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Surface effects in non-uniform nanobeams: continuum vs. atomistic modeling. (English)

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Summary: Nanobeams are expected to be one of the key structural elements in nanotechnology. Contrary to macroscopic structures, surface effects can strongly influence the stress and deformation properties of nano-devices. In addition, at such small scales, material non-uniformity becomes significant and must be considered. In this work, a continuum model for nanobeams, including both surface effects and material heterogeneity is developed. The model treats the surfaces as separate material layers with finite thickness. The continuum solution is compared with atomistic simulations, from which the effective bulk and surface properties are computed independently. A special case of self-deflection due to surface non-uniformities, which is important for design of nanosensors, is studied. A comparison between continuum and atomistic solutions reveals differences, which originate from local transition effects in the neighborhood of strong non-uniformities. This discrepancy is addressed by defining an effective length, found by correlating the beam deflections from both methods.

MSC:

74A25 Molecular, statistical, and kinetic theories in solid mechanics
74K10 Rods (beams, columns, shafts, arches, rings, etc.)

Keywords:

surface effects; nanosensors; nanobeams; nanomechanics

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References:

[1] Bar On, B., 2010. Ph.D. thesis, Israel Institute of Technology.

[2] Bar On, B., Altus, E., 2010. Stochastic surface effects in nano-beam sensors, Probabilistic Engineering Mechanics, in press, doi:10.1016/j.probengmech.2009.12.001.

[3] Cammarata, R. C.: Surface and interface stress effects in thin films, Progress in surface science 46, 1-38 (1994)

[4] Cuenot, S.; Fretigny, C.; Demoustiere-Champagne, S.; Nysten, B.: Surface tension effect on the mechanical properties of nanomaterials measured by atomic force microscopy, Physical review B 69, 165410 (2004)

[5] Gurtin, M. E.; Murdoch, I.: A continuum theory of elastic material surface, Archive of rational mechanics and analysis 57, 291-323 (1975) · Zbl 0326.73001 · doi:10.1007/BF00261375

[6] Haiss, W.: Surface stress of clean and adsorbate-covered solids, Reports on progress in physics 64, 591-648 (2001)

[7] Huang, D. W.: Size-dependent response of ultra-thin films with surface effects, International journal of solids and structures 45, 568-579 (2008) · Zbl 1167.74497 · doi:10.1016/j.ijsolstr.2007.08.006

[8] Lavrik, N.; Spaniak, M.; Datskos, P.: Cantilever transducers as a platform for chemical and biological sensors, Review of scientific instruments 75, 2229-2253 (2004)

[9] Lim, C. W.; He, L. H.: Size-dependent nonlinear response of thin elastic films with nano-scale thickness, International journal of mechanical science 46, 1715-1726 (2004) · Zbl 1098.74640 · doi:10.1016/j.ijmecsci.2004.09.003

[10] Lu, P.; He, L. H.; Lee, H. P.; Lu, C.: Thin plate theory including surface effects, International journal of solids and structures 43, 4631-4647 (2006) · Zbl 1120.74602 · doi:10.1016/j.ijsolstr.2005.07.036

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

[12] Müller, P.; Saúl, A.: Elastic effects on surface physics, Surface science reports 54, 157-258 (2004)

[13] Reddy, J. N.: Theory and analysis of elastic plates, (1999)

[14] Reddy, J. N.: Mechanics of laminated composite plates and shells – theory and analysis, (2003)

[15] Sader, J. E.: Surface stress induced deflections of cantilever plates with applications to the atomic force microscope: rectangular plates, Journal of applied physics 89, 2911-2921 (2001)

[16] Sader, J. E.: Surface stress induced deflections of cantilever plates with applications to the atomic force microscope: V-shaped

plates, Journal of applied physics 91, 9354-9361 (2002)

[17] Shenoy, V. B.: Atomistic calculations of elastic properties of metallic fcc crystal surfaces, Physical review B 71, 094104 (2005)

[18] Tsai, D. H.: Virial theorem in molecular dynamics, Journal of chemical physics 70, 1375-1382 (1978)

[19] Wallace, D. C.: Thermodynamics of crystals, (1972) · Zbl 0242.15005