A CONCURRENT MULTISCALE METHOD FOR COUPLING ATOMISTIC AND CONTINUUM AT FINITE TEMPERATURES

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In this work, a concurrent multi-scale simulation method for finite temperature simulation of solids is developed. The aim is to capture far from equilibrium phenomena using an atomistic model and near equilibrium phenomena using a continuum model employing constitutive equations. The domain is partitioned into atomistic and continuum regions which are coupled through an interface region. The underlying problem of coupling between different time and length scales, spanning multiple physics is approached here with the idea of partitioning the phonon spectrum into the continuum notions of thermal energy represented by the higher frequencies and mechanical energy represented by lower frequencies. This is achieved by use of the generalized Langevin equation in the interface to function as a low pass filter. The problem of spurious reflections of high frequency components from the interface of the two models is avoided by proper decoupling of the modes and ensuring the continuity of displacements in the interface region. This is achieved by modifying the continuum nodal displacements through kinematic constraints and slaving atomistic displacements to continuum. The underlying thermal problem is coupled by imposing a flux input into atomistic and using a temperature boundary condition for continuum. Proper flow of energy between the continuum and atomistic models is ensured by this bi-directional coupling.