Increasing Thermoelectric ZT Using Interfacial Patterning

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With ~60% of all generated energy wasted as heat[1], energy harvesting is an important avenue of study. Thermoelectrics (TEs) offer the unique opportunity to recover this wasted energy, and improve performance, via a direct solid state conversion of heat to electricity. The key limitation of TEs is their poor power conversion efficiency, characterised by the dimensionless figure of merit, ZT. This value depends on both the electron and phonon transport characteristics, which themselves are interdependent. This interdependence has effectively limited the maximum ZT to its current value of ~3[2]. Therefore the ideal technique for raising ZT further would optimise these characteristics independently. With this in mind, we investigate interfacial patterning as a method for controlling the transport properties of phonons. This method utilises the fundamental difference in electron and phonon wavelengths to selectively scatter phonons and hence reduce thermal conductivity. Using density functional theory, we demonstrate the effectiveness of patterning on Si/Ge structures. We investigate three differently patterned interfaces, noting how subtle changes in the patterning can have dramatic effects on properties such as the effective mass and the lattice thermal conductivity. This patterning provides a technique to enhance ZT and a framework for producing more viable devices from any heterostructure-based TE materials.

1. M. Zebarjadi, K. Esfarjani, M. S. Dresselhaus, Z. F. Ren, G. Chen *En.Env. Sci.*, **2012**, 5, 5147

2. J. He, T. M. Tritt, *Science*, **2017**, 357, 6358, 9997