Effect of intrinsic defects on the thermal conductivity of PbTe

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Despite PbTe being the archetypal thermoelectric material, still today some of the most exciting advances in the efficiency of this and related materials are being achieved by tuning their properties at the nanoscale. Its inherently low lattice thermal conductivity can be lowered to its fundamental limit by designing a structure capable of scattering phonons over a wide range of length scales. Intrinsic defects, such as vacancies or grain boundaries, can and do play the role of these scattering sites. Here we assess the effect of these defects by means of molecular dynamics simulations. For this we purposely parametrized a Buckingham potential that provides an excellent description of the thermal conductivity of this material over a wide temperature range [1] (see Figure 1). Our results show that intrinsic point defects and grain boundaries can reduce the lattice conductivity of PbTe down to a quarter of its bulk value (see Figure 2). By studying the size dependence, we also show that typical defect concentrations and grain sizes realized in experiments normally correspond to the bulk lattice conductivity of pristine PbTe. We then address the issue of the survival of nanostructuring against thermal coarsening using a phase field model [2].

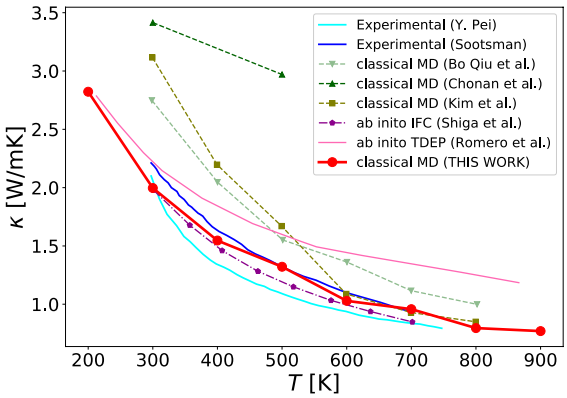

Figure 1: Thermal conductivity of bulk PbTe

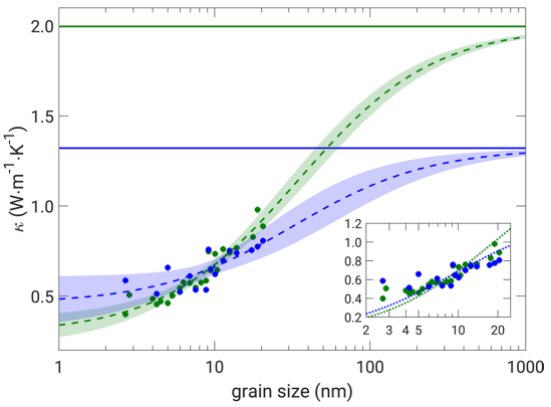

Figure 2: Thermal conductivity of polycrystalline PbTe

References

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[2] J. Fernández Troncoso, P. Chudzinski, T. N. Todorov, P. Aguado Puente, M. Grüning, and J. Kohanoff, ***Thermal Conductivity of Porous Polycrystalline PbTe***, Phys. Rev. Materials **5**, 014604 (2021).

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