PHONONIC EXCITATIONS DURING SLIDING FRICTION

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ABSTRACT
The Prantl-Tomlinson model is frequently used to explain friction phenomena on the atomistic scale [1]. In this model energy dissipation is often modelled as viscous damping. The associated damping parameter is typically guessed or fitted to experimental data. This description lumps all microscopic dissipation channels into a single constant and allows no conclusion on the atomistic mechanism of energy dissipation.

Fundamentally, energy dissipation in friction is due to the excitation of lattice vibrations, the phonons. We study the coupling of external sliding to the phononic modes by means of large-scale molecular dynamics (MD) simulations for both crystalline and amorphous solids. The atomic interaction in our model systems are modelled using a modified Lennard-Jones potential.

In order to understand which phonons are excited by the external action of a sliding object, we carry out non-equilibrium MD simulations of a sliding Hertzian indenter. Decomposition of the resulting displacement field into contributions from vibrational modes allows to extract the excitation of phonon modes due to the external sliding action. Figure 1(a) shows typical displacement fields of selected phonon modes for an amorphous solid. We show that in particular low-frequency modes are excited. While low frequency modes in crystals are plane waves and follow the Debye prediction, plane-wave like phonons and quasi-localized modes coexist in amorphous solids [2,3,4]. The type of phonon mode in the amorphous solid plays a crucial role for energy dissipation.

By additionally measuring lifetimes of normal modes, we predict the energy dissipated by the sliding indenter. The lifetimes are computed from total-energy autocorrelation functions [5]. Figure 1(b) and (c) demonstrate the lifetimes of the crystalline and the amorphous solid. We show that the empirical viscous dissipation constant in the Prantl-Tomlinson model can be described by the collective decay of phononic modes excited during sliding.

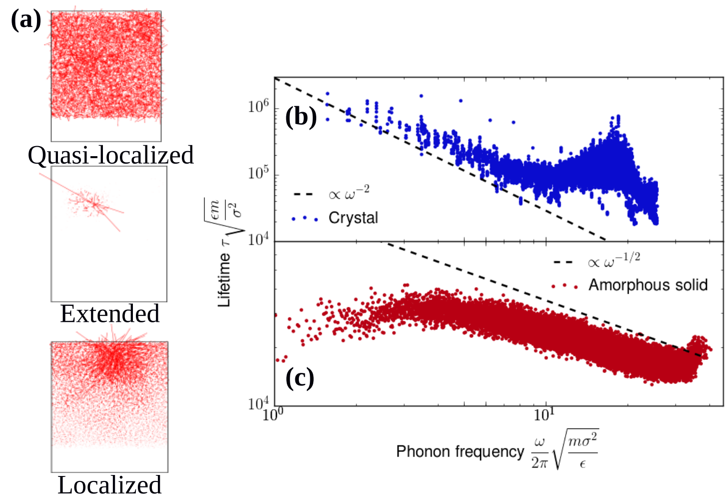

Fig.1: (a) Displacement field of normal modes in a model amorphous solid showing exemplary a low-frequency quasi-localized, an intermediate frequency extended and a high-frequency localized mode. (b) Measured lifetimes of vibrational modes of the crystal. (c) Measured lifetimes of vibrational modes of the amorphous solid.

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