

Peak thermal conductivity measurements of boron arsenide crystals

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Figure S1 shows the schematic illustration of differential thin film resistance thermometry measurements of Boron Arsenide (BAs) crystals and photograph of the sample. To maintain an adequate distance between the two thermometers to achieve a measurable temperature drop and one-dimensional (1D) temperature distribution, a serpentine thin film heater patterned on a silicon bar is joined to one end of the sample with silver epoxy. In addition, each of the two thermometers on the BAs surface is patterned at a position at least 3 times the thickness away from the nearby silver epoxy joint with the heater or the copper heat sink.

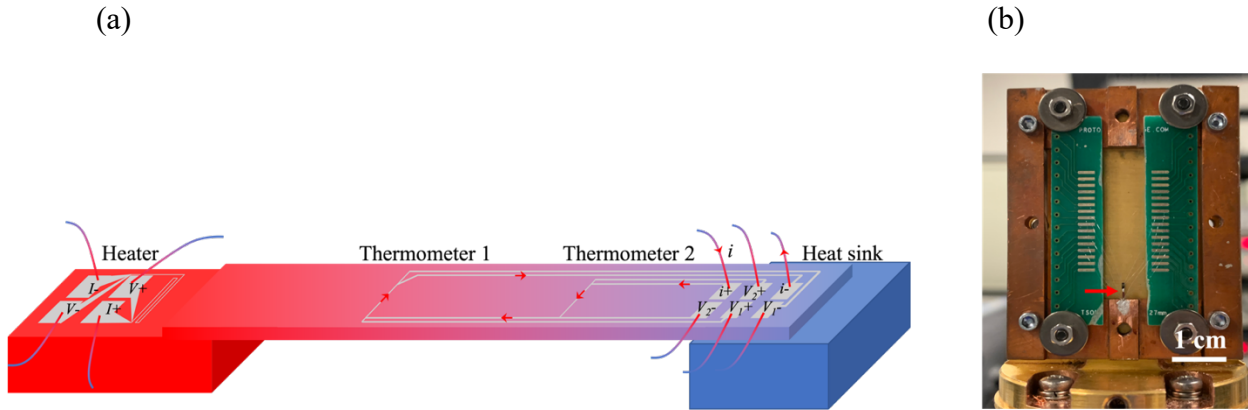


FIG. S1. (a) Schematic illustration of the sample design showing the current (i or I) source (+) and drain (-) and voltage (V) contacts to the heater and two thermometers (1 and 2) [1]. (b) Photograph of the patterned BA sample S1 assembled with a thin film Au/Cr serpentine heater on a silicon piece and a copper heat sink and connected to a printed circuit board (PCB) with bonding wires. The arrow in (b) indicates the BA sample location.

Figure S2 shows the oxygen impurity concentration variation among the samples measured by time-of-flight secondary ion mass spectroscopy (TOF-SIMS) profiling.

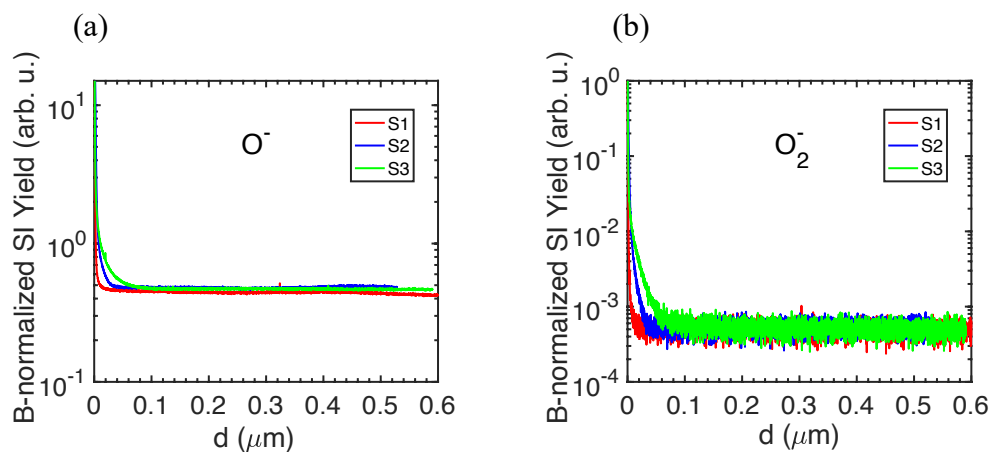


FIG. S2. (a) O^- and (b) O_2^- impurity depth profile normalized by B for the three samples measured by TOF-SIMS.

Figure S3 shows the original magnetic field scans for S1, S2, and S3 with a magnetic field sweeping between ± 3 T.

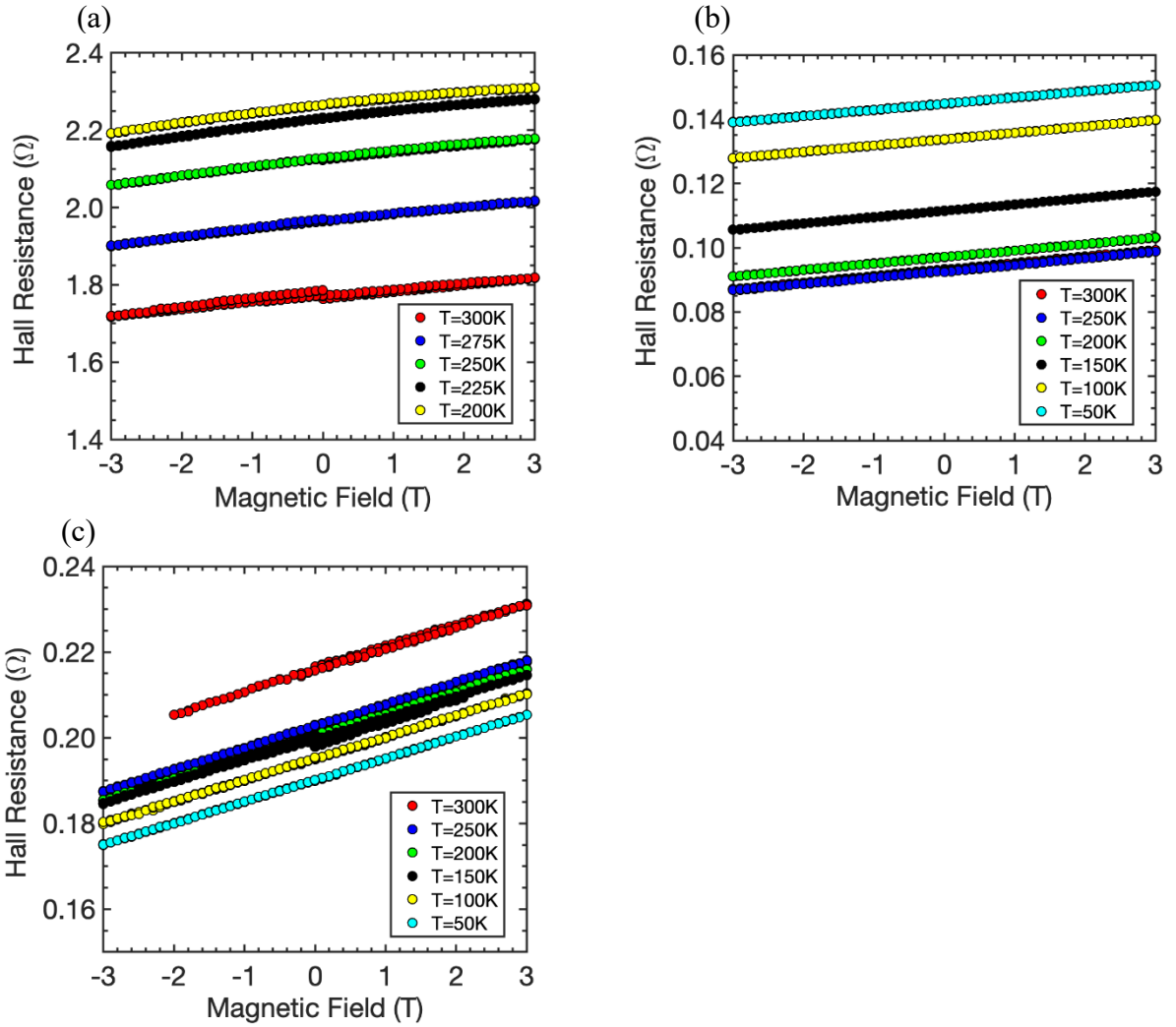


FIG. S3. Original magnetic field scans for (a) S1, (b) S2, and (c) S3. Y-axis represents the measured hall resistance of sample. In (b), measurement results at 300 K and 250 K overlap.

In cubic compounds, the scattering rates of phonons resulting from the mass disorder can be expressed in a closed form [2]:

$$\frac{1}{\tau_{\lambda}^{pd}} = \frac{\pi}{6} \omega_{\lambda}^2 \Omega \sum_s g_s |\hat{e}_s^{\lambda}|^2 D_s(\omega_{\lambda}) \quad (\text{S1})$$

Here, ω_{λ} is the frequency in phonon mode $\lambda = j, \mathbf{q}$, where j is the phonon branch and \mathbf{q} is the phonon wave vector, the sum in Eq. S1 is over each atom, $s = B, As$, in the unit cell whose volume is Ω , \hat{e}_s^{λ} is the phonon eigenvector for atom s , $D_s(\omega_{\lambda})$ is the partial density of states:

$$D_s(\omega) = \frac{1}{V} \sum_{\lambda} |\hat{e}_s^{\lambda}|^2 \delta(\omega - \omega_{\lambda}) \quad (\text{S2})$$

with V being the volume of the crystal, and g_s is the mass variance parameter for atom s :

$$g_s = \sum_i f_{is} (1 - M_{is}/\bar{M}_s)^2 \quad (\text{S3})$$

where M_{is} is the mass of the i^{th} type of atom on site s (host atom or point defect) whose relative concentration is f_{is} , and $\bar{M}_s = \sum_i f_{is} M_{is}$ is the average mass on site s . Since As is isotopically pure, the isotopic mixture occurs only on the B site (19.9% ^{10}B , 80.1% ^{11}B) giving $g_B = 1.36 \times 10^{-3}$. All extrinsic point defects are taken to occupy the As sites, which is consistent with the lower formation energies found on As sites compared with those on the B sites [3]. Since the specific defects and their concentrations are only known approximately, we treat g_{As} as a variable parameter that is adjusted to best fit the measured data.

References:

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- [2] S. Tamura, Isotope Scattering of Large-Wave-Vector Phonons in GaAs and InSb: Deformation-Dipole and Overlap-Shell Models, *Phys. Rev. B* 30, 849 (1984).
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