NANOMECHANICS: A CONTINUUM THEORY BASED ON THE INTERATOMIC POTENTIAL

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Abstract. It is commonly believed that continuum mechanics theories may not be applicable on the nanometer scale due to the discrete nature of atoms. Here we develop a nano-continuum theory based on the interatomic potential for nanostructured materials. The interatomic potential is directly incorporated into the continuum theory through the constitutive models. The nano-continuum theory is then applied to study the mechanical deformation of carbon nanotubes, including (1) the pre-deformation energy; (2) linear elastic modulus; (3) fracture nucleation; (4) defect nucleation; (5) electrical property change due to mechanical deformation; (6) binding energy between carbon nanotubes; (7) coefficient of thermal expansion; and (8) specific heat. The nano-continuum theory agrees very well with the atomistic models without any parameter fitting, and therefore has the potential to be applied to complex nanoscale material systems (e.g., nanocomposites) and devices (e.g., nanoelectronics).