Mechanical properties of irradiated metal nanowires

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Summary Recently, ion beam is proposed to be a powerful way to modify the properties of nanowires. We study the mechanical properties of copper nanowires irradiated with swift heavy ions by molecular dynamics simulations. The Cu nanowires are irradiated with Cu ions with energies ranging from 0.2 to 8.0 keV, and both the elastic properties and yields under compressive and tensile loading are simulated. The results show that two kinds of defects, namely point defects and stacking faults, appear in the irradiated nanowire depending on the incident ion energy. The Young modulus is significantly reduced by the ion irradiation, and the reduction magnitude depends on the vacancy number. Moreover, the irradiated nanowires yield at a smaller strain, compared with the pristine nanowire. The reduced Young modulus and the small yield strain result in a significant drop in yield stress of the irradiated nanowires.

Introduction

Metallic nanowires have attracted considerable attention in the last decade because of their special physical properties and potential applications in future nanoelectromechanical systems (NEMS) [1-3]. For example, they have found applications in the next-generation electronics, opto-electronics, superconducting devices and sensor system [4]; they also can be used as contact tip of atomic force microscope (AFM) and scanning tunneling microscope (STM) [5]. To realize all these applications, it is important to understand mechanical properties of the nanowires, which directly affect their functionalities.

Ion beam irradiation has been found helpful for growth of metallic nanowires, and their size and shape can be controlled by irradiation conditions [6,7]. Besides, irradiation has also been used to tailor the mechanical, electronic and magnetic properties of nanowires [8], while not much work explore its effect on metallic nanowires. Therefore, in this work, we carry out molecular dynamics (MD) simulation to study the mechanical property of irradiated nanowires under tension and compression. During irradiation process, the [001]-oriented Cu nanowires are irradiated by four different incident energies, which generate different numbers of defects on the surface and in the interior. We find irradiation decreases both Young's modulus and yield stress, and the induced surface defects serve as dislocation source.

Simulation details

We consider the [001]-oriented nanowires, which are cut from bulk fcc Cu. The aspect ratio of 5 is selected since the wire tends to buckle under compression with larger ratio value. Fig. 1 shows the atomic pictures of the nanowire under study, with the size of $2.89\times2.89\times14.46$ nm^3. Free boundary conditions are used in all three dimensions to simulate the free-standing nanowire, and the embedded-atom-method (EAM) potential developed for Cu by Mishin et al. [9] is chosen to describe the atomic interactions.

The freshly cut nanowires are first relaxed at 0 K using the conjugate gradient method. Due to the tensile surface stress, the relaxed nanowires are under the compressive state. Then the wires are equilibrated at 300 K with both ends of the wire fixed. Each fixed end contains four atomic layers. The strain load is applied by displacing the fixed top atoms repeatedly and the displacement of the fixed top atoms is chosen to make sure the strain increment is 0.2%. After each loading step, the wire is fully relaxed at 300 K for 400 ps, with both ends fixed. The mean stress over the last 100 ps of the relaxation period is taken as the stress of the nanowire. The stresses are calculated using the Virial theorem, which is equivalent to the Cauchy stress in the continuum theory [10].

In the irradiation simulation, three Cu ions irradiate the nanowire one by one at an angle of 15°to the normal direction of <010> plane (Fig. 1a), the angle is to avoid the ion channelling effect. Ten incident energies, ranging from 0.2 keV to 5 keV, are used. NVE ensemble is firstly used during the collision, after the ions stop in the nanowire or penetrate the nanowire, the nanowire is relaxed at 300 K under NVT ensemble until equilibrium is achieved. The interactions between the incident ions and the nanowire atoms are described with a combined EAM/ZBL potential, in which the Ziegler−Biersack−Littmark (ZBL) potential [10] is joined with the EAM potential, when inter-atomic distance is shorter than 0.05 nm.

Defect in nanowires with irradiation

The nanowire is irradiated by ions with four different energies: 200, 500, 1000, and 5000 eV, and in Fig. 1b) we show the defects induced by irradiation. We can see for small incident energy, defects locate near the incident plane.

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With higher incident energy, defects are generated in deeper layers. The biggest incident energy generates the largest number of defects in the nanowire.

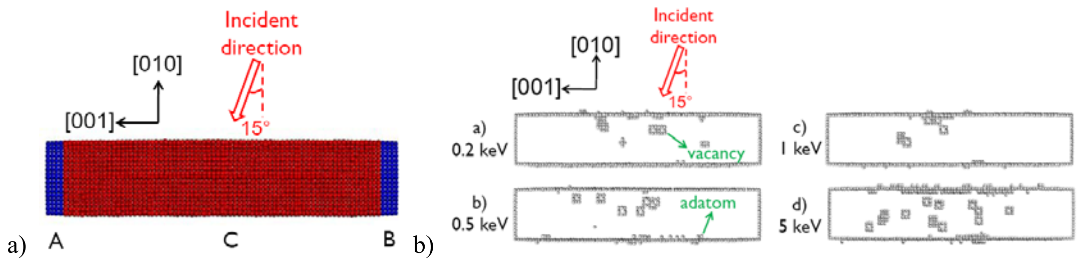

FIG. 1. a) Atomic pictures of the [010]-oriented Cu nanowire equilibrated at 300 K. Red arrow denotes the incident direction of the ions in the irradiation simulation. Blue atoms denote the fixed atomic layers at both ends. b) Defects distribution in the nanowire after irradiation, incident energies are given in front of each figure. Surface atoms (the outermost two atomic layers) and perfect fcc atoms are removed to visualize the defects. Red arrow on top of the figure denotes the incident direction.

Mechanical property of nanowires with and without irradiation

Fig.2 shows the stress-strain curve (before yield) of the irradiated wires, comparing with the unirradiated one. We find the mechanical response of the irradiated nanowire is similar as that of the perfect nanowire. The stress first linearly increases with strain during the elastic region, and it decreases after passing a threshold value. From the figure, we can see defects induced by irradiation decrease Young’s modulus. By performing quadratic fitting, Young’ modulus of the irradiated nanowires can be obtained.

We find irradiation reduces the Young’s modulus (Fig. 2b), and the reduction amount is proportional to incident energy, which in turn indicates the Young’s modulus depends on the number of defects.

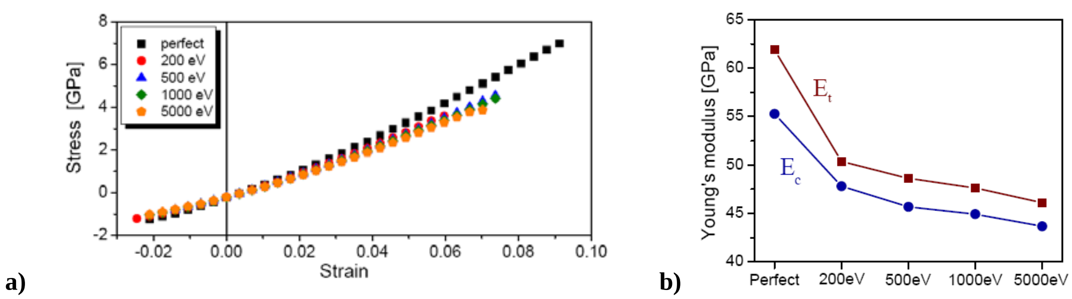

FIG. 2. a) The stress-strain curves obtained from the irradiated nanowires without irradiation-induced stacking faults, comparing with the one of unirradiated nanowires. For clarity, results before yield are shown in the figure. b) The Young moduli of the irradiated and unirradaietd nanowires.

References

[1] C. M. Lieber, Z. L. Wang. MRS Bull 32 (2007) 99.
[2] H. S. Park, W. Cai, H. D. Espinosa, H. Huang. MRS Bull 34 (2009) 178.
[3] H. G. Craighead, Science 290 (2000) 1532.
[4] N. S. Ramgir, Y. Yang, and M. Zacharias, Small 6 (2010) 1705.
[5] A. B. H. Tay, J. T. L. Thong, Appl. Phys. Lett. 84, 1940 (2004).
[6] S. S. Oh et al., Journal of Physics: Conference Series 61 (2007) 884.
[7] W. L. Jiang et al., Adv. Mater. 17 (2005) 1602.
[8] A. V. Krasheninnikov, K. Nordlund, Journal of Applied Physics 107 (2010) 071301.
[9] Y. Mishin, M. J. Mehl, D. A. Papaconstantopoulos, A. F. Voter and J. D. Kress, Phys. Rev. B 63 (2001) 224106.
[10] Ziegler, J.F., J.P. Biersack, and U. Littmark, Stopping and Ranges of Ions in Matter. Pergamon Press, 1985. 1.