Supporting Information

Strain tuning high thermal conductivity in Boron Phosphide at nanometer length scales– A first-principles study

Rajmohan Muthaiah and Jivtesh Garg

School of Aerospace and Mechanical Engineering, University of Oklahoma, Norman, OK 73019, USA.

Relative contributions of different scattering channels in scattering of acoustic phonons over the entire Brillouin zone

Magnitudes of dominant scattering channels - a) $a + a \rightarrow o$ b), $a + o \rightarrow o$, c) $a + a \rightarrow a$, and d) $a \rightarrow a + a$ involved in scattering of LA and TA modes, over the entire Brillouin zone, are presented in Fig. S1.

For LA phonons, an increase in $a + a \rightarrow o$ scattering is observed near the Brillouin zone edge. This can be explained by a shift of the optical phonons to higher frequencies in strained BP (as seen in phonon dispersion in Fig. 2c) which induces new scattering channels for high frequency LA phonons. As an example, in the 2% biaxially strained BP, an LA phonon of frequency ω=500 cm^{-1} can scatter by absorbing another LA phonon of frequency ω'=340 cm^{-1}, yielding optical phonon of frequency ω''=840 cm^{-1} ($\omega+\omega'=\omega''$). Presence of higher frequency optical phonons in strained BP (spanning frequency range of 711 cm^{-1} – 848 cm^{-1}) makes such a channel feasible in the 2% strained BP, since ω''=840 cm^{-1} lies within the optical frequency range of strained BP. In the unstrained case, however, optical phonon frequencies are lower (688 cm^{-1} – 820 cm^{-1}), and an optical phonon of frequency ω''=840 cm^{-1} does not exist, making the above channel infeasible in unstrained case. The presence of additional scattering channels for higher energy LA phonons near the zone edge (in strained BP), increases their linewidths in strained case.

Above outlined increase in LA phonon scattering, in strained BP, near the Brillouin zone edge at frequencies exceeding ~ 500 cm^{-1}, however, does not significantly impact thermal conductivity, since contribution of phonons with frequencies > 500 cm^{-1} to overall thermal conductivity is negligible in unstrained BP itself (Fig. 6c in main manuscript). Moreover, the effect of increase in LA phonon scattering is somewhat offset by an increase in LA phonon group velocities (Fig. 4b).

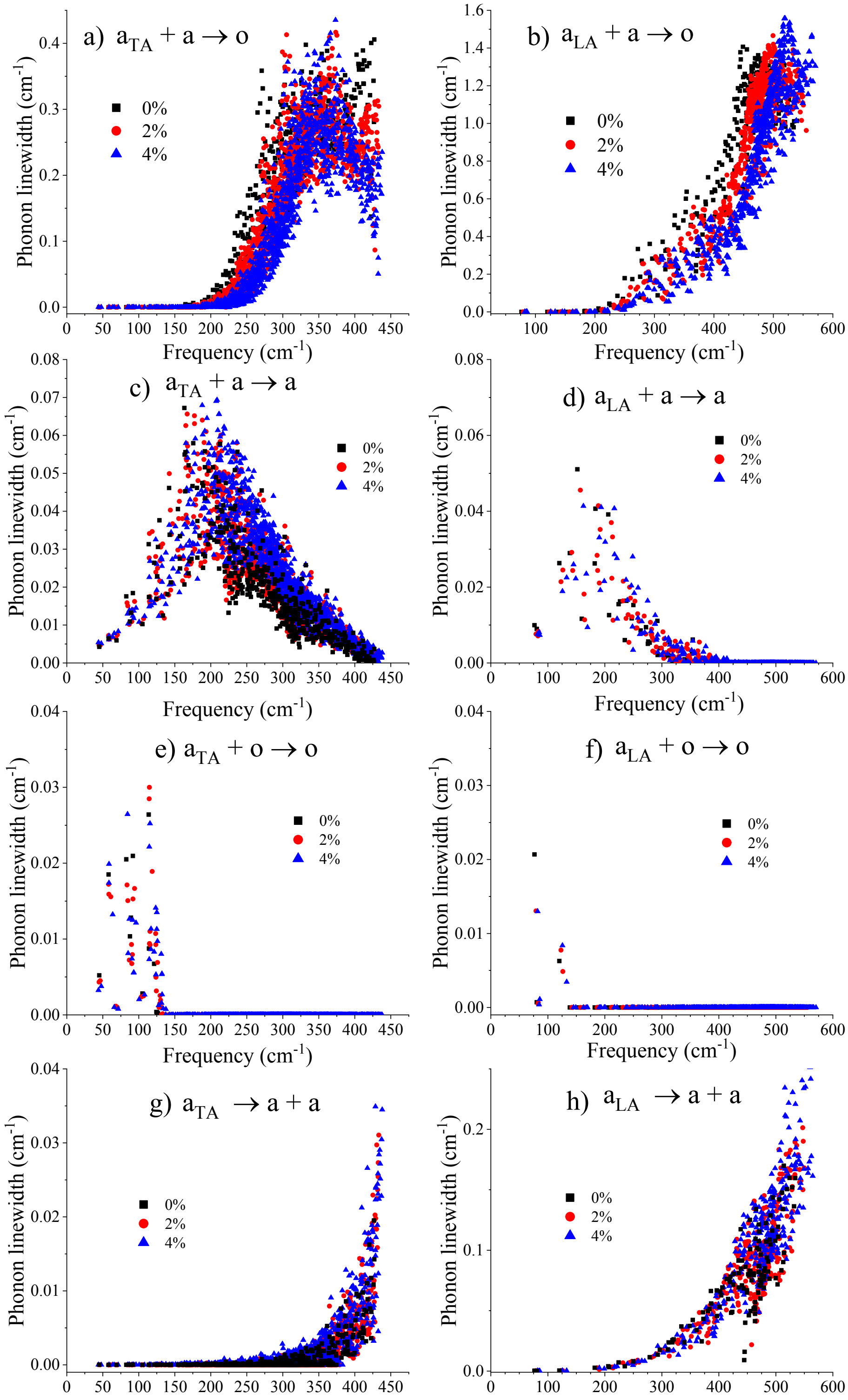
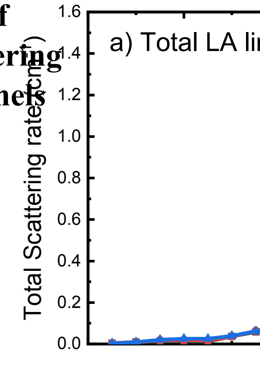


Figure S1: Effect of strain on dominant scattering channels involved in scattering of LA and TA modes.

Relative contributions of scattering channels for



acoustic phonons along Γ-Z

Length dependence of thermal conductivity of unstrained and strained BP for long lengths

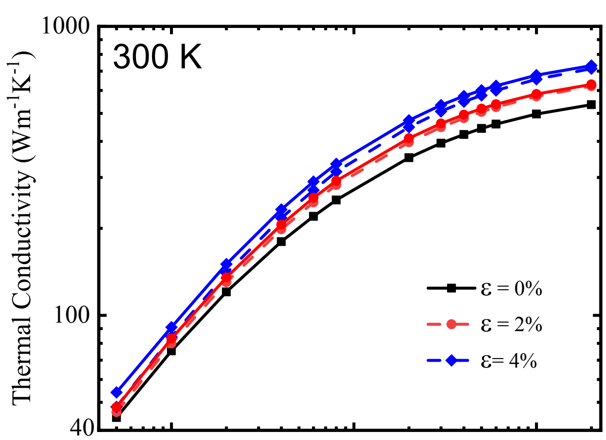


Figure S3: Length dependence of thermal conductivity of unstrained and strained BP showing convergence towards bulk values. For strained BP, solid lines are out-of-plane (perpendicular to the plane in which bi-axial strain is applied) values, while dashed lines are in-plane result.