Power Factor Improvements in Thermoelectric PbTe under Stress

Gavin Woolman[1*] and Ingo Loa[1]

[1]*SUPA, School of Physics and Astronomy, and Centre for Science at Extreme Conditions, The University of Edinburgh, Edinburgh, UK*

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*e-mail: gavin.woolman@ed.ac.uk

Thermoelectric materials have been attracting renewed scientific interest because they provide a means of generating electricity directly from waste heat. Efficient thermoelectric materials require a delicate balance between the electrical conductivity, σ, the Seebeck coefficient, *S*, and the thermal conductivity. Lead telluride is one of the most efficient thermoelectric materials known, partly due to its high thermoelectric power factor, σS^2. Previous experiments [1] suggested that hydrostatic pressure can greatly improve the power factor of lead telluride, but the origin of this change has remained unknown.

We have conducted *ab initio* electronic structure and transport calculations in the framework of density functional theory (DFT) in order to model how high hydrostatic pressure and uniaxial stress can tune the direction-dependent electrical transport properties and enhance the power factor of PbTe.

The electronic band structure and thermoelectric properties of *p*- and *n*-doped PbTe were calculated as a function of hydrostatic pressure as well as uniaxial stress along several crystal directions. We found that significant enhancements of the thermoelectric power factor can be obtained, and we analysed the underlying changes in the electronic band structure (Fig. 1). We identified the key effects in PbTe, which allowed us to deduce a few more general rules for identifying stress conditions that may improve other thermoelectric materials. These will be presented along with the specific results for PbTe.

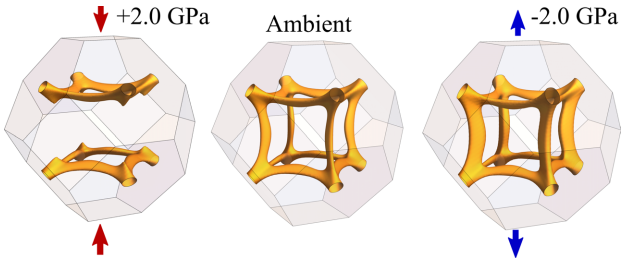

Figure 1. Constant-energy surfaces in the Brillouin zone of PbTe under uniaxial stress. The change in topology observed for compressive stress indicates changes to band extrema near the Fermi level, which play a crucial role for thermoelectricity.

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