Abstract No: 06

Prediction of Mechanical Properties of Steel Nanowires using Molecular Dynamics

Nadeesha Tharundi M. D.[1], Liyanage J. K.[2], Laalitha S. I. Liyanage[*]

1. Department of Applied Computing, Faculty of Computing and Technology, University of Kelaniya, Sri Lanka

**Corresponding author: laalitha@kln.ac.lk*

ABSTRACT

Nanowires have received increasing interest due to their unique properties and potential applications [1]. Limited studies have been conducted on tensile strength and mechanical properties of pure iron and iron alloy-based nanowires using simulations. In this study, the dependence of the mechanical properties of steel nanowires with different carbon percentages at varying temperatures is investigated. Atomic interactions between Fe and C atoms are modelled using interatomic force fields for molecular dynamics (MD) simulations. Four interatomic potentials were evaluated [2][3][4][5][6] using their bulk properties. Modified embedded atom method (MEAM) potential by Liyanage et al. was selected due to its accuracy in predicting properties of BCC Fe, Fe-C in B1 rock salt structure, and properties of BCC iron structure with varying C percentages.

Uniaxial tensile test simulations at varying C atom percentages and different temperatures are conducted using MD simulations with the LAMMPS package. The amount of C was varied from 0 – 10 % at temperatures ranging from 0.1 K – 900 K. Mechanical properties of steel nanowires were extracted from the stress-strain curves generated by the tensile simulations. Young's modulus of the steel nanowires increased in the temperature range of 0.1 K – 300 K while decreased in the range of 600 K - 900 K with respect to the C %. Yield stress and Ultimate Tensile Stress gradually decreased with the increase of C atoms from 0 – 10 %. Predicted results were compared with the results of bulk steel experimental values [7]. The micro-structural changes in the nanowires were analysed with common neighbor analysis (CNA). CNA showed the rapid formation of slip planes with increasing C% and increased propagation of slip planes contributes to the reduction in the strength of the nanowires.

Keywords: *Nanowires, Uniaxial tensile test*

REFERENCE

[1] L. Li and M. Han, "Molecular dynamics simulations on tensile behaviors of single-crystal bcc Fe nanowire: effects of strain rates and thermal environment," *Appl. Phys. A Mater. Sci. Process.*, vol. 123, no. 6, Jun. 2017, doi: 10.1007/s00339-017-1062-7.

[2] L. S. I. Liyanage *et al.*, "Structural, elastic, and thermal properties of cementite (Fe<inf>3</inf> C) calculated using a modified embedded atom method," *Phys. Rev. B - Condens. Matter Mater. Phys.*, vol. 89, no. 9, 2014, doi: 10.1103/PhysRevB.89.094102.

[3] K. O. E. Henriksson, C. Björkas, and K. Nordlund, "Atomistic simulations of stainless steels: A many-body potential for the Fe-Cr-C system," *J. Phys. Condens. Matter*, vol. 25, no. 44, Nov. 2013, doi: 10.1088/0953-8984/25/44/445401.

[4] D. J. Hepburn and G. J. Ackland, "Metallic-covalent interatomic potential for carbon in iron," *Phys. Rev. B - Condens. Matter Mater. Phys.*, vol. 78, no. 16, pp. 1–6, 2008, doi: 10.1103/PhysRevB.78.165115.

[5] W. Xu and W. K. Kim, "Molecular dynamics simulation of the uniaxial tensile test of silicon nanowires using the MEAM potential," Mech. Mater., vol. 137, no. May, p.103140, 2019, doi: 10.1016/j.mechmat.2019.103140.

[6] B. J. Lee, "A modified embedded-atom method interatomic potential for the Fe-C system," *Acta Mater.*, vol. 54, no. 3, pp. 701–711, 2006, doi: 10.1016/j.actamat.2005.09.034.

[7] B. L. Bramfitt, "Structure/Property Relationships in Irons and Steels," 1998, Accessed:Aug. 04, 2021. [Online]. Available: www.asminternational.org.