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Investigation of the effect of hydrogen on the properties of fcc nanowires

M D Starostenkov, O V Yashin, A V Yashin

Altai State Technical University, Lenin Str. 46, 656038 Barnaul, Russia

E-mail: frs22@mail.ru

Abstract. In the present work, the features of the processes of structure-energy transformations observed during deformation of fcc Ni nanowires containing hydrogen atoms in octahedral and tetrahedral pores are studied. As a result of the investigation at temperatures of 50, 100, 300, 600, 900 and 1200 K, the effect of the concentration of hydrogen atoms on the strength characteristics of fcc Ni nanowires having a cylindrical shape was revealed.

1. Introduction

The scenario of the strain-induced structure-energy transformations of fcc Ni nanowires containing hydrogen atoms was studied by means of the molecular dynamics method. The axis of the tensile direction corresponded to the <100> direction. Ni nanowires had a cylindrical shape (figure 1a). The interaction of atoms was calculated using the Morse pair potential, adopted from [1], approved in [2].

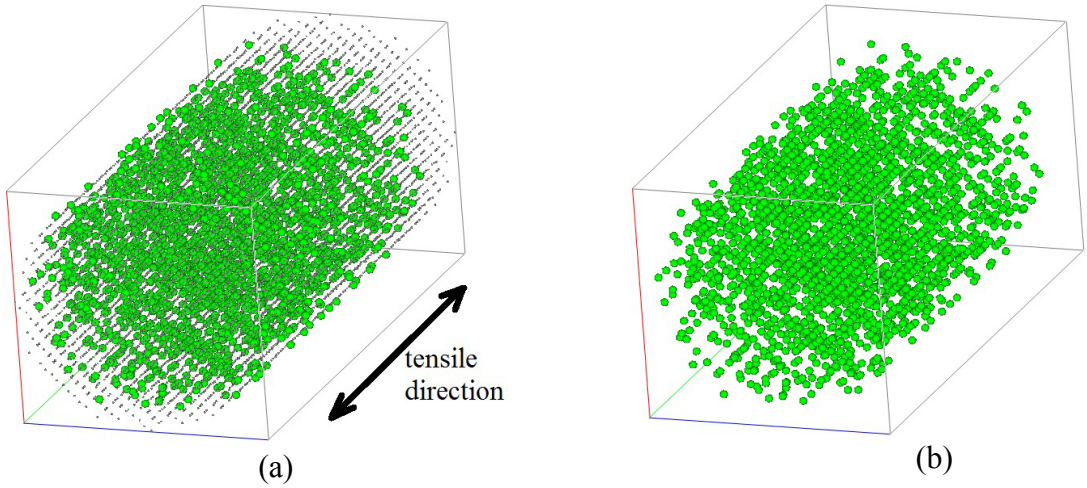

Figure 1. Cylindrical <100> oriented Ni nanowires with 40% of pores filled with hydrogen. (a) atomic structure of the wire before the deformation begins (small dots stand for Ni, large ones for H), (b) hydrogen sub-lattice

Hydrogen atoms of were placed in octahedral and tetrahedral pores of the wire (figure 1b). In the present work 0, 20, 40, 60 and 80% of the pores of the nanowires were filled with hydrogen, one

hydrogen atom in each pore. The ratio of the number of hydrogen atoms in the octahedral and tetrahedral pores of the nanowires corresponded to the ratio of the total volume of the octahedron and tetrahedral pores in the unit cell.

A periodically repeated translational displacement of the atoms constituting absolutely rigid grips along the axis of stretching of the nanowires in opposite directions from each other was performed to simulate the straining of the nanowires. The total velocity of the gripper movement was 20 m / s and corresponded to the strain rate of the order of $\cdot 10^9$ s^{-1}. The numerical experiment was performed at temperatures of 50 K, 300 K, 600 K, 900 K and 1200 K. At the beginning of the computer experiment, the temperature was set through the initial velocities of the atoms. During deformation, thermal stabilization was performed in accordance with the Berendsen algorithm [3]. The described model of the experiment was approved earlier in studies of the deformation dynamics of nanowires of such alloys as CuAu [4], Ni_3Al [5,6] and Ni_3Fe [7].

2. Results and discussion

As a result of the study of structure-energy transformations of fcc Ni with 0, 20, 40, 60, and 80% of pores filled with hydrogen, four basic stages of deformation were revealed: quasi-elastic (I), plastic (II), flows (III) and fracture (IV). The deformation stages are clearly seen on the graphs of the dependence of the stored deformation energy on the experiment time (figure 2).

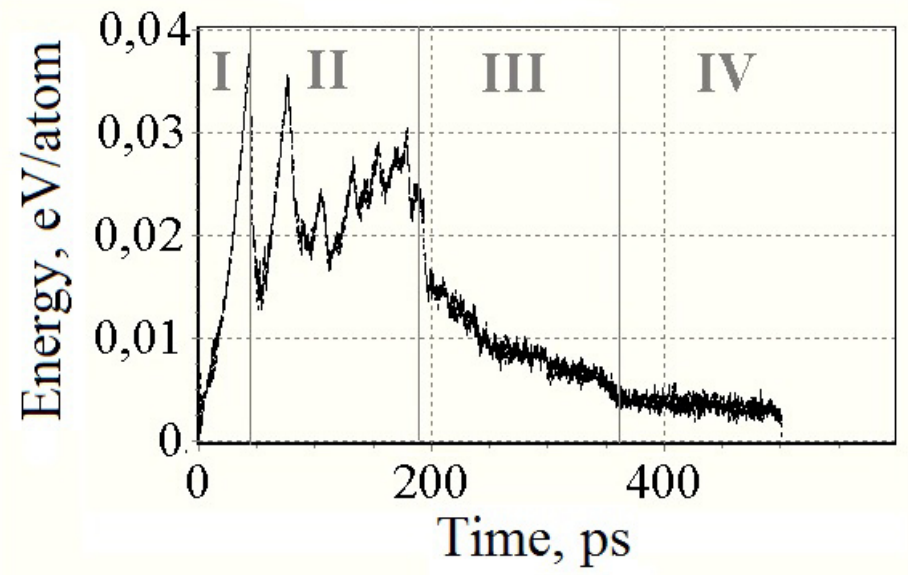

Figure 2. Dependence of stored energy of deformation per 1 atom on the experiment time, obtained at T=300 K for nanowires <100> Ni with 40% of pores filled with hydrogen

At the same time, the behavior of this graph is reflected in the graph of the dependence "stress on the grips / time of the experiment", where the deformation stages can be indicated as well (figure 3). At high temperatures (900 and 1200 K) for <100> Ni nanowires with a large proportion of hydrogen filled pores (more than 40%), it was impossible to distinguish the deformation stages due to the fact that the material acquired an amorphous state.

In the course of the study, the points of maximum stress on the grips, which were reached at the end of the first stage (figure 3), were of the greatest interest

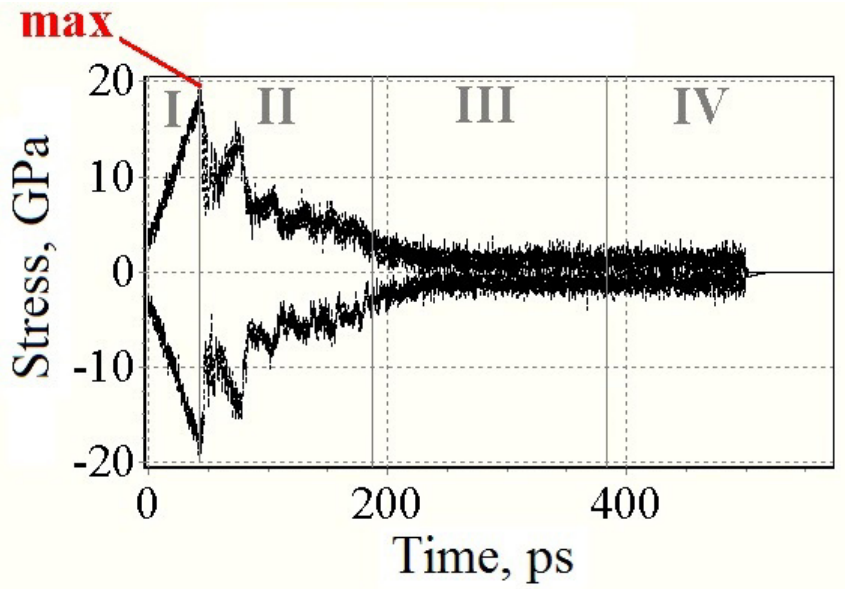

Figure 3. Dependence "stress on the grips / the experiment time", obtained at T=300 K for nanowires <100> Ni with 40% of pores filled with hydrogen. The stress applied to the left grip is indicated as negative for better display on the graph.

The next graph was build using the obtained values of the maximum stress on the grips for nanowires of cylindrical shape <100> Ni at different temperatures. The dependence shows the change in the value of the maximum stress on the grips from the temperature for nanowires with 0, 20, 40, 60 and 80% of pores filled with hydrogen.

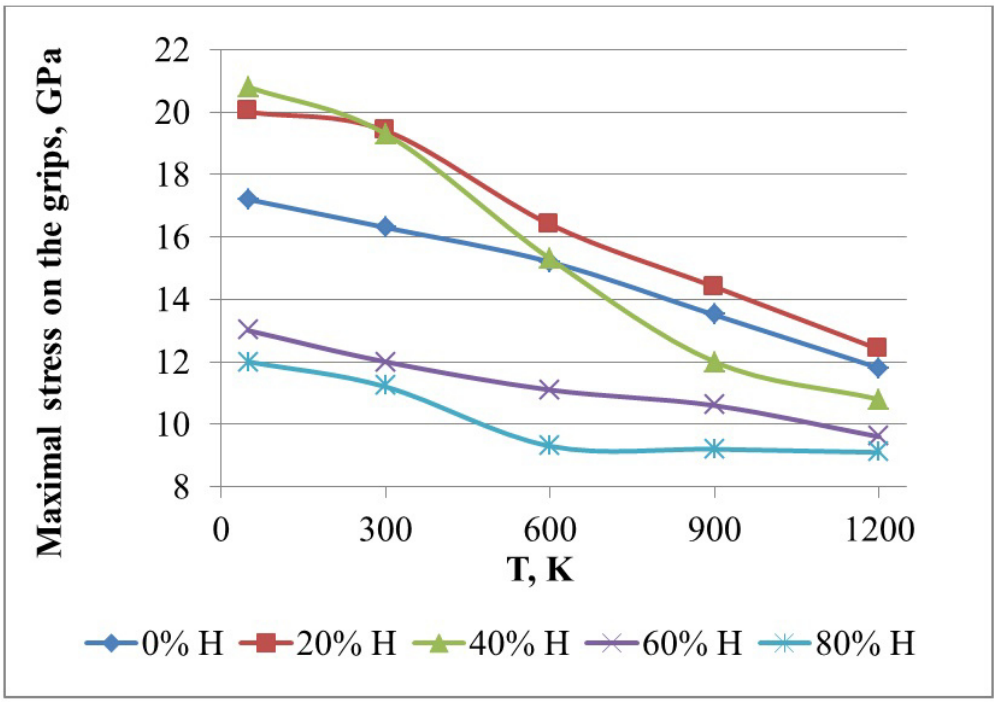

Figure 4. Dependence of maximal stress value on the grips at different temperatures in nanowires with 0, 20, 40, 60 and 80% of pores filled with hydrogen

The obtained results show that when hydrogen filled up to 20% of the pores, the strength of nanowires at different temperatures is higher than in nanowires without hydrogen. At the same time the filling of more than 40% of pores with hydrogen results in the degradation of the strength properties of nanowires. This fact is associated with the formation of clusters of hydrogen atoms in the form of globules at the stage of plastic deformation. The obtained results are in accordance with the data presented in [9-14].

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