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Polarization-dependent force driving the E_g mode in bismuth under optical excitation: comparison of first-principles theory with ultrafast x-ray experiments[1] STEPHEN FAHY, EAMONN MURRAY, Tyndall National Institute, University College Cork — Using first principles electronic structure methods, we calculate the induced force on the E_g (zone centre transverse optical) phonon mode in bismuth immediately after absorption of a ultrafast pulse of polarized light. To compare the results with recent ultra-fast, time-resolved x-ray diffraction experiments [1], we include the decay of the force due to carrier scattering, as measured in optical Raman scattering experiments [2], and simulate the optical absorption process, depth-dependent atomic driving forces, and x-ray diffraction in the experimental geometry. We find excellent agreement between the theoretical predictions and the observed oscillations of the x-ray diffraction signal, indicating that first-principles theory of optical absorption is well suited to the calculation of initial atomic driving forces in photo-excited materials following ultrafast excitation.

[1] S. L. Johnson et al, Phys. Rev. B 87, 054301 (2013).
[2] J.J. Li et al, Phys. Rev. Lett. 110, 047401 (2013).

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Stephen Fahy
Tyndall National Institute, University College Cork

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