EPSRC Thermoelectric Network UK Meeting, 2nd May 2019, Kings College, London.

Nanostructuring for reducing the bipolar effect in thermoelectric materials

Samuel Foster[a] and Neophytos Neophytou[b]

School of Engineering, University of Warwick, CV7 4AL, Coventry, UK

[a]S.Foster@warwick.ac.uk (corresponding author), [b]N.Neophytou@warwick.ac.uk

Abstract

Many thermoelectric materials (e.g. BiTe, PbTe and SnSe) suffer from degraded performance at high temperatures due to their narrow band gaps which give rise to an additional term in the thermal conductivity and a reduction in the Seebeck coefficient [1, 2]. Efforts to reduce this phenomenon (the bipolar effect) have included alloying to increase the band gap [3], and superlattice barriers to filter minority carriers [4]. In addition, a large number of studies are currently devoted to nanostructuring such materials in order to reduce their lattice thermal conductivity.

In this work we theoretically address the possibility of reducing bipolar effects in low bandgap nanostructured materials by employing the quantum mechanical Non-Equilibrium Green's Function (NEGF) method. We simulate electron transport through two-dimensional systems embedded with densely packed nanoinclusions. We then extract the materials electrical conductivity, Seebeck coefficient and electronic thermal conductivity including its bipolar contribution. 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 can provide indeed provide some reduction in the bipolar thermal conductivity. Importantly, however, we show that suppressing the bipolar conduction is accompanied by an additional improvement in the overall power factor on the order of 10% [5]. 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 by proper optimisation.

References:

[1] F. Hao *et.* al. E. & E. Sci., **9**, 3120, 2016
[2] R. Liu *et.* al. J. Appl. Phys., **109**, 023719, 2011
[3] L. D. Zhao *et.* al. E. & E. Sci., **6**, 3346, 2013
[4] J. Bahk *et.* al. Phys. Rev. B, **93**, 165209, 2016
[5] S. Foster and N. Neophytou, Comp. Mat. Sci., 164, 91, 2019.