Boron Arsenide Phonon Dispersion from Inelastic X-Ray Scattering: Potential for Ultrahigh Thermal Conductivity

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Cubic boron arsenide (BAs) was predicted to have an exceptionally high thermal conductivity (k) ~2000 $Wm^{-1}K^{-1}$ at room temperature, comparable to that of diamond, based on first-principles calculations. Subsequent experimental measurements, however, only obtained a k of ~200 $Wm^{-1}K^{-1}$. To gain insight into this discrepancy, we measured phonon dispersion of single crystal BAs along high symmetry directions using inelastic x-ray scattering (IXS) and compared these with first-principles calculations. Based on the measured phonon dispersion, we have validated the theoretical prediction of a large frequency gap between acoustic and optical modes and bunching of acoustic branches, which were considered the main reasons for the predicted ultrahigh k. This supports its potential to be a super thermal conductor if very high-quality single crystal samples can be synthesized.

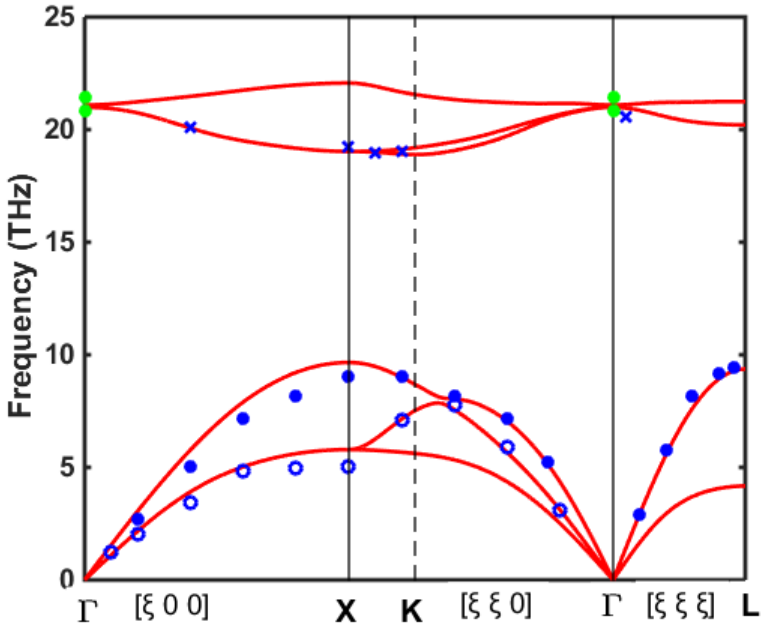

Fig. 1: Bottom: Experimental (markers) and theoretical (solid lines) phonon dispersion of BAs. Green circle makers are Raman data. Filled markers are for LA modes and unfilled ones are for TA modes

[1] Hao Ma, Chen Li, Shixiong Tang, Jiaqiang Yan, Ahmet Alatas, Lucas Lindsay, Brian C. Sales, and Zhiting Tian, *Physical Review B* **94** (22), 220303 (2016)