A Generalized Continuum Theory and Its Applications in Nano/Micro Materials

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This work will present a generalized continuum field theory formulated from classical N-body dynamics, in which a continuum is viewed a continuous collection of lattice points with each of its points endowed with a group of bonding atoms. Atomistic definitions and the corresponding field representations of fundamental physical quantities in multi-element systems will be introduced. Balance equations and the constitutive relations obtained through atomistic formulation will be presented, from which a well-defined continuum field theory will be found. The relation of the newly formulated theory with various nonlocal and generalized continuum theories will be discussed. Numerical implementation of the generalized theory as well as computational results on ferroelectric materials, microporous ziolites and silicon carbide will be presented. Comparison with results obtained from atomic-level molecular dynamics simulations will also be presented and discussed.

References

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