MAS20-2020-000029

Abstract for an Invited Paper for the MAS20 Meeting of the American Physical Society

Unusual electronic and vibrational behavior in the high thermopower antimonides FeSb_2 and CrSb_2^1 CHRISTOPHER HOMES, Condensed Matter Physics and Materials Science Dept., Brookhaven National Laboratory

The antimonides FeSb₂ and CrSb₂ both exhibit an extraordinarily high thermoelectric power factor at low temperature; however, the origin of this behavior is still a subject of some debate, having been variously attributed to either electronic correlations or the phonon drag effect. The optical properties of a material provide information about both the electronic and vibrational properties of a material; accordingly, the temperature dependence of the complex optical properties of single crystals of FeSb₂ and CrSb₂ have been measured along the principle optical axes over a wide frequency range. At room temperature, the low-frequency optical conductivity of FeSb₂ is anisotropic, with the conductivity along the *b* axis significantly larger than along either the *a* or *c* axes. Below $\simeq 100$ K the low-frequency conductivity decreases dramatically, but a step-like feature emerges along the *b* axis at $\simeq 75$ meV in agreement with first principle calculations, suggesting one-dimensional behavior and signalling the presence of electronic correlations. The infrared-active modes are extremely narrow; curiously, the character of the lattice modes changes between $\simeq 100 - 200$ K, possibly indicating a weak structural distortion.² The high thermopower observed in CrSb₂ is attributed to the phonon drag effect. The behavior. No phonon anomalies are observed in this material; however, just below $T_{\rm N} \simeq 273$ K a peculiar electronic mode appears at $\simeq 50$ meV, which rapidly softens and decreases in intensity at low temperature.

¹This work done in collaboration with Q. Du, C. Petrovic, W. H. Brito, S. Choi, and G. Kotliar. Supported by the Office of Science, U.S. Department of Energy, under Contract No. DE-SC0012704. ²C. C. Homes, Q. Du, C. Petrovic, W. H. Brito, S. Choi, and G. Kotliar, Sci. Rep. 8, 11292 (2018).