

Dingreville, Rémi; Qu, Jianmin; Cherkaoui, Mohammed

Surface free energy and its effect on the elastic behavior of nano-sized particles, wires and films. (English) [Zbl 1120.74683](#)

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Summary: Atoms at a free surface experience a different local environment than do atoms in the bulk of a material. As a result, the energy associated with these atoms will, in general, be different from that of the atoms in the bulk. The excess energy associated with surface atoms is called surface free energy. In traditional continuum mechanics, such surface free energy is typically neglected because it is associated with only a few layers of atoms near the surface and the ratio of the volume occupied by the surface atoms and the total volume of material of interest is extremely small. However, for nano-size particles, wires and films, the surface to volume ratio becomes significant, and so does the effect of surface free energy. In this paper, a framework is developed to incorporate the surface free energy into the continuum theory of mechanics. Based on this approach, it is demonstrated that the overall elastic behavior of structural elements (such as particles, wires, films) is size-dependent. Although such size-dependency is negligible for conventional structural elements, it becomes significant when at least one of the dimensions of the element shrinks to nanometers. Numerical examples are given in the paper to illustrate quantitatively the effects of surface free energy on the elastic properties of nano-size particles, wires and films.

MSC:

74M25 Micromechanics of solids

74Q15 Effective constitutive equations in solid mechanics

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Keywords:

Surface energy; surface stress; nano-fiber; nano-wire; nano-film

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References:

- [1] Ackland, G.J.; Finnis, M.W., Semi-empirical calculation of solid surface tensions in B.C.C. transition metals, *Philos. mag. A*, 54, 301-315, (1986)
- [2] Adams, J.B.; Wolfer, W.G.; Foiles, S.M., Elastic properties of grain boundaries in copper and their relationship to bulk elastic constants, *Phys. rev. B*, 40, 9479-9484, (1989)
- [3] Alber, I.; Bassani, J.L.; Khantha, M.; Vitek, V.; Wang, G.J., Grain boundaries as heterogeneous systems: atomic and continuum elastic properties, *Philos. trans. R. soc. London A*, 339, 555-586, (1992)
- [4] Alymov, M.I.; Shorshorov, M.K., Surface tension of ultrafine particles, *Nanostruct. mater.*, 12, 365-368, (1999)
- [5] Aris, R., *Vectors, tensors, and basic equations of fluid mechanics*, (1962), Prentice-Hall Englewood Cliffs, NJ · [Zbl 0123.41502](#)
- [6] Baker, S.P., Small, M.K., Vlassak, B.J., Daniels, B.J., Nix, W.D., 1993. The search for the supermodulus effect. In: Nastasi, M., Parkin, D. M., Gleiter, H., (Eds.), *Mechanical Properties and Deformation Behavior of Materials Having Ultra-Fine Microstructures*. Kluwer Academic Publishers, Netherlands, pp. 53-67.
- [7] Banerjea, A.; Smith, J.R., Continuum elasticity analysis of the enhanced modulus effect in metal – alloy superlattice films, *Phys. rev. B*, 35, 5413-5420, (1987)
- [8] Bassani, J.L.; Vitek, V.; Alber, I., Atomic-level elastic properties of interfaces and their relation to continua, *Acta metall. mater.*, 40, S307-S320, (1992)
- [9] Blakely, J.M., *Introduction to the properties of crystal surfaces*, (1973), Pergamon Press New York
- [10] Buerger, M.J., *Elementary crystallography*, (1963), Wiley New York, (Chapter 11) · [Zbl 0098.44605](#)
- [11] Cammarata, R.C., Surface and interface stress effects on interfacial and nanostructured materials, *Mater. sci. eng. A*, 237, 180-184, (1997)
- [12] Cammarata, R.C.; Sieradzki, K., Effects of surface stress on the elastic moduli of thin films and superlattices, *Phys. rev. lett.*, 62, 2005-2008, (1989)
- [13] Cammarata, R.C.; Sieradzki, K., Surface and interface stresses, *Annu. rev. mater. sci.*, 24, 215-234, (1994)
- [14] Cammarata, R.C.; Trimble, T.M.; Srolovitz, D.J., Surface stress model for intrinsic stresses in thin films, *J. mater. res.*, 15, 2468-2474, (2000)
- [15] Capolungo, L.; Jochum, C.; Cherkaoui, M.; Qu, J., Homogenization method for strength and inelastic behavior of nanocryst-

- talline materials, *Int. J. plasticity*, 21, 67-82, (2005) · [Zbl 1112.74472](#)
- [16] Capolungo, L.; Cherkaoui, M.; Qu, J., 2005, A self consistent model for the inelastic deformation of nanocrystalline materials. *ASME J. Eng. Mater. Technol.*, to appear. · [Zbl 1112.74472](#)
- [17] Catlin, A.; Walter, W.P., Mechanical properties of thin single-crystal gold films, *J. appl. phys.*, 31, 2135-2139, (1960)
- [18] Diao, J.; Gall, K.; Dunn, M.L., Surface-stress-induced transformation in metal nanowires, *Nat. mater.*, 2, 656-660, (2003)
- [19] Diao, J.; Gall, K.; Dunn, M.L., Atomistic simulation of the structure and elastic properties of gold nanowires, *J. mech. phys. solids*, 52, 1935-2186, (2004) · [Zbl 1115.74303](#)
- [20] Dingreville, R.; Qu, J.; Cherkaoui, M., 2005. Calculating surface energy using molecular static simulations., in preparation. · [Zbl 1120.74683](#)
- [21] Fartash, A.; Fullerton, E.E.; Schuller, I.K.; Bobbin, S.E.; Wagner, J.W.; Cammarata, R.C.; Kumar, S.; Grimsditch, M., Evidence for the supermodulus effect and enhanced hardness in metallic superlattices, *Phys. rev. B*, 44, 13760-13763, (1991)
- [22] Fougere, G.E.; Riester, L.; Ferber, M.; Weertman, J.R.; Siegel, R.W., 1995. Young's Modulus of nanocrystalline Fe measured by nanoindentation. *Mater. Sci. Eng. A* 2004, 1-6.
- [23] Gibbs, J.W., *The collected works of J. willard Gibbs*, (1928), Longmans New York
- [24] Gleiter, H., Nanocrystalline materials, *Prog. mater. sci.*, 33, 223-315, (1989)
- [25] Gurtin, M.E.; Murdoch, A.I., A continuum theory of elastic material surfaces, *Arch. rat. mech. anal.*, 57, 291-323, (1975) · [Zbl 0326.73001](#)
- [26] Gurtin, M.E.; Murdoch, A.I., Surface stress in solids, *Int. J. solids struct.*, 14, 431-440, (1978) · [Zbl 0377.73001](#)
- [27] Gurtin, M.E.; Weissmuller, J.; Larche, F., A general theory of curved deformable interfaces in solids at equilibrium, *Philos. mag. A*, 78, 1093-1109, (1998)
- [28] Itozaki, H., 1982. Mechanical properties of composition modulated copper – palladium foils. Ph. D. Thesis, Northwestern University.
- [29] Kluge, M.D.; Wolf, D.; Lutsko, J.F.; Phillpot, S.R., Formalism for the calculation of local elastic constants at grain boundaries by means of atomistic simulation, *J. appl. phys.*, 67, 2370, (1990)
- [30] Korn, D.; Morsch, A.; Birringer, R.; Arnold, W.; Gleiter, H., Measurements of the elastic constants and the specific heat and the entropy of grain boundaries by means of ultrasound, *J. phys.*, 49, C5-769, (1988)
- [31] Kosevich, Y.U.; Kosevich, A.M., On the possibility of measuring the tensor of surface stress in thin crystalline plates, *Solid state commun.*, 70, 541-543, (1989)
- [32] Krstic, V.; Erb, U.; Palumbo, G., Effect of porosity on Young's modulus of nanocrystalline materials, *Scr. metall. mater.*, 29, 1501-1504, (1993)
- [33] Marinopoulos, A.G.; Vitek, V.; Bassani, J.L., Local and effective elastic properties of grain boundaries in silicon, *Phys. stat. sol. A*, 166, 453-473, (1998)
- [34] Miller, R.E.; Shenoy, V.B., Size dependent elastic properties of nanosized structural elements, *Nanotechnology*, 11, 139-147, (2000)
- [35] Murdoch, A.I., A thermodynamical theory of elastic material interfaces, *Q. J. mech. appl. math.*, 29, 245-275, (1976) · [Zbl 0398.73003](#)
- [36] Nieman, G.W.; Weertman, J.R.; Siegel, R.W., Mechanical behavior of nanocrystalline cu and pd, *J. mater. res.*, 6, 1012-1027, (1991)
- [37] Nix, W.D.; Clemens, B.M., Crystallite coalescence: a mechanism for intrinsic tensile stresses in thin films, *J. mater. res.*, 14, 3467-3473, (1999)
- [38] Nix, W.D.; Gao, H., Atomistic interpretation of interface stress, *Scr. mater.*, 39, 1653-1661, (1998)
- [39] Pan, Z.W.; Dai, Z.R.; Wang, Z.L., Nanobelts of semiconducting oxides, *Science*, 291, 1947-1950, (2001)
- [40] Pei, Z.W.; Hwang, H.L., Formation of silicon nano-dots in luminescent silicon nitride, *Appl. surf. sci.*, 212, 760-764, (2003)
- [41] Phillpot, S.R.; Wolf, D.; Gleiter, H., Molecular dynamic study of the synthesis and characterization of a fully dense, three-dimensional nanocrystalline material, *J. appl. phys.*, 78, 847-860, (1995)
- [42] Sander, D., Surface stress: implications and measurements, *Curr. opin. solid state mater. sci.*, 7, 51-57, (2003)
- [43] Schiøtz, J.; Di Tolla, F.D.; Jacobsen, K.W., Softening of nanocrystalline metals at very small grain sizes, *Nature*, 391, 561-563, (1998)
- [44] Sharma, P.; Ganti, S., 2003. Size-dependent Eshelby's tensor for embedded nano-inclusions incorporating surface/interface energies. Private Communications. · [Zbl 1111.74629](#)
- [45] Shuttleworth, R., The surface tension of solids, *Proc. R. soc. London A*, 63, 444-457, (1950)
- [46] Streitz, F.H.; Cammarata, R.C.; Sieradzki, K., Surface-stress effects on elastic properties, I: thin metal films, *Phys. rev. B*, 49, 10699-10706, (1994)
- [47] Streitz, F.H.; Cammarata, R.C.; Sieradzki, K., Surface-stress effects on elastic properties, II: metallic multilayers, *Phys. rev. B*, 49, 10707-10716, (1994)
- [48] Suryanarayana, C., Nanocrystalline materials, *Inter. mater. rev.*, 40, 41-64, (1995)
- [49] Vitek, V.; Wang, G.J.; Alber, I.; Bassani, J.L., Relationship between modeling of the atomic structure of grain boundaries and studies of mechanical properties, *J. phys. chem. solids*, 55, 1147-1156, (1994)

- [50] Wolf, D.; Kluge, M., Relationship between shear resistance and local atomic structure at grain boundaries in FCC metals, *Scr. metall.*, 24, 907-914, (1990)
- [51] Wolf, D.; Lutsko, J.F., Structurally-induced elastic anomalies in a superlattice of (001) twist grain boundaries, *J. mater. res.*, 4, 1427-1443, (1989)
- [52] Wolf, D.; Lutsko, J.F.; Kluge, M., Physical properties of grain-boundary materials: comparison of EAM and central-force potentials, (), 245-264
- [53] Yang, F., Size dependent effective modulus of elastic composite materials: spherical nanocavities at dilute concentrations, *J. appl. phys.*, 95, 3516-3520, (2004)
- [54] Zhou, L.G.; Huang, H., Are surfaces elastically softer or stiffer?, *Appl. phys. lett.*, 84, 1940-1942, (2004)

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