Effect of the Length on the Tensile Deformation of Nickel Nanowires Using Molecular Dynamics Simulations

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In the recent years, with the fast advancement in the fields associated with nanoscience and nanotechnology, metal nanowires, in specific have received enormous attention among researchers due to their fascinating properties and applications. In this study, the Young Modulus and failure behavior of Nickel (Ni) nanowires 7.04 nm in diameter with eight (8) different lengths (17.60, 21.12, 24.64, 28.16, 31.68, 35.20, 52.80 and 70.40 nm) were successfully modeled for uniaxial tensile tests using Molecular Dynamic (MD) simulations. MD simulations were performed at a fixed point of the temperature of 300 K and a constant strain rate of 0.0001 ps^{-1}. The finding showed that these Ni nanowires have a Young Modulus between 140.02 to 142.5 GPa. We strongly believe that the variation of the length model has no significant influence on neither the Young Modulus nor the failure behavior. All the investigated nanowires demonstrated ductile failure behavior type, in which represents a typical behavior of Ni at bulk scales.

Keywords: Young Modulus, mechanical behavior, nickel nanowire, uniaxial testing, molecular dynamics