International Journal of
Science Inventions Today
www.ijsit.com
ISSN 2319-5436
Research Article

# MOLECULAR DYNAMIC SIMULATION OF 12X12X36 NICKEL NANOWIRE AT DIFFERENT TEMPERATURES

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The mechanical properties of Nickel nanowire have been studied at different temperatures using molecular dynamics simulations. Morse potential is employed to carry out three dimensional molecular dynamics simulations. The stress–time relation of nanowire under extension is obtained. Temperature effect on the mechanical property of metal nanowire is discussed in detail. At high temperature a wide range of plastic region takes place. The simulation results at nanoscale play an important role on the mechanical behaviors of nanostructures.

## 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:

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

Where $\alpha_{KL}$, $\beta_{KL}$, $D_{KL}$ - 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:

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

Where $r_i$ - radius vectors of i-th atom.When considering a closed system, the force acting on the i-th atom, willbe:

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

Mathematical model of the molecular dynamics method [2] describes a system of ordinary differential equations of motion of Newton. The equation of motion in the classical form is represented by:

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

Where $m_i$ 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:

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

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

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 10K to 1500K, which is adjusted every $10^{-13}$ seconds. The estimated size of the crystal unit was for this experiment of **2592** atoms (12 atoms along the edges and 36 atoms in height).

## RESULTS AND DISCUSSION, TEMPERATURE EFFECT

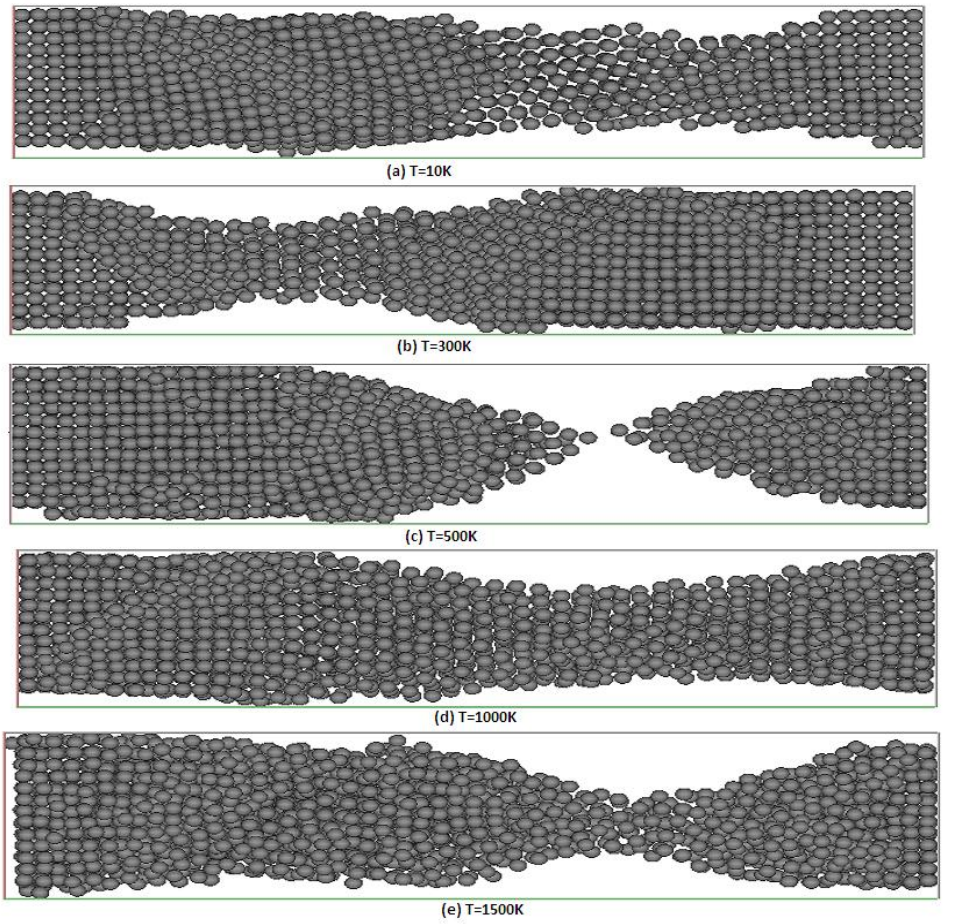


**Figure 1:** Atomic configurations of 12x12x36 nanowire Nickel under extension loading at time 175 ps at different temperatures (a) T=10 K, plastic deformation occur (b) T=300K , plastic deformation occur (c)T =500K, break-up occur(d) T=1000K , plastic deformation occur (e) T=1500K , plastic deformation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

| Temperature | Ultimate strength (GPa ) | Strain at max. stress | Strain to failure |
|---|---|---|---|
| 10 | 25 | 0.25 | 0.76 |
| 300 | 21 | 0.222 | 0.7 |
| 500 | 19 | 0.61 | 0.58 |
| 1000 | 12 | 0.1 | 0.86 |
| 1500 | 8 | 0.05 | 0.61 |

**Table 1:**Results of MD simulation of uniaxial tensile loading with 12x12x36 Nickel nanowire. Number of atoms=2592.

Table 1. gives the measured (from MD simulation) tensile strength and strain to fracture of the 12x12x36 Nickel nanowire at different temperature. It is observed that the first yield stress decreases as the temperature increases. the first yield strain (Ɛ) decreases when the temperature increases. From 0 to 1500 K**,** an abrupt decrease is identified and the first yield strains are 0.25 (10 K) and 0.05 (1500 K) with Ni alloy 12x12x36.It is observed that the first yield strain decreases as the temperature increases (Table.1). When the plastic deformation of the nanowire begins, the drop of the first yield stress also decreases.

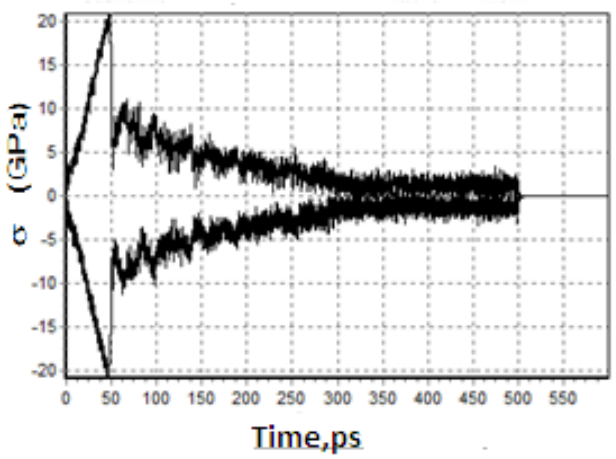


**Figure 2:**The stress–time relationships of the 12x12x36 nanowires subjected to uniaxial tension at temperatures 300 K.

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

## 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 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.

## REFERENCES

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