## Abstract Submitted for the MAR06 Meeting of The American Physical Society

Calculation of the Phonon Lifetime of Photoexcited Bismuth<sup>1</sup> EAMONN MURRAY, Department of Physics and Tyndall National Institute, University College, Cork, Ireland, DAVID PRENDERGAST<sup>2</sup>, TADASHI OGITSU, Lawrence Livermore National Laboratory, STEPHEN FAHY, Department of Physics and Tyndall National Institute, University College, Cork, Ireland — Phonon lifetimes of the zone-center longitudinal optical phonon in bismuth are calculated with respect to the fraction of valence band electrons excited into the conduction bands. Second order density-functional perturbation theory (DFPT), combined with the frozen phonon technique, is used to calculate the third-order anharmonic couplings between phonons. Calculations on the photoexcited system are performed by constraining the occupations of the valence and conduction bands, giving a certain excited electron-hole plasma density. It is found that the calculated decrease in the phonon lifetime with excitation is due both to the reduction of the phonon frequency and an increase in the coupling to other phonons.

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