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Dynamics of Phononic Dissipation at the Atomic Scale¹ HALDUN SEVINCLI, SOMA MUKHOPADHAY, R. TUGRUL SENGER, SALIM CIRACI, Department of Physics, Bilkent University — Dynamics of dissipation of a local phonon distribution to the bulk is a key issue in boundary lubrication and friction between sliding surfaces. We consider a highly excited molecule which interacts weakly with the substrate surface. We study different types of coupling and substrates having different types of dimensionality and phonon densities of states. We propose three different methods to solve the dynamics of the combined system, namely the equation of motion technique, Fano-Anderson method and the Green's function method. Using this theoretical framework we present an analysis of transient properties of energy dissipation via phonon discharge at the microscopic level. The methods allow the theoretical calculations to be extended to include any density of states for the substrate including experimental ones and any type of molecule that represent the lubricant or the asperity.

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