ВЛИЯНИЕ ВАКАНСИИ НА ДЕФОРМАЦИЮ И МЕХАНИЧЕСКИЕ НАПРЯЖЕНИЯ СТРУКТУРЫ УЛЬТРАТОНКИХ НИКЕЛЕВЫХ НАНОВОЛОКОН

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EFFECT OF VACANCY ON THE STRUCTURAL DEFORMATION AND MECHANICAL STRENGTH OF ULTRATHIN NICKEL NANOWIRES

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Molecular Dynamics (MD) simulations have been carried out on ultrathin 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 of ultrathin Ni nanowires containing various vacancy defects. We performed MD simulations to study the yield mechanisms in ultrathin Ni nanowires. The coupled effects in various shapes, sizes, and locations of vacancy defects on the mechanical strength and structural deformation of nanowires are presented. The formation energies of Vacancy defects are also evaluated. As the number of vacancies increases, the yield strength decreases. The results showed that breaking time also decreases with increasing number of vacancy.

Analysis

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:

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

Where r_i – radius vectors of i-th atom.

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

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

Mathematical model of the molecular dynamics method [2, 3] describes a system of ordinary differential equations of motion of Newton. The equation of motion in the classical form is represented by:

$$m_i\frac{dx_i}{dt} = F_i\frac{dr_i}{dt} = x_i i = 1,2,..., \quad N \quad (4)$$

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:

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

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 for different number of vacancies at 300 K, which is adjusted every 10^{-13} seconds. The estimated size of the crystal unit was for various experiments of 500 atoms (10 atoms along the edges and 10 atoms in height)

It is assumed that the specimens have some random vacancies within materials in the simulation. The random distribution of vacancies is modeled by: (i) first calculating the number of vacancies according to the given vacancy fraction and the total atomic numbers; (ii) numbering the random vacancies in order; (iii) obtaining the occupation positions of the vacancies; (iv) converting the atoms and the vacancies to their actual positions in simulation. To understand the effects of the vacancies on the mechanical properties of nanowire Nickel, the tensile tests are simulated.

Results and discussion:

In this paper, the mechanical properties of nanoscale Nickel were studied. Since the breaking and the Yielding of Ni nanowires are of main interest in this work (table 1), 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. The nature of deformation, slipping, twinning and necking were studied.

Four stages 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 simulations, 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 10 x 10 x 10 Ni nanowire without vacancies and 7 ps for 10 x 10 x 10 with vacancy equal 200. The sharp fall takes place only at the point of transition from the first to second stages of deformation (figure 2 a and 2 c). Experiments have shown that when the vacancy number increases the first stage of deformation was narrowed, and also the second stage was also narrowed (figure 1).

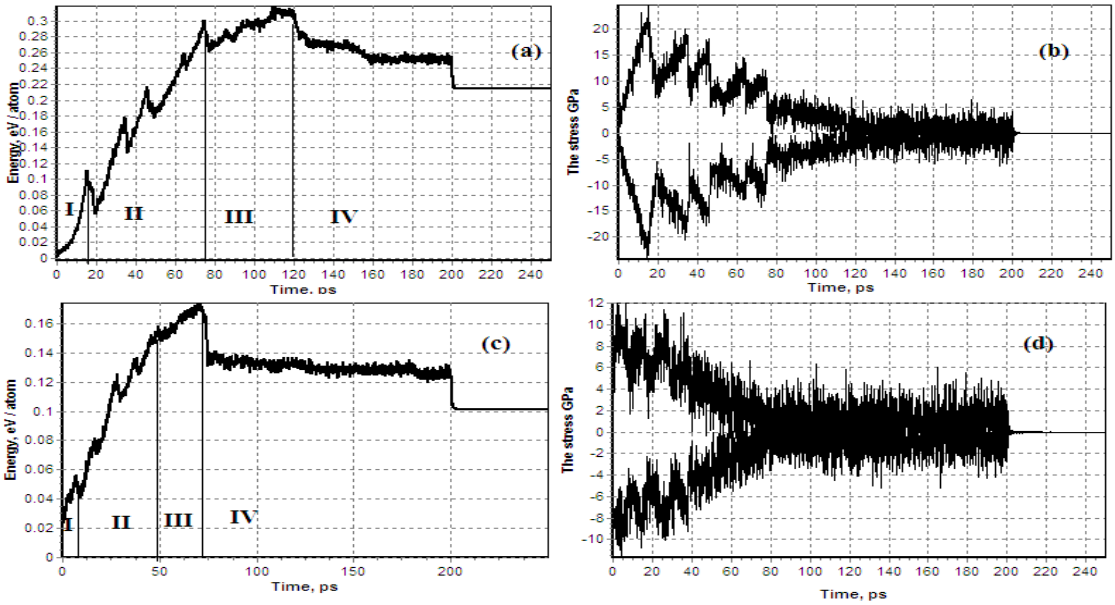

Figure 1 – the dependence of the stored energy of deformation of the experiment at 300 K for nickel-10 x 10x 10 without vacancies (a), the relation of stress with time at temperatures 300 K for nickel-10 x 10 x 10 without vacancies (b), the dependence of the stored energy of deformation of the experiment at 300 K for nickel-10 x 10x 10 with vacancy number =200 (c) and the relation of stress with time at temperatures 300 K for nickel-10 x 10x 10 with vacancy number =200 (d)

Tensile deformation

The mechanical property at different vacancy number With MD simulations are studied (table 1), the uniaxial tension of the nickel nanowires are studied with different vacancy number at 300 K. Figure 2 gives the stress–strain relationships of the 10 x 10 x 10 nanowire subjected to uniaxial tension for different vacancies at temperatures 300 K.

The strain was defined as:
$$\varepsilon = \frac{l - l_0}{l_0} \quad (7)$$
where *l* was the stretching length and l_0 was the length just after relaxation.

The stress in the tensile direction was calculated as:

$$\sigma = \frac{1}{NV_i}\sum_i^N F_i r_i \quad (8)$$

Where V_i refers to volume of atom i.

With the increasing initial strain, stress increases linearly at vacancies. 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 no vacancies, whereas, some ‘‘minipeaks’’ exhibit with increasing vacancy number. The results demonstrate that the tensile strength decreases with increasing vacancy number.

Table 1 – The typical MD results of uniaxial tensile loading with 10 x 10 x 10 ultra-thin Nickel nanowire at vacancy number including the time required to attain atomic break, the number of atoms, initial length, breaking length, yielding time, yielding stress and the calculated final breaking position

	Number of vacances V	l_0	breakdown			Yielding point		
			t,Ps	$l_{b,\ nm}$	position	σ(Gpa)	t,ps	$l_{z1.nm}$
1	0.0	4.6	120	11	5.5	24	15	5.3
2	50	4.6	95	9.5	4.7	23	13	5.2
3	100	4.6	93	9.8	4.8	20	12	5.1
4	150	4.6	75	8.4	4.4	16	7	4.9
5	200	4.6	72	8.5	4.5	11	4	4.7
6	300	4.6	40	6.8	3.8	9	3	4.65
7	400	4.6	2	4.7	2.1	2	2	4.7

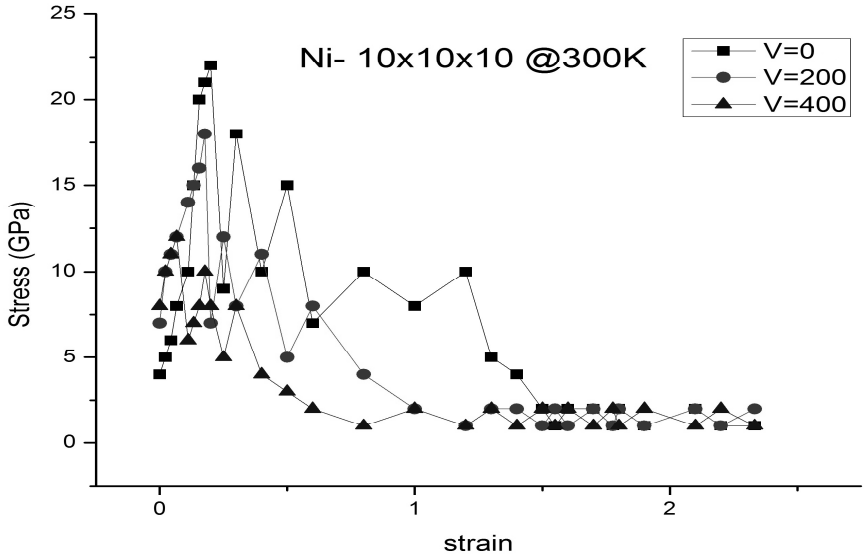

Figure 2 – Relationship between tensile stress with tensile strain for Ni nanowires at different vacancies at T=300 K

Deformation of the nanowire is in a fast stage of the atomic damage process. It is observed that the first yield stress decreases as the vacancy number increases (figure 3). When the plastic deformation of the nanowire begins, the drop of the first yield stress also decreases. In this work, MD simulations are performed for ultrathin Ni nanowire subject to uniaxial tensile strain loading. Figure 3 shows the simulated ultimate strength of ultrathin Ni nanowires as a function of vacancy number. As expected, the nanowire strength decreases with increase of vacancy number. The average result is from 300 samples at 300 K.

Breaking position

The results showed that the breaking position depended on the vacancy number figure 4. The most probable breaking position was located at the center of the nanowires as in table 1. Figure 4 presents the calculated breaking position for ultrathin Ni nanowires as a function of vacancy number.

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. Figure 5 presents the representative snapshots of 10 x 10 x 10 Ni nanowires with different vacancies at the breaking moment. In most cases, the final breaking position occurs at the central part of this nanowire.

Conclusions

The tensile and fatigue behavior of Ni nanowire with vacancies at 300K has been studied by means of molecular-dynamics simulation. The stress–strain curve for Ni nanowire was obtained. It can be seen from the curve that the tensile stress decreases with increasing vacancy fraction of the material and the maximum stress occurs at about V=0. The Ni nanowire shows very high ultimate tensile stress and elongation rate. Increasing vacancy fraction was also found to decrease the stress. It was observed that the Ni nanowire has a higher fatigue limit when the vacancy fraction is lower, and when the value of applied stress is less-than-critical.

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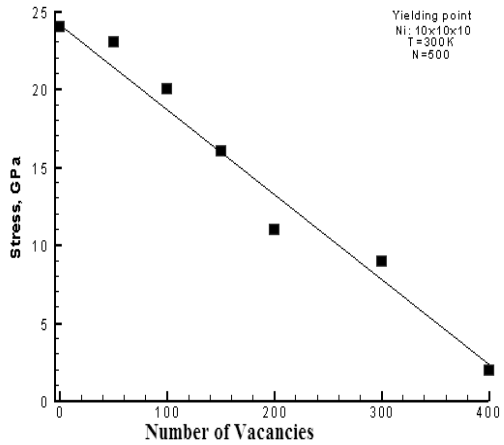

Figure 3 – Relationship between tensile stress for Ni nanowires with various vacancies at T=300 K

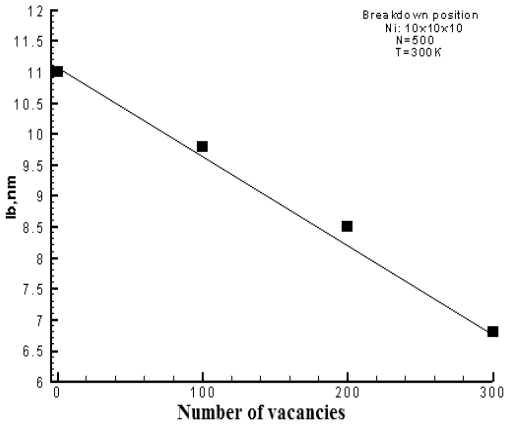

Figure 4 – Relationship between breaking position for Ni nanowires with various vacancies at T=300 K

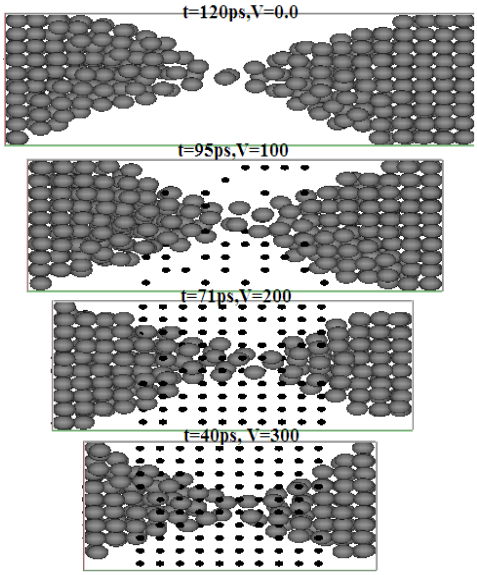

Figure 5 – Snapshots of 10 x 10 x 10 Ni nanowires with different vacancies and the breaking moment at 300 K