Thermoelectric Efficiency of Zero-dimensional Nanocomposites

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Abstract

Thermoelectrics are a promising area of materials research recently revitalised by the introduction of nanocomposites. In this project, we aim to derive a theoretical mechanism, through which new, high efficiency thermoelectric materials can be designed. This will involve a detailed understanding of the fundamental theories of solid-state physics, of which the phonon model plays a critical role. This theoretical project aims to guide expierment, keeping within practical limits and computationally modelling potential designs.

1 Introduction

1.1 Motivation

Energy and its use defines human society. Throughout history we have seen an upwards trend of energy consumption and with it we transform our environment and our lives.

Thermoelectric materials have great potential to revolutionise our energy harvesting methods due to their ability to convert heat directly into electricity. This potential has motivated decades of research, resulting in; radioisotope thermonuclear generators, solid state refrigerators and laser temperature control systems.

The main limitation of thermoelectric materials is their heat to electricity conversion efficiency. In modern applications, this is approximately 7% [1], roughly $4\times$ lower than what is currently possible for internal combustion engines [2].

Recent advances in nano-fabrication have facilitated the development of new nanocomposites. Closely resembling the principles behind metamaterials; nanocomposites are typically periodic arrays of nanoscale sheets, wires or particles. Arranging materials like this has shown [**?**]reat potential to increase the thermoelectric figure of merit ZT, a key parameter in the conversion efficiency discussed above.

1.2 Investigation

1.3 Approach

2 Background

All the theories discussed in this report are transport processes. Fundamental to them all are the non-equilibrium statistical mechanics of their particles.

2.1 Boltzmann Equation

2.2 Thermoelectricity

In 1821, Thomas Seebeck discovered that circuit made from two dissimilar metals, with junctions at different temperatures would deflect a compass magnet (**??**), he had discovered thermoelectricity. The temperature gradient ∇T between the junctions generates an electromotive force:

$$\mathbf{E_{emf}} = -S\nabla T \tag{1}$$

where S is the Seebeck coefficient, defined as the induced voltage per unit temperature difference, mathematically $\Delta S = \frac{\Delta V}{\Delta T}$ [**?**]. This coefficient is not only material dependent, but also temperature dependent, i.e., a temperature gradient produces an electromotive force gradient. This electromotive force gradient produces a current density gradient described macroscopically by a modified Ohm's law [**?**]:

$$\mathbf{J} = \sigma(-\nabla V - S\nabla T) \tag{2}$$

where $\mathbf{J}$ and σ are the current density $\frac{I}{A}$ and electrical conductivity at a given location in the material and ∇T and ∇V are the temperature and resultant voltage gradients across the material. If we were to repeat the experiment conducted by Seebeck (Figure **??**), using a probe to measure V between junctions and σ at each junction for one of the metals, assuming steady state, i.e., $I = 0$ so $\mathbf{J} = 0$, the metal's Seebeck coefficient can be determined.

Thermoelectricity, its uses and current nanocomposite research are well summarised by J. W. Bos [**?**] and A. J. Minnich *et al.* [5].

2.3 Nanocomposites

Composite materials are combinations of two or more materials, forming a new structure with significantly different physical or chemical properties than its constituent parts. In a similar way, nanocomposites are the seebeck-experiment-black.png

Figure 1: Thomas Seebeck's original thermoelectricity experiment diagram [?]. A compass needle lies on top of one metal, underneath a bridge of a different metal (K), connected by two junctions and heated at one of these junctions.

`graphene-superlattice.eps`

Figure 2: Superlattice of graphene and copper. Alternate layers of nanoscale copper and graphene are sandwiched together.

structuring of multiple materials, but at the nanoscale. As our nanocomposites are at a comparable size to the crystal lattices of their constituent materials, we can view nanocomposites as artificial defects in a larger crystal lattice. A simple example of a 2D nanocomposite, a copper-graphene superlattice, is pictured in Figure **??**. Examining one layer of the superlattice, the material in bulk form would be a 3D crystal structure, but by constraining the layer thickness we have introduced a boundary defect. The periodic array of these boundary defects forms a new 3D artificial crystal, which we define as a superlattice, a nanocomposite.

2.4 Kinetic Theory

Assumptions

3 Specifics

3.1 Thermoelectric Theory

Assumptions

4 Results and Analysis

5 Conclusion and Potential Development

`https://github.com/kahlos/thermoelectrics`

References

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