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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.