NANOSTRUCTURED SILICON THERMOELECTRICS

Thesis by

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To My Wife, Yi-Chun Iris Chen and My Parents,

Hsueh-Erh Hsu Yu and Jung-Tsung Yu

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ABSTRACT

The thesis discusses the thermoelectric properties of silicon nanostructures with a particular focus on their heat transport phenomenon. The aim of this thesis work is to design ultra-low thermal conductivity materials based on fundamental phonon physics. Silicon nanowires and silicon nanomeshes are the model nanostructure systems investigated in this thesis.

Degenerately boron-doped silicon nanowires (20 nm x 20 nm cross section) exhibit thermal conductivity, depending on the temperature of interest, roughly two orders of magnitude smaller than bulk silicon with similar impurity concentration. The reduction in thermal conductivity is presumably from increased boundary scattering of the thermal phonons. For smaller nanowire systems (e.g., 10 nm x 20 nm cross section), thermal conductivity lower than the amorphous limit is also observed. Dimensional crossover of the thermal phonons in these ultra-small nanowire systems is proposed to explain the thermal conductivity reduction. Thermoelectric figure-of-merit ZT~1, a two order of magnitude improvement is achieved in 20 nm x 20 nm silicon nanowires at 200K.

Silicon nanomeshes are designed to further reduce the thermal conductivity of silicon. The 2-D hole-array is patterned on the silicon nanomesh film as Bragg reflectors to slow down the phonon group velocity. From the direct thermal conductivity measurement via suspended microstructure platform, the coherent scattering mechanism effectively reduces the thermal conductivity of silicon by a factor of two from the nanowire value. In essence, the phononic metamaterial approach essentially creates a new class of silicon-based

material with distinct phonon properties, in other words, the theoretical lower limit of thermal conductivity of silicon based on bulk dispersions no longer applies to the phononic nanomeshes. In addition, silicon nanomeshes exhibit bulk-like electrical conductivity rendering them potential high efficiency thermoelectrics.

In Chapter 1, an introduction to the lattice thermal conductivity is given to point out the key parameters affecting the phonon transport, e.g., scattering mechanisms, phonon dispersions and phonon density-of-states. The thermoelectrics fundamentals are given in Chapter 2, as are the experimental results on silicon nanowires. The fabrication and measurement methodologies are also explained in this chapter. In Chapter 3, the phonon transport mechanism of the silicon nanomesh, a new class of phononic metamaterial, is investigated. A coherent phonon scattering mechanism is used to explain the unexpected phonon behaviors. A complete fabrication process flow is also developed in this chapter in order to fully release the nanostructure from the substrate for precise and accurate thermal conductivity measurement. In the last part of the thesis (Chapter 4), the phononic nanomesh approach is extended to a nanomesh superlattice structure. The architectural design is to incorporate interfacial thermal resistance or the Kapitza resistance to further reduce the thermal conductivity of silicon. In addition, device architecture consisting of self-assembled quantum dots is proposed to enhance the thermoelectric efficiency by energy-filtering mechanism.

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