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Damping of high amplitude phonons in bismuth: classical and quantum mechanical simulations EAMONN MURRAY, Rutgers University, AARON HURLEY, Universiry College Cork, Ireland, DAVID PRENDERGAST, Lawrence Berkeley Laboratory, TADASHI OGITSU, Lawrence Livermore National Laboratory, DAVID FRITZ, Stanford Linear Accelerator Center, DAVID REIS, University of Michigan, STEPHEN FAHY, University College Cork, Ireland — Using both classical and quantum mechanical simulations together with first-principles results, we investigate the damping mechanism of high amplitude excitations of the A_{1g} phonon mode in bismuth. Pump-probe experiments using ultrafast lasers can generate and measure large amplitude coherent oscillations of the A_{1g} phonon mode in bismuth. A substantial reduction in the lifetime of the phonon is observed when higher amplitude oscillations are produced. With third-order couplings obtained from first-principles we calculate the rate of energy loss from the A_{1g} mode over several picoseconds. We find that as the highly excited A_{1g} mode decays, it produces highly excited modes in relatively small regions of the Brillouin Zone, leading to an increase in the decay rate into these modes. We show how this can greatly affect the observed lifetime of the high amplitude excitation of the A_{1g} mode.

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