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Summary: We present an energy-based continuum model for the analysis of nanoscale materials where surface effects are expected to contribute significantly to the mechanical response. The approach adopts principles utilized in Cauchy-Born constitutive modelling in that the strain energy density of the continuum is derived from an underlying crystal structure and interatomic potential. The key to the success of the proposed method lies in decomposing the potential energy of the material into bulk (volumetric) and surface area components. In doing so, the method naturally satisfies a variational formulation in which the bulk volume and surface area contribute independently to the overall system energy. Because the surface area to volume ratio increases as the length scale of a body decreases, the variational form naturally allows the surface energy to become important at small length scales; this feature allows the accurate representation of size and surface effects on the mechanical response. Finite element simulations utilizing the proposed approach are compared against fully atomistic simulations for verification and validation.

MSC:

74A60 Micromechanical theories
74A25 Molecular, statistical, and kinetic theories in solid mechanics
74S05 Finite element methods applied to problems in solid mechanics

Keywords:

surface stress; potential energy decomposition; strain energy density

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