International Journal of Scientific and Innovative Mathematical Research (IJSIMR)
Volume 2, Issue 3, March 2014, PP 301-305
ISSN 2347-307X (Print) & ISSN 2347-3142 (Online)
www.arcjournals.org

Molecular Dynamic Simulations of Nickel Nanowires at Various Temperatures

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Abstract: *The mechanical properties of Nickel nanowires have been studied at various temperatures using molecular dynamics simulations. 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. The deformation corresponds to the direction <001>. To the calculated block of crystal - free boundary conditions are applied in the directions <100>, <010>. Morse potential was employed to carry out three dimensional molecular dynamics simulations. MD simulation used to investigate the effect of temperature of Ni nanowire on the nature of deformation and fracture. Temperature effect on the extension property of metal nanowire is discussed in detail. The mechanical strengths and the mechanical strain of the nanowires decrease linearly with the increasing temperature. The feature of deformation energy can be divided into four regions: quasi-elastic, plastic, flow and failure. Experiments have shown that when the temperature increases the first stage of deformation was narrowed, and the second stage was widened. The results showed that breaking position depended on temperature. The simulation results at nanoscale play an important role on the mechanical behaviors of nanostructures.*

Keywords: *mechanical properties, molecular dynamics simulations, nanowire, Morse potential.*

1. COMPUTER SIMULATION MODEL

The object of investigation is taken alloy Ni. Alloy structure is presented in the form of a face-centered cubic cell. In this paper for calculating the dynamics of the atomic structure of the molecular dynamics method using paired Morse potential function [1]. 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 - the distance between the atoms.
The potential energy of a system of N atoms is represented as:

$$E = \frac{1}{2}\sum_{i=1,i\neq j}^{N}\sum_{j=1}^{N}\varphi_{KL}\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right) \quad (2)$$

Where ri - radius vectors of i-th atom.

When considering a closed system, the force acting on the i-th atom, will be:

$$F_i = -\sum_{i=1,i\neq j}^{N}\sum_{j=1}^{N}\frac{d\varphi_{KL}\left(\left|r_i - r_j\right|\right)}{d(r_i - r_j)} \quad (3)$$

Mathematical model of the molecular dynamics method [2-5] describes a system of ordinary

differential equations of motion of Newton. The equation of motion in the classical form is represented by:

$$m_i \frac{dv_i}{dt} = F_i \frac{dr_i}{dt} = v_i i = 1,2,\ldots, N \quad (4)$$

Where mi and v_i - mass and velocity of i-th atom - time.

To solve the system of ordinary differential equations by numerical Euler method with half-step. Temperature of the atoms in a perfect crystal, calculated using the formula:

$$T = \frac{2k}{3Nk_b} = \frac{1}{3Nk_b}\sum_{I}^{N} m_i v_i^2 \quad (5)$$

Where k_b, Boltzmann constant and K, is the total Kinetic energy.

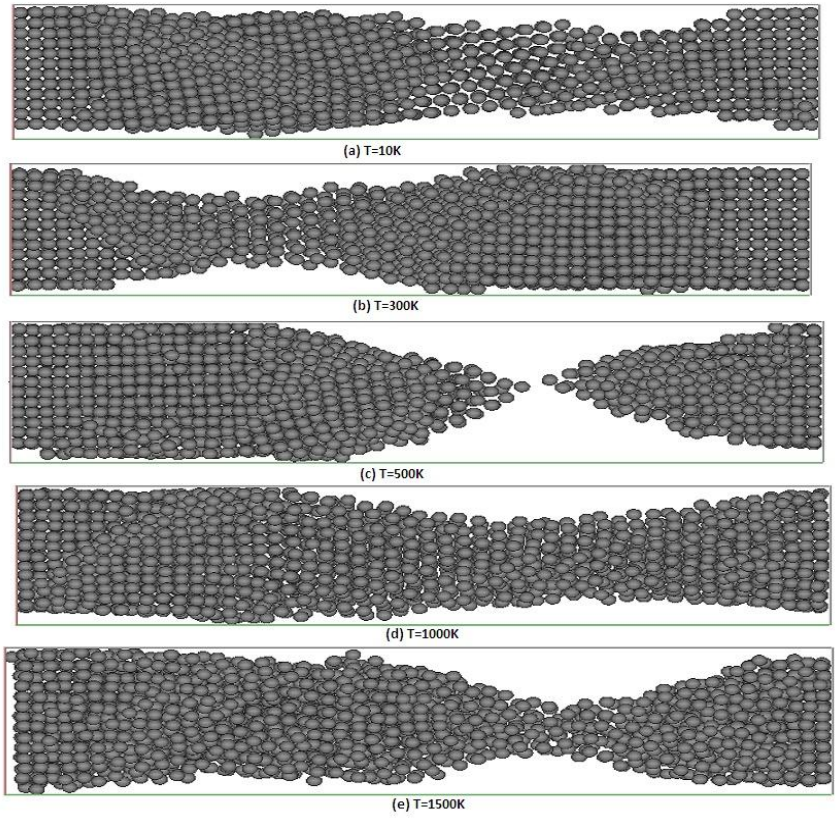

Fig 1. *Atomic configurations of 12x12x36 nanowire Nickel under extension loading at time 175 ps at different temperatures (a) T=10 K, plastic deformation occur (b) T=300K , plastic deformation occur (c)T =500K, break-up occur(d) T=1000K , plastic deformation occur (e) T=1500K , plastic deformation occur.*

Computer simulation using Morse potential is employed to carry out three dimensional molecular dynamics simulations of the mechanical properties of Nickel nanowire. We studied the extension properties of Nickel nanowires at different temperatures from 0 K to 1700 K, which is adjusted every 10^{-13} seconds. The estimated size of the crystal unit was for various experiments of 1728 atoms (6 atoms along the edges and 96 atoms in height), 2916 atoms (9 atoms along the edges and 72 atoms in height) and 3456 atoms (12 atoms along the edges at the bottom and 48 - in height).

The dependence of mechanical properties on simulation temperature has also been studied [6-9]. The yield strength decreases with increasing temperature. Low yield strength at high temperature is because of the fact that the thermal fluctuations overcoming the energy barrier for dislocation nucleation.

In the study the following parameters were monitored: the stored strain energy, the diffusion coefficients of the components in the directions, the overall diffusion coefficient, the kinetic and potential energy of the crystal.

2. RESULTS AND DISCUSSION, TEMPERATURE EFFECT

The mechanical property at different temperatures With MD simulations, the uniaxial tension of the nickel nanowires are studied at different temperatures from 0 to 1700 K. Figure 2 gives the stress–strain relationships of the 6x6x96 nanowires subjected to uniaxial tension at temperatures 300 K. The strain was defined as:

$$\varepsilon = \frac{l - l_0}{l_0} \tag{6}$$

Where l was the stretching length and l_0 was the length just after relaxation.

The stress in the tensile direction was calculated as:

$$\sigma = \frac{1}{NV_i} \sum_{i}^{N} F_i r_i \tag{7}$$

Where V_i refers to volume of atom i.

With the increasing initial strain, stress increases linearly at different temperatures. This process corresponds to the elastic deformation of the nanowire. With the increasing strain, stress decrease as shown in the stress–strain response of the nanowire, indicating the beginning of the plastic deformation of the nanowire. the stress–strain curves are smooth at low temperatures, whereas, some ‘‘minipeaks’’ exhibit at high temperatures.

It is observed that the first yield stress decreases as the temperature increases (Fig. 3). When the plastic deformation of the nanowire begins, the drop of the first yield stress also decreases. In order to clearly study these characters, in Fig. 4, we show the average statistical results of the first yield strain , the first yield stress (σ) at different temperatures.

The average result is from 300 samples at each temperature, and temperatures from 0 to 1700 K. As shown in Fig. 4, the first yield strain decreases when the temperature increases. From 0 to 1700 K**,** an abrupt decrease is identified and the first yield strains are 1.25 (100 K) and 0.2 (1700 K) with Ni alloy 12x12x48, 1.6 (10 K) and 0.07 (1700 K) with Ni alloy 9x9x72 and 1.46 (100 K) and 0.052 (1700 K) with Ni alloy 6x6x96. The bigger strain at low temperature indicates that the nanowire maintains its elastic deformation for long time. Whereas, the smaller strain at high temperature illustrates that the plastic deformation begins quickly. Deformation of the nanowire is in a fast stage of the atomic damage process at high temperature.

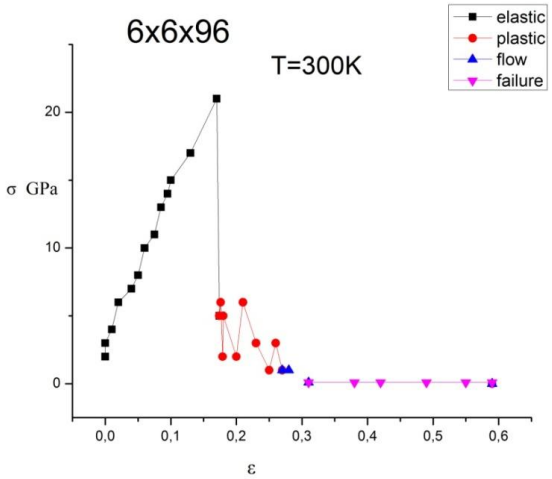

Figure.2. *The stress–strain relationships of the 6x6x96 nanowires subjected to uniaxial tension at temperatures 300 K.*

Table 1. *Results of MD simulation of uniaxial tensile loading with 12x12x28 Nickel nanowire. Number of atoms=3456.*

Temperature	Ultimate strength (GPa)	kinetic energy of the system, eV	Strain at max. stress
0	31	1	0.1
100	25	45	1.25
200	23	90	1.2
300	22	134	1.229
500	19	225	0.91
800	15	260	0.625
1000	14	325	0.479
1200	12	540	0.416
1500	**11**	690	0.208
1700	10	760	0.2

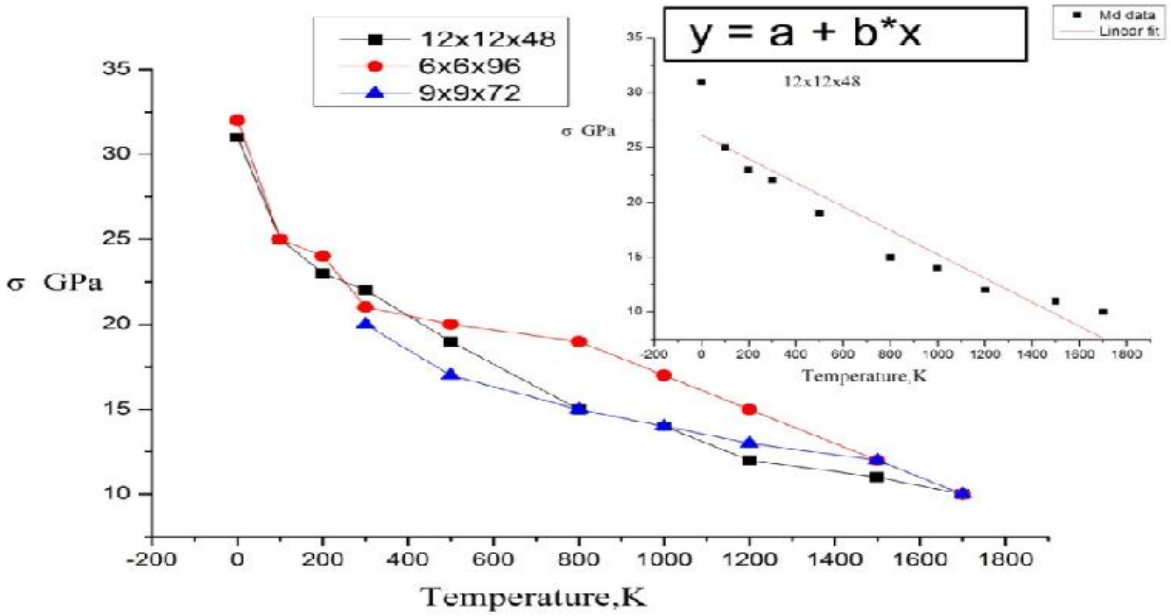

Fig. 3. *The curves of stress with temperatures.*

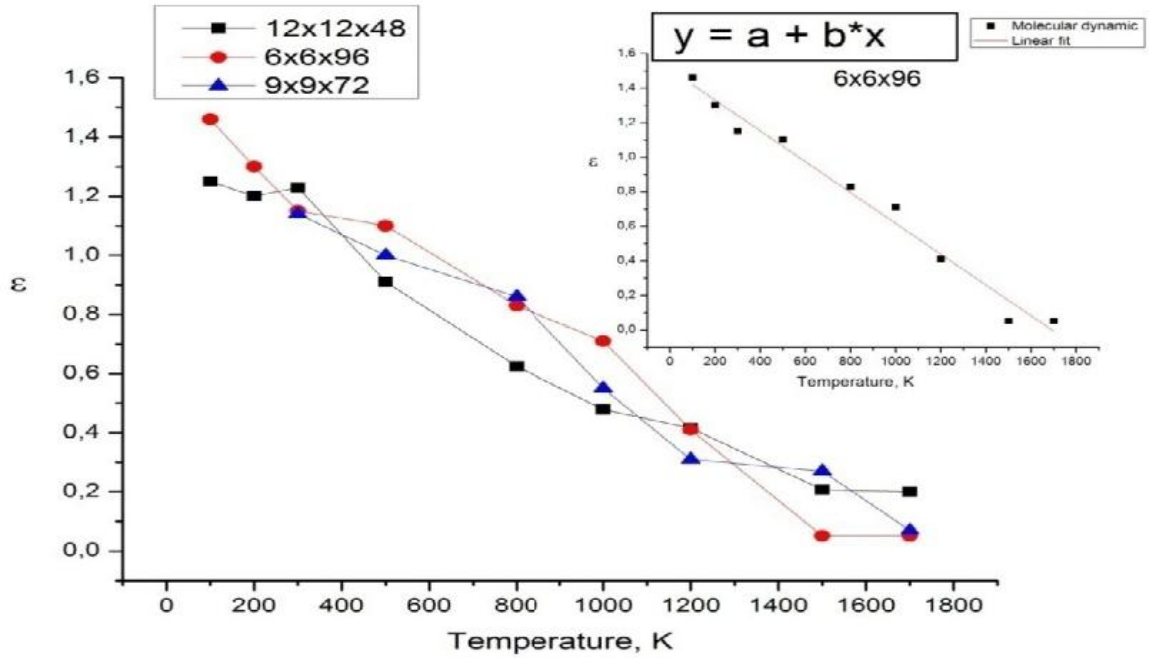

Fig 4. *The curves of strain with temperatures.*

3. CONCLUSION

The new concept of using nanowires as building blocks for logic and memory circuits makes it very necessary to fully understand the mechanical behaviors of these nanowires. Molecular dynamics simulations have been carried out to investigate the mechanical behaviors of Nickel nanowire. The effect of temperature on mechanical properties was investigated by MD simulations. The stress–strain relation of nanowire is obtained. The temperature effect on the extension properties is discussed in detail. Temperature exhibited a great effect on the mechanical properties of nanowires. Study on the mechanical properties of metal nanowires can give us more fundamental understanding of nanoscale machines from atomistic motions. The deformations of the nanowires were observed at low, middle, and high temperatures, respectively. The investigation on the configuration, stress, elasticity, yielding and deformation will contribute to the design, manufacture and manipulation of nano-devices. This study of mechanical properties of metal nanowires will be helpful to the design, manufacture and manipulation of nano-devices.

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