Nanocomposite Thermoelectric Materials

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ABSTRACT

We have studied the thermoelectric properties of nanoscale silicon spheres embedded within a germanium host. Our theory has identified that 10nm diameter spheres, with the densest possible packing, has the potential to improve thermoelectric efficiency 10x. If cost effective fabrication methods are found, this will enable a multitude of technological applications.

THERMOELECTRICITY

In any material, heat is conducted via two carriers; phonons and electrons. Thermoelectricity is simply a heat induced electrical potential, whereby electrons or holes are driven across a thermal gradient, producing a current.

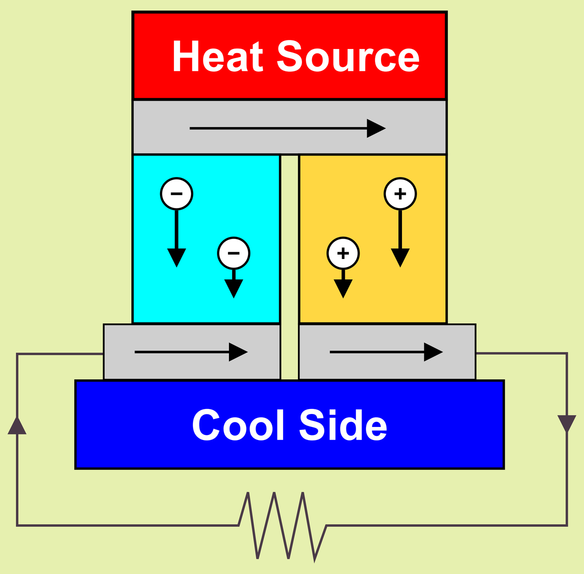

Figure 1. A thermoelectric circuit configured as an electrical generator. N and P-doped thermoelectrics are placed across a heat gradient, driving electrons and holes to recombine, generating a current.

NANOCOMPOSITES

Much like a traditional composite, a nanocomposite is comprised of two or more materials assembled to form a functionally distinct material. Typically, nanoscale sheets, wires or particles are dispersed into a bulk material, forming an artifical structure with significantly altered properties.

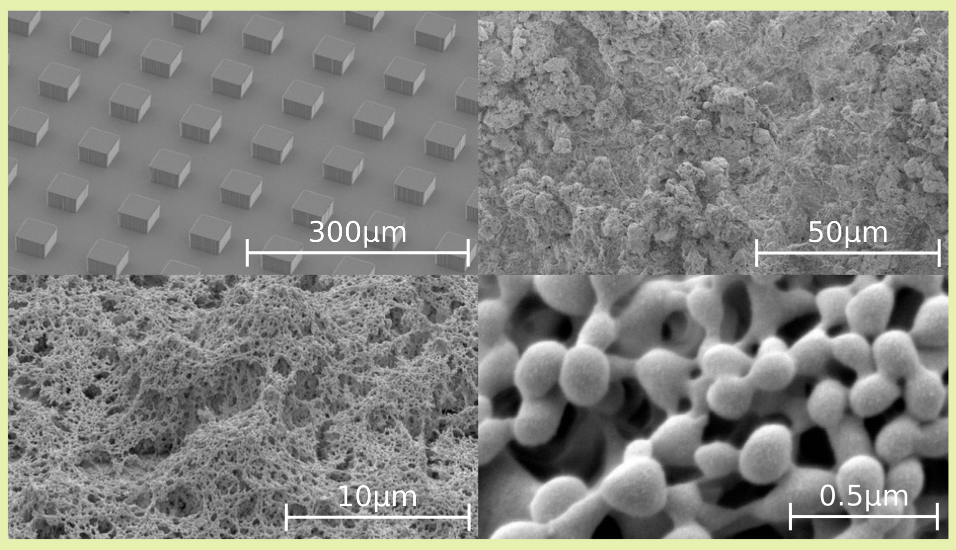

Figure 2. A STEM image of a nanocomposite at several different scales

APPLICATIONS

Thermoelectric materials have the potential to revolutionise current electricity generation and refridgeration methods. They are both simple to use and incredibly reliable; apply a heat gradient for electricity, apply electricity for cooling. Currently, their efficiency limits applications to space probes, where reliability is vitally important. But with the potential advancements of nanocomposite design, we could see utilisation in heat recovery systems, refridgeration and solar thermal generation.

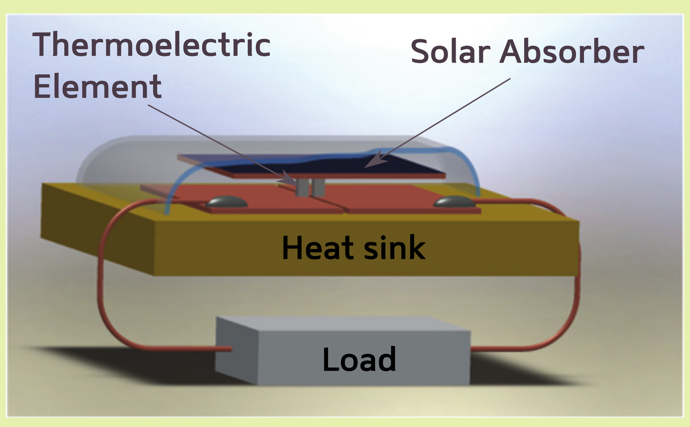

Figure 3. A solar thermal thermoelectric panel design. Sunlight heats the solar absorber, producing a thermal gradient across the two thermoelectric elements, generating a current across the load.

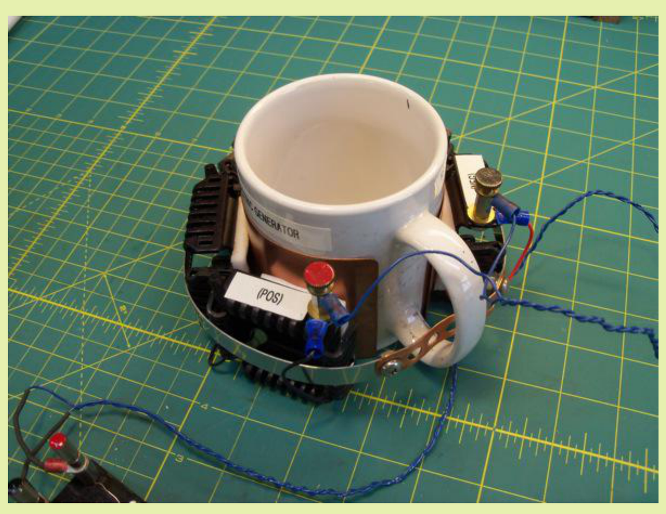

Figure 4. A prototype coffee cup heat recovery system. A thermal gradient between the heat sinks and the cup light a small bulb.

PHONON HEAT CONDUCTION

Key to our project, was the reduction of phonon thermal conductivity K_{ph} via nanocomposite structuring. A reduction in K_{ph}, will increase the total thermoelectric efficiency, as described by the figure of merit (ZT):

$$ZT = \frac{S^2 \sigma T}{K_{el} + K_{ph}}$$

Equation 1:
Defines the thermoelectric figure of merit (ZT) ∝ conversion efficiency. Seebeck cofficient (S), electrical conductivity (σ), temperature (T),

We investigated two different composite theories; the effective medium approximation (EMA) [2] and the phonon hopping model (PHM) [5]. From our analysis, the PHM model neglected crucial thermoelectric properties, so we adopted the EMA model.

The EMA considers the phonon thermal conductivity of a homogenous host medium (k_h), peterbed by a fluctuating particle inclusion conductivity (k_p), with a thermal boundry resistance (α). We assume the particle-host interface scatters phonons diffusively and is described by the acoustic mismatch model [6]. For spherical particle inclusions, the EMA simplifies to:

$$\frac{k_e}{k_h} = \frac{k_p(1+2\alpha)+2k_h+2\varphi[k_p(1-\alpha)-k_h]}{k_p(1+2\alpha)+2k_h-\varphi[k_p(1-\alpha)-k_h]}$$

Equation 2:
Defines phonon thermal conductivity (k_e) of a spherical macrocomposite. Thermal conductiviy of the host medium (k_h), thermal boundry resistance (α), volume fraction of particle to host per unit cell (φ)

For nanocomposites, the EMA needs to be modified to account for increased scattering in and around particle inclusions. The mEMA [3] proposes a reduction of k_p and k_h based on the interface density of nanoparticles.

ELECTRICAL TRANSPORT

We derived from first principles, all the electrical properties to complete our ZT expression. Of upmost importance is the temperature dependent Fermi level (E_F), defined for an extrinsic semiconductor [7]:

$$E_F = E_g + \frac{3}{4}kT\ln\left(\frac{m_h^*}{m_e^*}\right) + kT\sinh^{-1}\left(\frac{N_d - N_a}{2\sqrt{U_c U_v}\exp - \frac{E_g}{2kT}}\right)$$

Equation 3:
Defines the Fermi level (E_F) of an extrinsic semiconductor.
Band gap (E_g), hole & electron effective mass (m*), donor & acceptor dopant concentration (N_d), effective conductance & valence band (U_c)

$$K_e = \frac{k_B^2}{e^2}\left(P + \frac{5}{2}\right)\sigma T$$

$$S = \frac{k_B}{e}\left(\frac{2E_F}{k_B T} - \left(P + \frac{5}{2}\right)\right)$$

RESULTS

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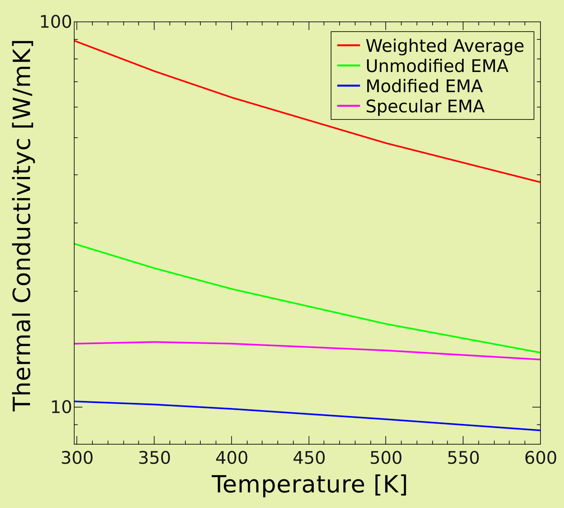

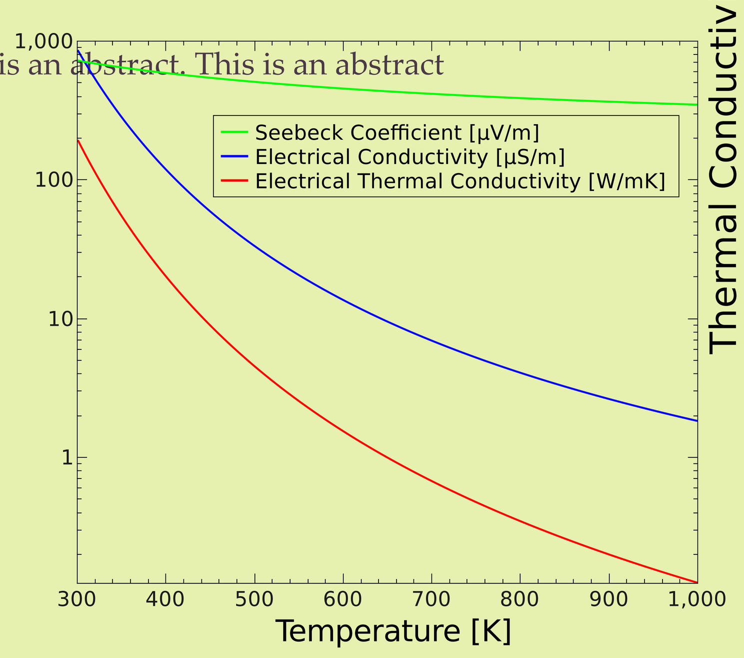

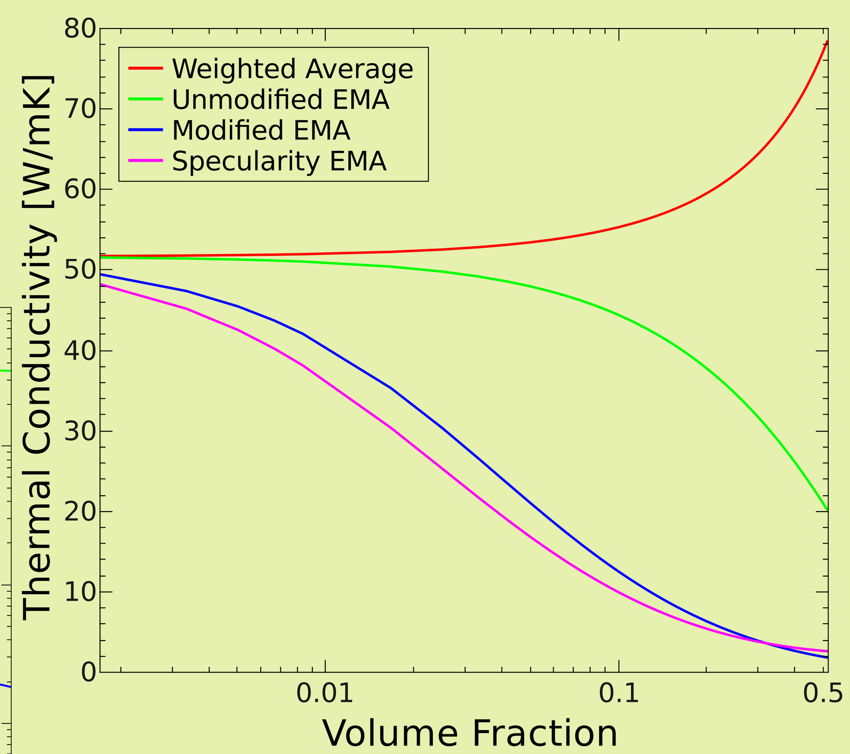

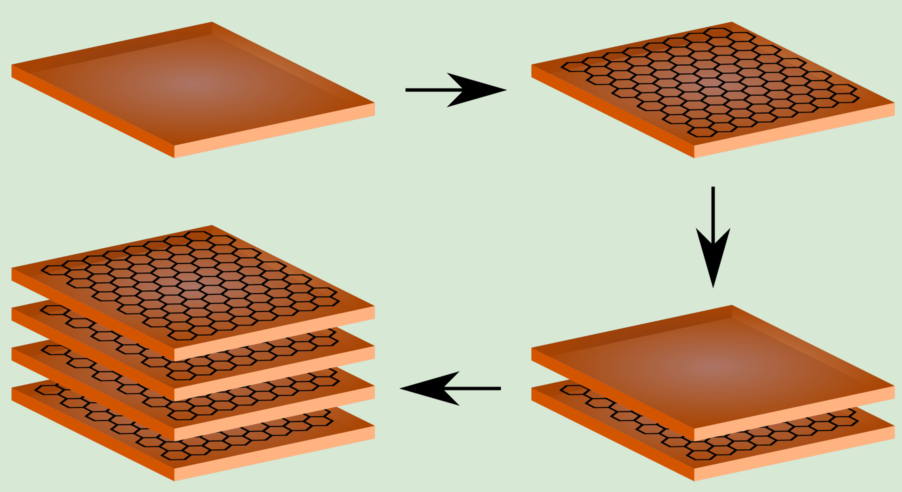

Figure 4. A nanocomposite of graphene and copper, known as a superlattice. Alternating layers of nanoscale copper and graphene are sandwiched together to produce a new material with altered properties.

FUTURE WORK

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