Diao, Jiankuai; **Gall, Ken**; **Dunn, Martin L.**
Atomistic simulation of the structure and elastic properties of gold nanowires. (English)
Zbl 1115.74303
J. Mech. Phys. Solids 52, No. 9, 1935-1962 (2004).

Summary: We performed atomistic simulations to study the effect of free surfaces on the structure and elastic properties of gold nanowires aligned in the ⟨100⟩ and ⟨111⟩ crystallographic directions. Computationally, we formed a nanowire by assembling gold atoms into a long wire with free sides by putting them in their bulk fcc lattice positions. We then performed a static relaxation on the assemblage. The tensile surface stresses on the sides of the wire cause the wire to contract along the length with respect to the original fcc lattice, and we characterize this deformation in terms of an equilibrium strain versus the cross-sectional area. While the surface stress causes wires of both orientations and all sizes to increasingly contract with decreasing cross-sectional area, when the cross-sectional area of a ⟨100⟩ nanowire is less than 1.83 nm×1.83 nm, the wire undergoes a phase transformation from fcc to bct, and the equilibrium strain increases by an order of magnitude. We then applied a uniform uniaxial strain incrementally to 1.2% to the relaxed nanowires in a molecular statics framework. From the simulation results we computed the effective axial Young's modulus and Poisson's ratios of the nanowire as a function of cross-sectional area. We used two approaches to compute the effective elastic moduli, one based on a definition in terms of the strain derivative of the total energy and another in terms of the virial stress often used in atomistic simulations. Both give quantitatively similar results, showing an increase in Young's modulus with a decrease of cross-sectional area in the nanowires that do not undergo a phase transformation. Those that undergo a phase transformation experience an increase of about a factor of three of Young's modulus. The Poisson's ratio of the ⟨100⟩ wires that do not undergo a phase transformation show little change with the cross-sectional area. Those wires that undergo a phase transformation experience an increase of about 10% in Poisson's ratio. The ⟨111⟩ wires show, with a decrease of cross-sectional area, an increase in one of Poisson's ratios and small change in the other.

MSC:

74A25 Molecular, statistical, and kinetic theories in solid mechanics
74A60 Micromechanical theories
74S30 Other numerical methods in solid mechanics (MSC2010)
82B21 Continuum models (systems of particles, etc.) arising in equilibrium statistical mechanics

Keywords:

Microstructure; Phase transformation; Elastic properties; Metallic material; Energy method

Full Text: DOI

References:

[1] Baskes, M.I., Modified embedded-atom potentials for cubic materials and impurities, Phys. rev. B, 46, 5, 2727-2742, (1992)

[2] Baskes, M.I.; Angelo, J.E.; Bisson, C.L., Atomistic calculations of composite interfaces, Modell. simul. mater. sci. eng., 2, 505-518, (1994)

[3] Binnig, G.K.; Rohrer, H.; Gerber, Ch.; Stoll, E., Real-space observation of the reconstruction of au(100), Surf. sci., 144, 321-335, (1984)

[4] Broughton, J.Q.; Meli, C.A.; Vashishta, P.; Kalia, R.K., Direct atomistic simulation of quartz crystal oscillatorsbulk properties and nanoscale devices, Phys. rev. B, 56, 2, 611-618, (1997)

[5] Buerger, M.J., Elementary crystallography, (1963), Wiley New York, 1963 (Chapter 11) · Zbl 0098.44605

[6] Cammarata, R.C.; Sieradzki, K., Effects of surface stress on the elastic moduli of thin films and superlattices, Phys. rev. lett., 62, 17, 2005-2008, (1989)

[7] Cheung, K.S.; Yip, S., Atomic-level stress in an inhomogeneous system, J. appl. phys., 70, 10, 5688-5690, (1991)

[8] Daw, M.S.; Baskes, M.I., Semiempirical, quantum mechanical calculation of hydrogen embrittlement in metals, Phys. rev. lett., 50, 17, 1285-1288, (1983)

[9] Daw, M.S.; Baskes, M.I., Embedded-atom methodderivation and application to impurities, surfaces, and other defects in

metals, Phys. rev. B, 29, 12, 6443-6453, (1984)

[10] Diao, J.; Gall, K.; Dunn, M.L., Surface stress induced phase transformation in metal nanowires, Nat. mater., 2, 10, 656-660, (2003)

[11] Egami, T.; Maeda, K.; Vitek, V., Structural defects in amorphous solidsa computer simulation study, Philos. mag. A, 41, 883, (1980)

[12] Fiorentini, V.; Methfessel, M.; Schoffler, M., Reconstruction mechanism of fcc transition metal (001) surfaces, Phys. rev. lett., 71, 1051-1054, (1993)

[13] Foiles, S.M.; Daw, M.S.; Baskes, M.I., Embedded-atom-method functions for the fcc metals cu, ag, au, ni, pd, pt, and their alloys, Phys. rev. B, 33, 7983, (1986)

[14] Frederick, M.; Rasky, D., Anharmonicity and symmetry in crystals, Philos. mag. A, 45, 1, 49-61, (1982)

[15] Gibbs, D.; Ocko, B.M.; Zehner, D.M.; Mochrie, S.G.J., Absolute X-ray reflectivity study of the au(100) surface, Phys. rev. B, 38, 11, 7303, (1988)

[16] Gülseren, O.; Ercolessi, F.; Tosatti, E., Noncrystalline structures of ultrathin unsupported nanowires, Phys. rev. lett., 80, 17, 3775, (1998)

[17] Gumbsch, P.; Daw, M.S., Interface stresses and their effects on the elastic moduli of metallic multilayers, Phys. rev. B, 44, 8, 3934, (1991)

[18] Haftel, M.I.; Rosen, M., Surface embedded atom model of the electrolyte – metal interface, Phys. rev. B, 64, 195405, (2001)

[19] Hall, B.D.; Flüeli, M.; Monot, R.; Borel, J.-P., Multiply twinned structures in unsupported ultrafine silver particles observed by electron diffraction, Phys. rev. B, 43, 3906-3917, (1991)

[20] Hasmy, A.; Medina, E., Thickness induced structural transition in suspended fcc metal nanofilms, Phys. rev. lett., 88, 096103, (2002)

[21] He, L.H.; Lim, C.W.; Wu, B.S., A continuum model for size-dependent deformation of elastic films of nano-scale thickness, Int. J. solids struct., 41, 3-4, 847-857, (2003) · Zbl 1075.74576

[22] Horstemeyer, M.F.; Baskes, M.I., Atomistic finite deformation simulationsa discussion on length scale effects in relation to mechanical stress, J. eng. mater. technol., 121, 114-119, (1999)

[23] Kondo, Y.; Takayanagi, K., Gold nanobridge stabilized by surface structure, Phys. rev. lett., 79, 3455-3458, (1997)

[24] Kondo, Y.; Takayanagi, K., Synthesis and characterization of helical multi-shell gold nanowires, Science, 289, 606-608, (2000)

[25] Kondo, Y.; Ru, Q.; Takayanagi, K., Thickness induced structural phase transition of gold nanofilm, Phys. rev. lett., 82, 751-754, (1999)

[26] Liang, H.Y.; Ni, X.G.; Wang, X.X., Acta metall. sin., 37, 8, 833-836, (2001)

[27] Liang, H.Y.; Wang, X.X.; Wu, H.G.; Wang, Y., Acta mecn. sinica, 34, 2, 208-215, (2002)

[28] Marks, L.D., Surface structure and energetics of multiply twinned particles, Philos. mag. A, 49, 81-93, (1984)

[29] Mays, C.W.; Vermaak, J.S.; Kuhlmann-Wilsdorf, D., On surface stress and surface tension 2. determination of the surface stress of gold, Surf. sci., 12, 134-140, (1968)

[30] Meyers, M.A., Chawla, K.K., 1999. Mechanical Behavior of Materials. Prentice-Hall, NJ, 91pp. · Zbl 1158.74300

[31] Miller, R.E.; Shenoy, V.B., Size-dependent elastic properties of nanosized structural elements, Nanotechnology, 11, 139-147, (2000)

[32] Needs, R.J.; Godfrey, M.J.; Mansfield, M., Theory of surface stress and surface reconstruction, Surf. sci., 242, 215-221, (1991)

[33] Segall, D.E.; Ismail-Beigi, S.; Arias, T.A., Elasticity of nanometer-sized objects, Phys. rev. B, 65, 214109, (2002)

[34] Streitz, F.H.; Sieradzki, K.; Cammarata, R.C., Elastic properties of thin fcc films, Phys. rev. B, 41, 17, 12285-12287, (1990)

[35] Streitz, F.H., Sieradzki, K., Cammarata, R.C., 1990b. Molecular dynamics study of (001) and (111) thin fcc films. In: Clemens B.M., Johnson, W.L. (Eds.), MRS Symposia Proceedings No. 187: Thin Film Structure and Phase Stability. Materials Research Society, Pittsburgh, pp. 299-304.

[36] Streitz, F.H.; Cammarata, R.C.; Sieradzki, K., Surface-stress effects on elastic properties. I. thin metal films, Phys. rev. B, 49, 15, 10699-10706, (1994)

[37] Tosatti, E.; Prestipino, S.; Kostlmeier, S.; Dal Corso, A.; Di Tolla, F.D., String tension and stability of magic tip-suspended nanowires, Science, 291, 288-290, (2001)

[38] Van Hove, M.A., The surface reconstructions of the (100) crystal faces of iridium, platinum and gold, Surf. sci., 103, 189-217, (1981)

[39] Wolf, D., Surface-stress-induced structure and elastic behavior of thin films, Appl. phys. lett., 58, 13, 2081-2083, (1991)

[40] Yamazaki, K.; Takayanagi, K.; Tanishiro, Y.; Yagi, K., Transmission electron microscope study of the reconstructed au(100) surface, Surf. sci., 199, 595-608, (1988)

[41] Zhou, M., A new look at the atomic level virial stresson continuum-molecular system equivalence, Proc. R. soc. London A, 459, 2347-2392, (2003) · Zbl 1060.81062

