Atomistic theory for the damping of vibrational modes in monoatomic gold chains - DTU Orbit (25/12/2018)

**Atomistic theory for the damping of vibrational modes in monoatomic gold chains**

We develop a computational method for evaluating the damping of vibrational modes in monatomic metallic chains suspended between bulk crystals under external strain. The damping is due to the coupling between the chain and contact modes and the phonons in the bulk substrates. The geometry of the atoms forming the contact is taken into account. The dynamical matrix is computed with density-functional theory in the atomic chain and the contacts using finite atomic displacements while an empirical method is employed for the bulk substrate. As a specific example, we present results for the experimentally realized case of gold chains in two different crystallographic directions. The range of the computed damping rates confirms the estimates obtained by fits to experimental data [T. Frederiksen et al., Phys. Rev. B 75, 205413 (2007)]. Our method indicates that an order-of-magnitude variation in the harmonic damping is possible even for relatively small changes in the strain. Such detailed insight is necessary for a quantitative analysis of damping in metallic atomic chains and in explaining the rich phenomenology seen in the experiments.

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