Quantum transport simulations for the thermoelectric properties of bipolar materials

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Abstract

Low bandgap thermoelectric materials (e.g. BiTe, PbTe and their alloys) suffer from degraded performance at high temperature due to an increase in the bipolar thermal conductivity [1, 2]. Efforts to reduce the bipolar effect have included alloying to increase the band gap [3], while theoretical studies have shown that superlattice barriers can filter minority carriers and consequently maintain ZT at high temperatures [4]. In addition, a large number of studies are currently devoted to nanostructuring such materials to reduce their overall thermal conductivity.

In this work we theoretically address the issue of reducing bipolar conduction effects in low bandgap nanostructured materials by employing the quantum mechanical Non-Equilibrium Green's Function (NEGF) method. We consider materials with embedded nanoinclusions, a typical deliberately included feature in experimentally realised materials. The NEGF method is most suitable for such studies as it is geometry flexible and can include electron phonon interactions, as well as all quantum mechanical effects at the nanoscale.

We show that nanoinclusions themselves (even up to the 15% densities that we examine), can provide some reduction in the bipolar thermal conductivity in certain cases, although the effect is small. Importantly, however, we show that suppressing bipolar conduction is accompanied by an improvement in the overall power factor of the order of 10%. Given the importance of nanoinclusions in reducing lattice thermal conductivity, this power factor improvement in the bipolar regime shows that additional benefits in the ZT of nanostructured materials can be achieved under proper optimisation.

References:

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