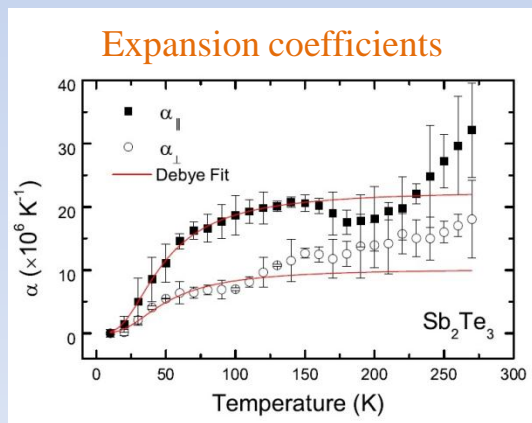
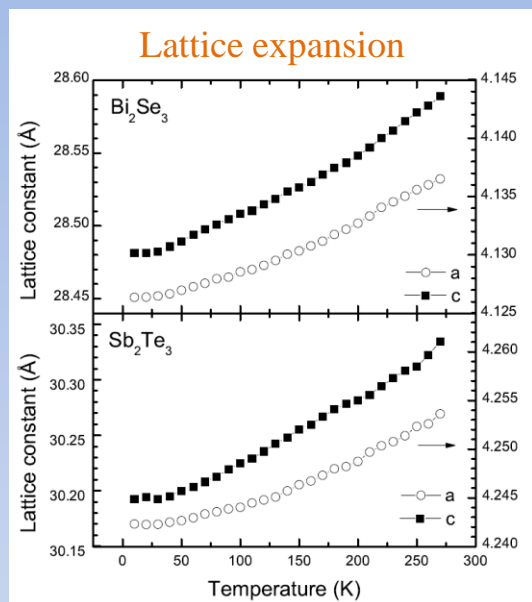


# Enhanced Thermoelectric Figure of Merit by Strong Anharmonicity

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The thermodynamic efficiency of thermoelectric devices can be enhanced by reducing the material thermal conductivity. Recently it has been shown that a very low thermal conductivity occurs in the semiconducting material, AgSbTe<sub>2</sub>, due to the strong anharmonicity of the bonding arrangement, which is largely responsible for its high thermoelectric figure of merit ( $ZT \sim 1.3$ , highest among simple semiconductors).

We have systematically studied the thermal expansion of a variety of thermoelectric materials, including AgSbTe<sub>2</sub>, Bi<sub>2</sub>Se<sub>3</sub>, Bi<sub>2</sub>Te<sub>3</sub> and Sb<sub>2</sub>Te<sub>3</sub>, using variable temperature X-ray powder diffraction, and extracted the Grüneisen parameters (a quantitative measure of the anharmonicity). Indeed, we find that the linear thermal expansion coefficients of these materials deviate from the standard Debye model at room temperature, indicative of higher-order anharmonic effects. The largest deviation is seen in Sb<sub>2</sub>Te<sub>3</sub>, leading to an unusually high Grüneisen parameter of 2.3.

In addition, we aim to further enhance the  $ZT$  of AgSbTe<sub>2</sub> materials via engineering nanostructures. It is known that properly embedded nanostructures help increase the  $ZT$  of the devices. Towards this end, we have investigated two AgSbTe<sub>2</sub> samples with different stoichiometry: (1) Sb-rich Ag<sub>16.7</sub>Sb<sub>30</sub>Te<sub>53.3</sub> and (2) Ag-rich Ag<sub>19</sub>Sb<sub>29</sub>Te<sub>52</sub>, where Sb<sub>2</sub>Te<sub>3</sub> and Ag<sub>2</sub>Te precipitates are found embedded within the single-phase AgSbTe<sub>2</sub>.