

Abstract Submitted
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A Multiscale Field Theory for Atomistic Multi-element Systems¹

YOUPING CHEN, JAMES LEE — Formulas for local densities of fundamental physical properties, including stress and heat flux fields, are derived for atomistic systems with many-body potentials. The obtained formulas are then generalized to multi-element systems and the field representation of the corresponding conservation equations is obtained. The resulting formulas are calculable within an atomistic simulation, in consistent with the conservation laws of the thermodynamics continuum, and can be applied to single- and multi-element systems involving general two- and three-body interaction forces. It is found that, for multi-element systems, fluxes are composed of homogeneous and inhomogeneous parts and the energy conservation equation takes a different form from single-element systems. At atomic level, stress is nonlinear and nonlocal in displacements and consists of higher order strain gradients, and heat flux is a function of both strain and temperature gradients. With the derived balance equations and constitutive relations, it is shown that the atomistic formulation is able to completely define a field theory that exactly represents the classical many-body dynamics and is able to work as an alternative to, but computationally more efficient than, atomic-level molecular dynamics simulations in studying statistical and finite temperature properties of finite size multi-element materials. Numerical examples will be presented. Potential applications of the obtained field theory will be discussed. .

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