8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

Deformation and Stability of Copper Nanowires under Bending

***Y. G. Zheng[1], H. W. Zhang[2] and Z. Chen[3]**

[1] State Key Laboratory of Structure Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Dalian 116024, China
ygzheng@student.dlut.edu.cn

[2] State Key Laboratory of Structure Analysis for Industrial Equipment, Department of Engineering Mechanics, Dalian University of Technology, Dalian 116024, China
zhanghw@dlut.edu.cn

[3] Department of Civil and Environmental Engineering, University of Missouri-Columbia, Columbia, Missouri 65211-2200, USA
chenzh@missouri.edu

Key Words: *Nanowire, Fivefold Deformation Twin, Molecular Dynamics Simulation.*

ABSTRACT

Materials with specific morphologies, such as nanowire, have been extensively studied in recent years because of the importance of the size and shape of materials in determining their physico-mechanical properties. That is, mechanical loading induced deformation and shape change can strongly affect the functionalities of nanowire-based devices and even lead to their failure. Therefore, the mechanical characteristics of nanowires need to be well characterized prior to any feasible applications. So far, a number of atomistic simulations and computational studies have been performed to investigate the tensile response of nanowires. However, the stability and deformation of such materials under bending and/or torsion loads have not yet to be well understood. Taking copper nanowires as an example, we investigate the size effect on stability and deformation mechanisms of such materials under bending loads.

Fig. 1. (a) The geometry of copper nanowires and (b) the formation of two conjoint fivefold deformation twins. The atoms in pink, white and blue are those in local fcc, hcp and icosahedral lattices, respectively; while disordered atoms in red represent surfaces and dislocation cores.

The geometry of the sample is shown in Fig. 1(a). The interactions between copper atoms were described by the EAM potential. The bending loads (20°/ns with a total time of 2.5 ns) were applied to the sample at its two ends after an initial equilibrium. All simulations were conducted using the molecular dynamics method with a Nose-Hoover thermostat to control the system temperature.

Simulation results show that atomic slip and deformation twin (DT) are the main mode to accommodate plastic deformation of copper nanowires. During the motions of various DTs, they meet and interact with each other, inducing the formation of two

conjoint fivefold DTs, as shown in Fig. 1(b). An intermediate icosahedral phase is detected to facilitate the transformation of a low dense (100) fcc plane to a (111) close-packed fashion.

Simulation results also show that the energy increases as increasing the bending angle in the early stage (elastic stage) while drops rapidly as the bending angle increases in a plastic deformation stage, as shown in Fig. 2(a) and (c). The effects of the length and thickness on the critical (transition) bending angle are also shown in Fig. 2(b) and (d). It can be seen that the critical bending angle has a linear dependence on the length while it has a power-law dependence on the thickness. The longer/thicker the nanowire, the larger the critical bending angle. For the longest nanowire, it can be seen from Fig. 2(a) that the energy curve has a very sharp change at ~ 40°. This is because that the global buckling occurs in a long wire while the local buckling and its accumulation are the main mode of instability in short wires.

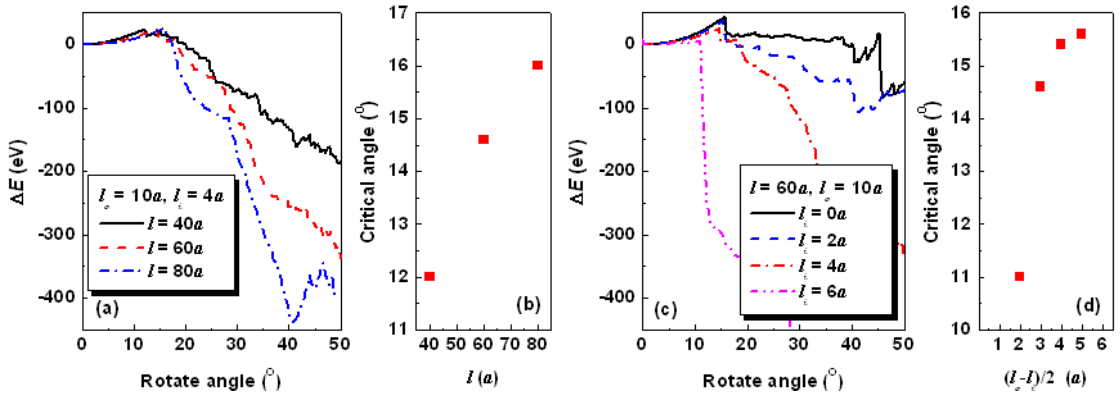

Fig. 2. Effect of length and thickness on the total energy change of copper nanowires: (a) Energy change *vs.* bending angle for three wires with different lengthes, (b) critical angle *vs.* length corresponding to (a); (c) Energy change *vs.* bending angle for four wires with different thicknesses and (d) critical angle *vs.* thickness corresponding to (c). Where *a* denotes the lattice constant for fcc copper.

REFERENCES

[1] Y. N. Xia, P. D. Yang, Y. G. Sun, Y. Y. Wu, B. Mayers, B. Gates, Y. D. Yin, F. Kim, and H. Q. Yan, "One-Dimensional Nanostructures: Synthesis, Characterization, and Applications", *Adv. Mater.*, 15, 353–389, (2003).

[2] X. Z. Liao, Y. H. Zhao, S. G. Srinivasan, Y. T. Zhu, R. Z. Valiev, and D. V. Gunderov, "Deformation twinning in nanocrystalline copper at room temperature and low strain rate", *Appl. Phys. Lett.*, 84, 592–594, (2004).

[3] H. Y. Liang, M. Upmanyu, and H. C. Huang, "Size-dependent elasticity of nanowires: Nonlinear effects", *Phys. Rev. B*, 71, 241403:1–4, (2005).

[4] H. S. Park and J. A. Zimmerman, "Modeling inelasticity and failure in gold nanowires", *Phys. Rev. B*, 72, 054106:1–9, (2005)

[5] A. J. Cao and Y. G. Wei, "Formation of fivefold deformation twins in nanocrystalline face-centered-cubic copper based on molecular dynamics simulations", *Appl. Phys. Lett.*, 89, 041919:1–3, (2006).