

LOCAL QUASICONTINUUM DENSITY FUNCTIONAL THEORY: AN AB-INITIO FINITE ELEMENT CONSTITUTIVE MODEL

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We present a method that utilizes ab-initio material properties computed in real-time during a finite element solid mechanics simulation. The material behavior is modeled, under the Cauchy-Born assumption, as individual non-interacting unit-cells at each mesh integration point. Density Functional Theory is used to compute stresses and energies, with the global solution fields obtained by energy minimization. This approach allows for the prediction of phase changes (with basis optimization), simulation under large ranges of stresses (including very high pressures) and the study of alloy composition, and models all material behaviors allowed by the chosen unit cell including plastic slip.

We demonstrate the algorithm with a simulation of the indentation of Aluminum by a spherical indenter. Stability analysis is used to provide an indication of the onset of strain localization and to identify the activated slip systems.