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# Deformation of different nickel nanowires at 300 K

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# Деформация различных нановолокон никеля при температуре 300 К

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The stress-time relation and energy-time relation for different nickel nanowires were studied under uniaxial deformation of tension. The stress-strain diagrams were obtained by the method of molecular dynamics (MD). Simulation of the tensile specimens of these Ni nanowires showed a rapid increase in stress up to a maximum followed by a gradual drop to zero when the specimen fails by ductile fracture. The stress-strain curve under extension loading and plastic deformation was studied. The maximum stress and strain at maximum stress had the same value for different Ni nanowires.

**Keywords:** stress, molecular dynamics, simulation, deformation, nanowires.

Исследованы зависимости напряжение-время и энергия-время для различных никелевых нанопроводов при одноосной деформации растяжения. Были получены диаграммы растяжения методом молекулярной (МД). Моделирование растяжения образцов из никелевых нанопроводов показало быстрый рост напряжения до максимума с последующим постепенным падением до нуля, когда образец вязко разрушается. Была исследована кривая напряжение-деформация под нагрузкой растяжения и пластической деформации. Максимумы напряжения и деформации имеют одинаковые значения для различных Ni нанопроводов.

**Ключевые слова:** напряжение, молекулярная динамика, моделирование, деформация, нанопроводы.

## 1.Introduction: Potential model andsimulation 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:

$$\varphi_{K}(r) = D_K\, \beta_K\, e^{-\alpha_K r}\left[\beta_K\, e^{-\alpha_K r} - 2\right],$$

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 object of investigation is taken seven nanowires of Ni alloy. Alloy structure is presented in the form of a face-centered cubic cell. We study the stress-strain curve of simulation nanowire at room temperature.

MD simulations [5-18] have been carried out on pure 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 potentials was employed to carry out three dimensional molecular dynamics simulations. The object of investigation is taken seven nanowires of Ni alloy. MD simulation used to investigate the nature of deformation and fracture. We addressed the stress-strain effects on the deformation characteristics and mechanical properties of the nanowire.

A computer experiment is performed at a temperature corresponding to 300K, at any stage of deformation involving the possibility of chilling calculation unit for detailed analysis of the structural changes occurring in it [19-22]. The estimated size of the crystal unit was for various experiments of 6912 atoms (24 atoms along the edges at the bottom and 24 – in height) to 27678 atoms (24 atoms along the edgesat the bottom and 96 – in height).

## 2. Results and discussion

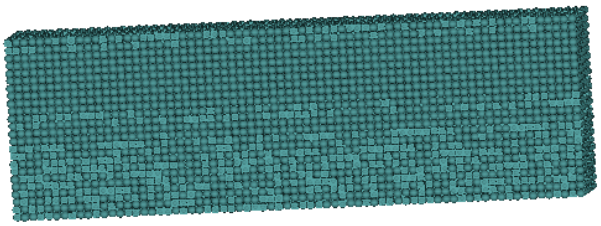

**Fig.1.** Simulation cell of Nickel 24×24×24 nanowire.

Fig.3 show the stress-Time relation and Energy-Time Relation for two different Ni nanowires. Experiments have shown that when the long of nanowire increases the first stage of deformation was widened, and the second stage was narrowed as in Fig.1. Figs.4-6 show the engineering stress–strain diagrams obtained by MD simulation of the tensile specimens of different system of Ni (FCC). Where the stress–strain diagram is essentially smooth with a linear slope in the elastic region, in nano-tensile testing, a series of steps of rise and fall in the stress values with engineering strain occurs in the initial elastic region. This is followed by a plastic region up to the maximum stress. Animation of the tensile tests indicated considerable reorganization of the atoms followed by rapid movement due to the generation of dislocations. Also, neither clear demarcation of linear elastic range nor the yield point is visible.

As can be expected, the maximum stress (ultimate strength of 20 GPa) and strain at maximum stress (earlier fracture at 0.16%) have the same value for different Ni nanowires. the maximum strain before fracture is different for different nanowire 1.5% for Ni-24×24×24 nanowire and 0.42% for Ni-24×24×96.

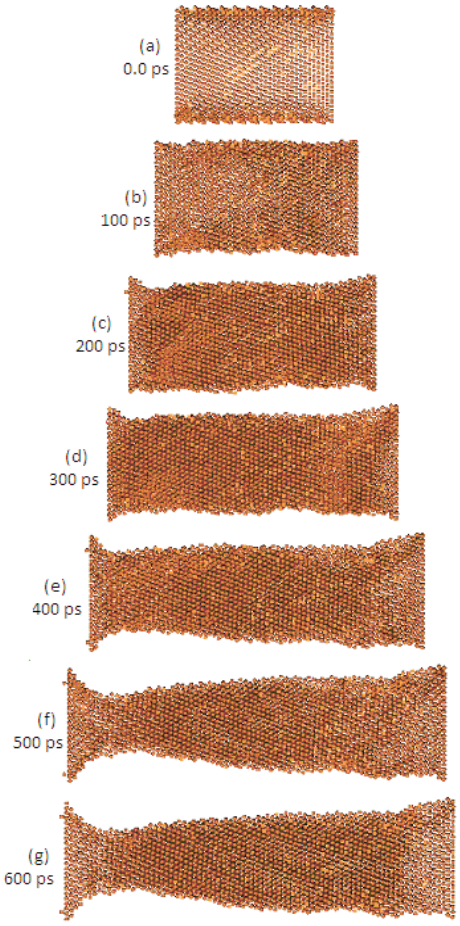


**Fig.2. (a)-(g)** The atomic configuration of Ni nanowire 24×24×36 system along X–Z section starting from a perfect fcc crystal at 300 K.

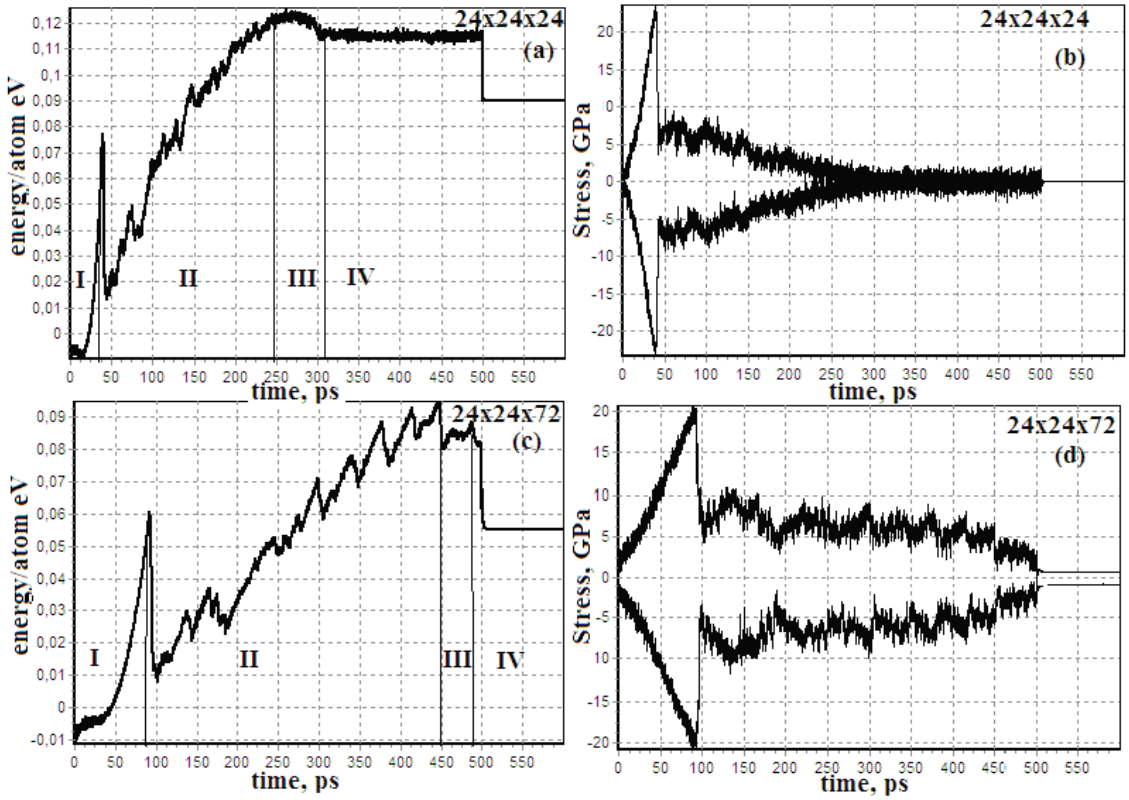


**Fig.3.** (a) The relation of stress with time at temperature 300K for nickel-24×24×24, (b) The dependence of the stored energy of deformation of the experiment at 300K for nickel-24×24×24, (c) The relation of stress with time at temperatures 300 K for nickel-24×24×72 and (d) the dependence of the stored energy of deformation of the experiment at 300K for nickel-24×24×72.

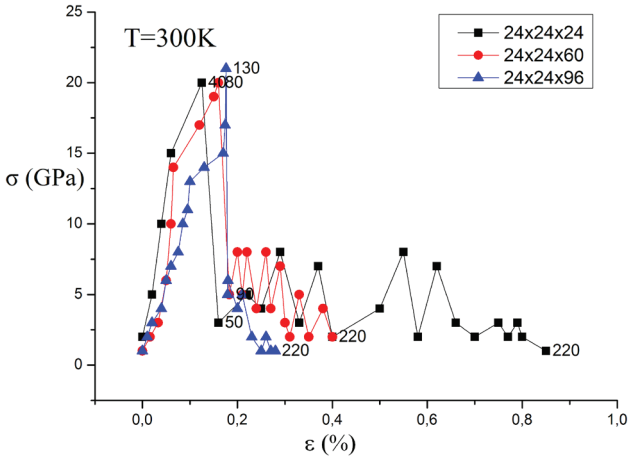


**Fig.4.** Stress-strain curve for three different nanowire of Nickel at 300 K. Elastic and plastic stages with labels of time at the first and end of these regions.

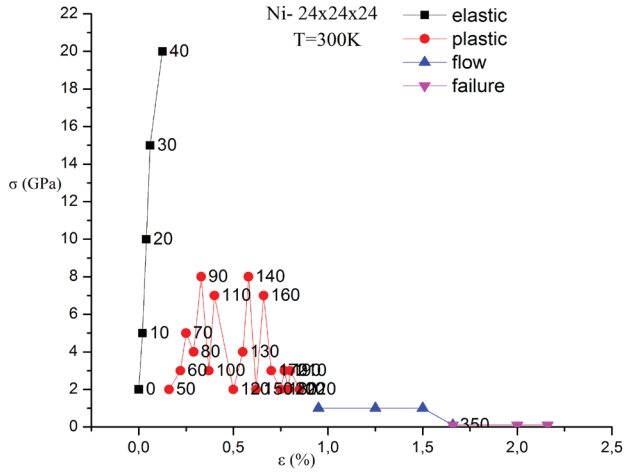


**Fig.5.** Stress-strain curve for 24x24x24 of Nickel nanowire at 300 K. Elastic, plastic, flow and failure stages with labels of time shown in this fig.

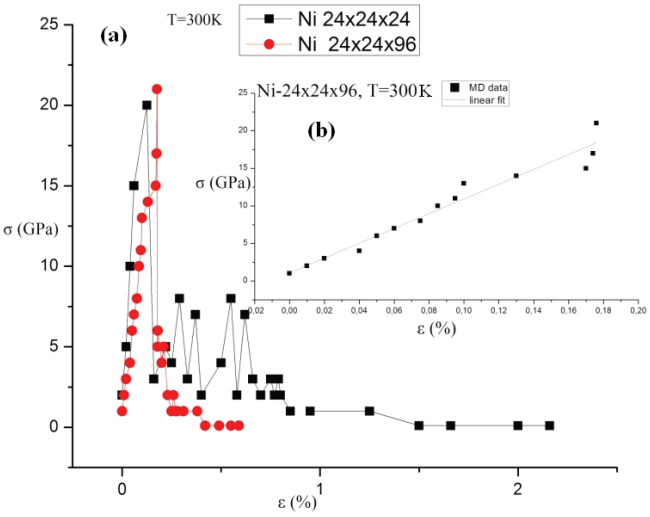


**Fig.6.** (a) Stress-strain curve for two different nanowire of Nickel at 300 K with (b) Stress-strain curve at the first stage for 24×24×96 nanowire of Nickel at 300 K.

**Table 1.**

Shows MD data of seven Ni nanowires.

| Crystal size, nanowires | No. of atoms | Time Ps (end of 1st stage) | Maximum strength (GPa) | Strain at max. stress % |
|---|---|---|---|---|
| 24×24×24 | 6912 | 40 | 21 | 0.15 |
| 24×24×36 | 10368 | 50 | 20 | 0.16 |
| 24×24×48 | 13824 | 60 | 20 | 0.15 |
| 24×24×60 | 17280 | 75 | 20 | 0.16 |
| 24×24×72 | 20736 | 90 | 20 | 0.16 |
| 24×24×84 | 24192 | 110 | 20 | 0.16 |
| 24×24×96 | 27678 | 120 | 20 | 0.16 |

Behavior stops after the elastic limit and once the yield point is reached. This is far below the position of maximum stress [23, 24]. In the MD simulations conducted here, we observed that in the case of FCC Nickel nanowire, even before the maximum stress point is reached the crystal has undergone significant amount of irreversible deformation.

## 3.Conclusion

In this paper, we have performed molecular dynamics simulations with the Morse potential field to study the structural evolution and deformation behavior of seven nanowires of nickel during the uniaxial tensile process. We addressed the stress-strain effects on the deformation characteristics and mechanical properties of the nanowire. The feature of stress-strain curve can be divided into four regions:

1) When the strain rate is below 0.16% for the nanowire, keeps its crystalline structure during the tensile process, the necking occurs in the last part of deformation. quasi-elastic deformation takes place at that region.

2) When the strain rate is below 0.8% for Ni-24×24×24 and 0.26% for Ni-24×24×96 part of nanowire transforms from a fcc crystal to amorphous state, and the other part still keeps its ordered structure during the tensile process. Several necks can be observed after certain strain. This is the plastic deformation of nanowire.

3) When the strain rate is below 0.95% for Ni-24×24×24 and 0.31% for Ni-24×24×96 the nanowire completely transforms into amorphous state during the deformation process beyond the elastic limit. This is the flow deformation of nanowire.

4) When the strain rate is above 1.5% for Ni-24×24×24 and 0.42% for Ni-24×24×96 stress goes to zero. This is the failure deformation of nanowire.

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