**Mechanical properties of Fe nanowires under uniaxial tests: a Molecular dynamic study**

Sajad Mousavi Nejad Souq1, Faramarz Ashenai Ghasemi1, Mir Masoud Seyyed Fakhrabadi2\*

1- Faculty of Mechanical Engineering, Shahid Rajaee Teacher Training University, Tehran, Iran

2- School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran, Iran

\* [mfakhrabadi@ut.ac.ir](mailto:mfakhrabadi@ut.ac.ir)

Abstract

The present study aimed to evaluate the mechanical properties of BCC Fe nanowires, including their elastic moduli, ultimate strengths, stress-strain diagrams, and structural evolutions from BCC to FCC and HCP under external loading. For this purpose, the effects of temperature and various shapes of cross-sections (with the same area) on the mechanical properties of Fe nanowires are evaluated using molecular dynamics simulation. The well-known embedded atom method potential function is employed in Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to model the metallic bonds between the Fe atoms. The Young's moduli are calculated based on the initial linear section of the stress-strain diagrams of uniaxial tension and compression of the nanowires. The comparison between the tensile and compressive results reveals that the strength values in compressive loading depend on the shapes of the cross-sections more than tensile loading following the order: circular> polygon> square> triangle. However, except for the triangular case, tensile strength values are less susceptible to the change of the cross-section shapes. On the other hand, for both loading states, increasing temperature results in reducing Young's moduli and ultimate strength values.

Keywords

Nanowire, BCC, Molecular Dynamics, Tension, Compression

1. **Introduction**

Iron is the most abundant metal in the universe and can be found in large quantities in liquid and solid forms in planetary cores, such as in the earth's case. Iron is frequently used in industry in various shapes such as beams, plates, shells, etc. Because of nanowires' unique properties to be used in nano and micro-electromechanical systems (respectively, NEMS and MEMS), many scientific investigations focused on their various properties [1, 2, 3, 4, 5, 6]. Among all, the examination of the mechanical behavior of nanowires is more critical for developing future technological applications [7]. The mechanical properties of metallic nanowires are different compared to the bulk counterparts [8, 9]. For example, many experiments and computer simulations clearly showed that elastic properties depend on the strain rate, temperature, and nanowire size [10, 11].

A study on the deformation behavior of Au nanowires subjected to uniaxial tension at high strain-rate under different temperatures showed that the magnitudes of Young's modulus and the maximum strength tend to decrease as the temperature increases [12]. Temperature and strain-rate effects on mechanical properties of Pt nanowires revealed that their Young's modulus is about 50% to 75% of its bulk counterpart, while according to Liang and Zhou [13], their Poisson’s ratio does not significantly change at the nano-scale. Greer and Kim studied the effect of temperature and geometric parameters (diameter, length) on the elastic properties of tungsten (W) nanowires and necking before the final fracture was successfully captured through molecular dynamics (MD) simulation [14]. Li and Han also studied the mechanical properties of polycrystalline W nanowire to analyze the impact of grain size, diameter, and temperature on the elastic properties [15]. In another study, the beat phenomenon in [110] oriented Ag nanowires was reported by using MD simulations [16].

In the present study, we investigate the effects of various cross-sectional shapes (with the constant area) and temperature on mechanical properties of a Fe nanowire with BCC structure using MD simulations through the embedded atom method (EAM) potential. In particular, the effects of the uniaxial loading modes (tension or compression), cross-section shapes (circular, square, polygon, and triangle), and temperature (0.1 - 600 K) are explored.

1. **Molecular Dynamics simulation**

In the present study, the molecular dynamics simulation of LAMMPS [17] software has been applied to study the deformation of single-crystal Fe nanowires. The temperature of the simulations is selected in the range of 0.1 to 600 K. A fixed lateral surface (8.55 nm2) and the length equal to 17.2 nm in four different shapes (triangle, square, polygon, and circle) are investigated to study the effects of the lateral surface (See Fig. 1.). The simulation box is assumed periodic in the z-direction, and for other directions, the faces are free of traction.

|  |
| --- |
|  |

**Fig. 1.** Cross-sectional shapes used in the MD simulations. L1 = 4.43 nm, L2 = 2.92 nm, L3=3.52nm and D = 3.38 nm.

All models were relaxed for 50 ps before loading under the NPT ensemble to remove residual stresses. Therefore, atoms' positions were updated with a step time equaling to 0.5 fs using the Velocity Verlet algorithm. A constant strain rate of 1.25 × 10−9 1/s in the z-direction was applied to the system for tension/compression during the simulations, which agrees with other works [18, 19]. The ultimate strain values of 0.20 and 0.25 were selected for the state of uniaxial tension and compression, respectively. Adaptive Common neighbor analysis (a-CNA) has been employed for the local segmentation of structures [20]. The embedded atom method (EAM) potential [21] has been proved to accurately capture the many-body atomic interactions in metallic systems. Hence, it was widely used to simulate the deformation behavior under various loading conditions [13, 18, 22]. Therefore, the interatomic forces in simulation systems were calculated using EAM potential. The BCC structures with a lattice constant of 2.86 Å [23 ] were studied.

1. **result and discussion**

The tensile test was conducted by displacing the atomic position uniformly with a constant strain rate in the z-direction. The system was equilibrated under the NPT ensemble for 50 ps before loading. Fig. 2 demonstrates the stress-strain diagram of the Fe nanowire with the lateral square surface at 0.1 K. As shown in Fig. 2, the strain stress diagram is completely consistent with Lee and Han simulations[15].

In this diagram, a couple of main peaks (points B and E) with an almost smooth area between them can be observed. We applied Ackland-Jones bond-angle method to observe the variations in the crystallographic structure types throughout the tensile test (Table 1).

|  |
| --- |
|  |

**Fig. 2.** Stress-Strain diagram of the lateral square area at 0.1 K.

**Table 1**. Structure type from Ackland-Jones bond-angle method during the tensile test.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | Structure Type (%) | | | |
|  | BCC | FCC | HCP | Other |
| A | 81.9 | 0.0 | 0.0 | 18.1 |
| B | 0.0 | 65.6 | 0.0 | 34.4 |
| C | 65.9 | 4.6 | 0.0 | 28.6 |
| D | 62.8 | 11.6 | 0.9 | 24.9 |
| E | 62.8 | 12.9 | 0.7 | 23.7 |

According to Ackland-Jones bond-angle analysis, the percentage of BCC structure was initially at its highest level, equalling 81.9%. The rest, 18.1%, was in other types of structures (mainly on the boundaries). This percentage of BCC structure remains approximately constant until the strain of 0.11 (point B). However, at point B, an increase in the percentage of atoms in FCC and HCP structures is observed, revealing a sudden transition from BCC to FCC and HCP structures. According to Fig.2, at this point, softening in the stress-strain diagram is seen, and the stress level is very close to a sudden decrease from about 15.5 GPa to about 3 GPa due to the start of the slip process of atomic layers on each other. We computed the percentage of BCC structure in point C at 65.9%, which was less than the initial BCC structure percentage. Between points D and E, the diagram shows a behavior similar to point A to B. In this part, the structural evolution from FCC to HCP and other structural types occurs (Table 1), but in the first section (between points A and B ) the structural evolution occurs from BCC to FCC, HCP, and others. So in the latest case, the percentage of BCC structure is at a constant value of 62.8%.

Fig. 3 demonstrates the stress-strain diagrams of the Fe nanowire for various lateral areas at 0.1 K. As seen in this figure, the charts of the square and polygon cross-sections are very similar to each other. For the lateral circular area, the diagram is considerably similar to the square cross-section's behavior up to a strain of 0.55. However, its action is different after this point. Also, despite the lower ultimate strength, the lateral triangular surface diagram is similar to the other cross-sections up to the strain of 0.3. Due to the triangular shape of the lateral area causing higher stress intensity, the movement of the dislocations during the fracture started from the edges, and the failure of the structure happened earlier than the other geometries.

|  |
| --- |
|  |

**Fig. 3**. Tensile stress-strain diagrams of the nanowires with different cross-sections at 0.1 K.

Fig. 4. shows the stress-strain diagrams of the Fe nanowires with various cross-sections. According to this figure, the elastic behavior of nanowires is identical for all analyzed cross-sections, and the only difference is in their ultimate stress/strain values. Fig. 4 reveals that the nanowires with the triangular, square, polygon, and circular lateral surfaces reach their ultimate values in the strains of 0.16, 0.16, 0.21, and 0.226, respectively. These results can be related to the cross-section symmetry. As the numbers of lines and planes of symmetry increases, the fracture strain and stress, and consequently, the strain energy, are also increased.

|  |
| --- |
|  |

**Fig. 4**. Stress-strain diagrams of the Fe nanowires with different lateral surfaces under compressive loading at 0.1 K.

In this section, a single-crystal BCC Fe nanowire behavior under tension/compression in various temperatures is investigated. Fig. 5 represents the tensile stress-strain diagrams in 150-600 K and the variations of their corresponding Young’s moduli in 0.1-600 K. According to Fig. 5(a), increasing temperature decreases the ultimate strength/strain values, uniformly. Also, as the temperature gradually increases (150-450 K), the tensile stress-strain diagrams of different cross-sections become closer and more similar. However, by increasing the temperature more, the ultimate strain values move away from each other, and the similarities decrease. The diagrams at low temperatures (here, 150 K) show a hardening-type behavior vs. strain. In comparison, at higher temperatures (450-600 K), this behavior first becomes flattened and subsequently changes to the softening type. Moreover, based on Fig. 5(b), increasing temperature, similar to the strength values, decreases Young’s moduli of all cross-sections, uniformly.

|  |
| --- |
|  |
| a |
|  |
| b |

**Fig. 5**. a. Stress-strain diagrams of the different lateral surfaces at 150-450 K for tensile loading, b. Effects of temperature on tensile Young’s moduli

On the other hand, Fig. 6 demonstrates the compressive stress-strain diagrams and Young's moduli of different cross-sections in 150-600 K. As seen in Fig. 6(a), with increasing temperature, the ultimate strength/strain values decrease. This decrease results in the reduction of the diagrams non-linearity so that their hardening parts disappear at high temperatures. Unlike tensile loading, which did not have a particular sequence for the strength values of different cross-sections, in the compressive loading, the ultimate strengths in all temperatures have a series as circle *>*polygon *>*square *>*triangle. Moreover, the variation of ultimate strengths of all lateral surfaces is the same as the variation in their corresponding strain values.

|  |
| --- |
|  |
| a |
|  |
| b |

**Fig. 6** . **a**. Stress-strain diagrams of different lateral surfaces at 150-600 K for compressive loading, **b**. Effects of temperature on compressive Young’s moduli.

Unlike Fig. 5(b), the compressive elastic moduli of various lateral cross-sections do not change considerably and uniformly versus the temperature increase. Hence, with increasing the temperature, they can be considered almost constant (Fig. 6(b)), and their average values for different cross-sections are square: 101.39±1.16, circle: 101.15±1.65, triangle: 97.41±1.43, and pentagon: 101.34±1.17 GPa. Although the variations of compressive elastic moduli with increasing the temperature are not significant, it can be seen that, on the contrary to their tensile counterparts, the lowest elastic moduli of all cross-sections, in the studied range of temperatures, are at 0.1 K.

Fig. 7 represents the behavior of ultimate strengths vs. the changes in the temperature. According to this figure, as the temperature increases, the corresponding stress and strain decrease, consistent with other materials [15]. In the compressive loading case, with increasing the temperature, the ultimate strengths approach to constant values, but they still tend to decrease more in the tensile loading state.

|  |
| --- |
|  |

**Fig. 7.** Ultimate strengths of the different lateral surfaces in the tensile/compressive loading.

1. **conclusion**

In the present study, the mechanical behavior of Fe nanowires with a BCC structure was investigated using the MD method based on EAM potential function. The effects of various cross-sections, i. e., circle, square, polygon, and triangle, and the impact of temperature on the elastic moduli and ultimate strength values, were scrutinized. The following observations and results were obtained:

The ultimate strength values depend on the cross-sectional shape as circle> polygon> square> triangle in compressive loading. However, such a correlation could not be observed in tensile loading.

Increasing temperature generally decreases both of Young’s moduli and ultimate strengths of Fe nanowires with all cross-sections.

1. **References**

[1] F. Sedona *et al.*, “Substrate involvement in dioxygen bond dissociation catalysed by iron phthalocyanine supported on Ag (100),” *Chem. Commun.*, vol. 54, no. 68, pp. 9418–9421, 2018.

[2] F. Sedona *et al.*, “Tuning the catalytic activity of Ag (110)-supported Fe phthalocyanine in the oxygen reduction reaction,” *Nat. Mater.*, vol. 11, no. 11, pp. 970–977, 2012.

[3] D. Dragoni, D. Ceresoli, and N. Marzari, “Vibrational and thermoelastic properties of bcc iron from selected EAM potentials,” *Comput. Mater. Sci.*, vol. 152, pp. 99–106, 2018.

[4] H. W. C. Postma, I. Kozinsky, A. Husain, and M. L. Roukes, “Dynamic range of nanotube-and nanowire-based electromechanical systems,” *Appl. Phys. Lett.*, vol. 86, no. 22, p. 223105, 2005.

[5] P. Yang, “The chemistry and physics of semiconductor nanowires,” *MRS Bull.*, vol. 30, no. 2, pp. 85–91, 2005.

[6] Y. Zhang, S. Rohani, and A. K. Ray, “Numerical determination of competitive adsorption isotherm of mandelic acid enantiomers on cellulose-based chiral stationary phase,” *J. Chromatogr. A*, vol. 1202, no. 1, pp. 34–39, 2008.

[7] S. Suresh and J. Li, “Materials science: Deformation of the ultra-strong,” *Nature*, vol. 456, no. 7223, p. 716, 2008.

[8] W. F. McDonough and S.-S. Sun, “The composition of the Earth,” *Chem. Geol.*, vol. 120, no. 3–4, pp. 223–253, 1995.

[9] C. M. Lieber, “Nanoscale science and technology: building a big future from small things,” *MRS Bull.*, vol. 28, no. 7, pp. 486–491, 2003.

[10] H. Liu and J. Zhou, “Plasticity in nanotwinned polycrystalline Ni nanowires under uniaxial compression,” *Mater. Lett.*, vol. 163, pp. 179–182, 2016.

[11] H. A. Wu, “Molecular dynamics study on mechanics of metal nanowire,” *Mech. Res. Commun.*, vol. 33, no. 1, pp. 9–16, 2006.

[12] S. Xu, Y. Su, D. Chen, and L. Li, “An atomistic study of the deformation behavior of tungsten nanowires,” *Appl. Phys. A*, vol. 123, no. 12, p. 788, 2017.

[13] W. Liang, M. Zhou, and F. Ke, “Shape memory effect in Cu nanowires,” *Nano Lett.*, vol. 5, no. 10, pp. 2039–2043, 2005.

[14] J. R. Greer, J.-Y. Kim, and M. J. Burek, “The in-situ mechanical testing of nanoscale single-crystalline nanopillars,” *Jom*, vol. 61, no. 12, p. 19, 2009.

[15] 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.*, 2017, doi: 10.1007/s00339-017-1062-7.

[16] A. Cao, “Shape memory effects and pseudoelasticity in bcc metallic nanowires,” *J. Appl. Phys.*, vol. 108, no. 11, p. 113531, 2010.

[17] S. Plimpton, “Fast parallel algorithms for short-range molecular dynamics,” *J. Comput. Phys*., vol. 117, no. 1, pp. 1–19, 1995.

[18] G. Sainath and B. K. Choudhary, “Deformation behaviour of body centered cubic iron nanopillars containing coherent twin boundaries,” *Philos. Mag.*, vol. 96, no. 32–34, pp. 3502–3523, 2016.

[19] S. Li, X. Ding, J. Li, X. Ren, J. Sun, and E. Ma, “High-efficiency mechanical energy storage and retrieval using interfaces in nanowires,” *Nano Lett.*, vol. 10, no. 5, pp. 1774–1779, 2010.

[20] H. Zhan, Y. Gu, and H. S. Park, “Beat phenomena in metal nanowires, and their implications for resonance-based elastic property measurements,” *Nanoscale*, vol. 4, no. 21, pp. 6779–6785, 2012.

[21] Y. Gao and H. M. Urbassek, “Evolution of plasticity in nanometric cutting of Fe single crystals,” *Appl. Surf. Sci.*, vol. 317, pp. 6–10, 2014.

[22] S. Plimpton, “Fast parallel algorithms for short-range molecular dynamics,” *J. Comput. Phys.*, vol. 117, no. 1, pp. 1–19, 1995.

[23] M. S. Daw, S. M. Foiles, and M. I. Baskes, “The embedded-atom method: a review of theory and applications,” *Mater. Sci. Reports*, vol. 9, no. 7–8, pp. 251–310, 1993.