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Multiscale analysis of phonon mediated dissipation in crystalline solids

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ABSTRACT

In this study, we develop a multiscale method to study intrinsic damping in nano-structure. Vibrational frequencies in the range of few GHz are considered. Deformation of the structure, at such high rates of vibration, results in a nonequilibrium phonon distribution. The condition of local equilibrium, as is often used in the existing mutli-scale approaches, no longer remains valid. The nonequilibrium phonon population results in the absorption of energy from the mechanical deformation and manifests itself as macroscopic dissipation. In this study, we develop constitutive relation for the stress tensor under such nonequilibrium condition. The stress tensor is decomposed into equilibrium and nonequilibrium components. The equilibrium component of the stress tensor is obtained using finite temperature quasi-harmonic methods (QHM). A visco-elastic relation is obtained for the nonequilibrium component. The different parameters, for the developed constitutive law, are obtained from the underlying interatomic potential. A modified QHM approach is used to obtain the stress relaxation rate. We first consider the case of ideal crystalline solids and study dissipation rate as a function of frequency and different strain state. Dissipation rate is computed in terms of dimensionless Q factor. The results from the analyses are compared with those obtained from nonequilibrium molecular dynamics simulations. The case of nano-structure is, then, considered. The role of surface on the Q factor is studied and compared with atomistic results.