10, 11]:

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

where Ns 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, cross-sectional area of the nanofilms and temperature.

The object of investigation is taken different size of Ni nanofilms. Nanofilms structure is presented in the form of a face-centered cubic cell. We study the effect of cross-sectional area on the mechanical properties of simulation nanofilms 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 length) to 20250 atoms (90 atoms along the edges at the bottom and 5 - in length).

3. Results and discussion

Since the breaking and the Yielding of Ni nanofilms are of main interest in this work (Tables 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 L_z =5 and L_x=L_y, changes from 5 to 90. The nature of deformation, slipping, twinning and necking were studied.

Table.1. The typical MD results of different system at 300 K , depending on the yield strength (σ_T), the starting time of plastic deformation (t_{pl}), the starting time for failure of the sample (t_f), the length of start failure of the sample (l_f) and the relative position of the sample breaking (l_b).

	system	σ_T, GPa	t_{pl}, ps	t_f, ps	l_f, nm	l_b, nm
1	5x5x5	28	9	66	5,8	2,6
2	10x10x5	26	9	70	6	3
3	15x15x5	25	12	100	7,5	3,5
4	25x25x5	26	16	110	8	4
5	40x40x5	26	17	140	8.2	5
6	50x50x5	27	18	115	8,3	4,4
7	60x60x5	26	19	110	8	4
8	70x70x5	27	20	110	8	4
9	90x90x5	28	21	100	7,5	3,5

Table 2. The typical MD results of different system at 1000 K, depending on the yield strength (σ_T), the starting time of plastic deformation (t_{pl}), the starting time for failure of the sample (t_f), the length of start failure of the sample (l_f) and the relative position of the sample breaking (l_b).

	system	σ_T, GPa	t_{pl}, ps	t_f, ps	l_f, nm	l_b, nm
1	5x5x5	25	9	51	5,1	2,7
2	10x10x5	23	9	83	6,8	3,3
3	15x15x5	20	12	101	7,8	4,2
4	25x25x5	22	16	116	8,5	4,2
5	40x40x5	23	17	110	8,3	4
6	50x50x5	24	18	115	8,5	4,2
7	60x60x5	24	19	115	8,5	4,2
8	70x70x5	24	20	115	8,5	4,2
9	90x90x5	25	21	110	8,3	4,2

3.1. Four stages of deformation. In the experiments the plots of the stored energy of deformation on the time were obtained. There are four stages of deformation: the quasi-elastic deformation (I), plastic deformation (II), the breaking (flow) (III), and failure (IV). At all cross-sectional area, in the first stage there was almost linear increase in stress. In the initial stage quasi-elastic there was only relative displacement of atoms and there were no defects. Therefore, in this region the energy stored varies periodically. This stage is completed in 9 ps for 5 x 5 x 5 Ni nanofilm. The sharp fall takes place only at the point of transition from the first to second stages of deformation (Fig. 2a). Experiments have shown that when the cross-sectional area increases the first stages of deformation have the same value, Tables 1, 2. If you change the cross-section of the samples, structural rearrangements in them take place in time.

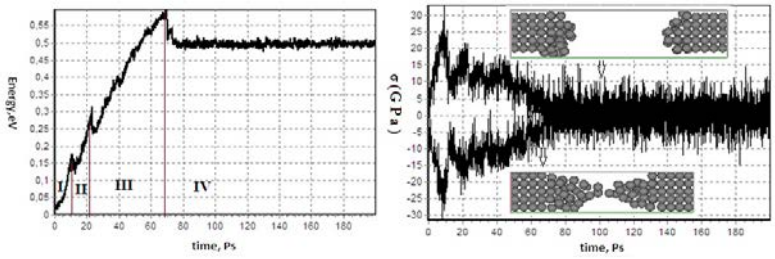

Fig. 2. The stored energy of deformation of the experiment at 300 K for nickel-5 x 5 x 5 (a), the relation of stress with time at temperatures 300 K for nickel-5 x 5 x 5 (b).

The neck of the nanofilm 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 with time of deformation. 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 nanofilm, the bond between the two atoms lying in the one-atom breaks and then the rupture happens.

Analysis of the graphs in Figure 3 shows that the average duration of the first stage of deformation for nanofilms with cross-section 10x10, 25x25, 50x50 and 70x70 equals 9, 16, 18 and 21 ps, respectively. Duration of the plastic deformation steps are 41, 34, 37, 41 ps, respectively.

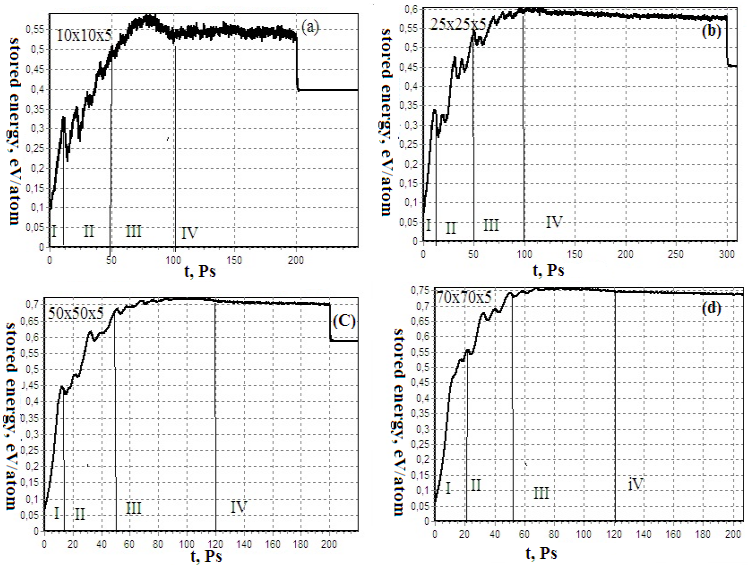

Fig. 3. The stored energy of deformation of the experiment at 1000 K for nanofilms with cross-section (a) 10x10, (b) 25x25, (c) 50x50, and (d)70x70.

Values of the stored energy at the peak of the graph deformation at the end of the first stage for the studied samples are 0.32, 0.34, 0.45 and 0.55 eV/atom, respectively. The values of stored energy at the end of plastic deformation of studied samples are 0.5, 0.55, 0.68, and 0.74 eV/atom, respectively.

3.2. Stress– cross-sectional area relations. Figure 4 shows the stress– length relations obtained from the simulations for temperature at 300 K as listed in Table 1. As can be seen from the figure the yield strength depends on the length. However, further analysis at 1000 K (Table 2) shows that the stress– length results exhibit a large oscillation about a mean curve (Fig. 4).

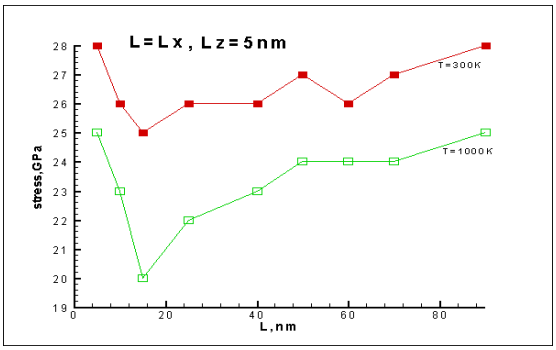

Fig. 4. The simulated ultimate strength of Ni nanofilms as a function of nanofilm cross-sectional area for different temperatures.

3.3. Breaking. Figure 5 represents the breaking position for Ni nanofilms. Unlike the stress, the breaking position increases with increasing of cross-sectional area. Figure 5 shows the variation of breaking position with the cross-sectional area (indicated by the side length). Surface atoms play an important role in the mechanical behaviors of nano-structures, and the cross-sectional area effect commonly found in small-scale systems is the surface effect. If the breaking position is predictable, the nanofilm 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.

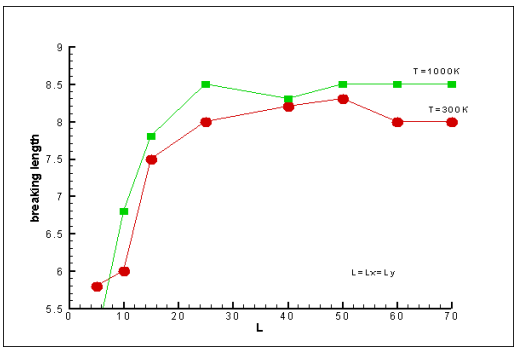

Fig. 5. The breaking length with length L of the Ni at T=300 K.

Figure 6 represents the representative snapshots of Ni nanofilms with different cross-sectional area at the breaking moment. In most cases, the final breaking position occurs at the central part of the nanofilm because it is length small.

4. Conclusions

Molecular dynamics simulation results about Ni nanofilm at 300 K and 1000 K temperatures are presented. There are four stages of deformation: the quasi-elastic deformation (I), plastic deformation (II), the breaking (flow) (III), and failure (IV).

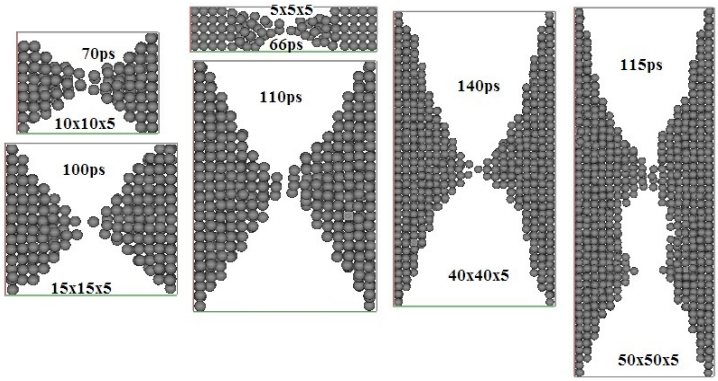

Fig. 6. Snapshots of Ni nanofilms with different cross-sectional area at the breaking moment.

The mechanical properties of Ni nanofilms depends on size and temperature. Atomic configurations as well as energy of deformation were calculated as a function of time of deformation. These quantities clearly revealed four distinct structural transformations that take place during the tensile deformation, namely: the quasi-elastic, plastic, flow and fracture. The breaking and yield stress of nanofilms are dependent on the cross-sectional area and the temperature. Stress has the dramatically change with increasing nanofilm cross-sectional area and temperature. The final breaking position occurs at the central part of the nanofilm because it's length is small.

Acknowledgments

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