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14. ABSTRACT

In this project, we have studied, through computer simulation, how the three dimensional (3D) phononic crystal structures can confine phonon and thus reduce thermal conductivity significantly leading to an enhancement of efficiency of energy conversion in thermoelectric applications. In particular, we have studied a nanoscale 3D Si phononic crystal (PnC) with spherical pores, which can reduce thermal conductivity of bulk Si by a factor up to 10,000 times at room temperature. The phonon participation ratio spectra demonstrate that more phonons are localized as the porosity increases. The thermal conductivity is found insensitive to the temperature changes from room temperature to 1,100K. The effect of period length and mass ratio on thermal conductivity is also studied.

15. SUBJECT TERMS
phonon transport , Thermoelectric, nano structures, nano photonics

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Final Report for AOARD Grant 124047

"Manipulating heat flow through three dimensional (3D) nanoscale phononic crystal structure"

Date: June 2, 2014

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Abstract:

In this project, we have studied, through computer simulation, how the three dimensional (3D) phononic crystal structures can confine phonon and thus reduce thermal conductivity significantly leading to an enhancement of efficiency of energy conversion in thermoelectric applications. In particular, we have studied a nanoscale 3D Si phononic crystal (PnC) with spherical pores, which can reduce thermal conductivity of bulk Si by a factor up to 10,000 times at room temperature. The phonon participation ratio spectra demonstrate that more phonons are localized as the porosity increases. The thermal conductivity is found insensitive to the temperature changes from room temperature to 1,100K. The effect of period length and mass ratio on thermal conductivity is also studied.

Details of the main project can be found in the publication:

L-N Yang, N Yang, and B Li, Extreme Low Thermal Conductivity in Nanoscale 3D Si Phononic Crystal with Spherical Pores, *Nano Letters* **14**, 1734 Published on 21 Feb (2014). dx.doi.org/10.1021/nl403750s

List of Publications and Significant Collaborations that resulted from your AOARD supported project:

a. Two papers have been published in peer-reviewed journals,

   1. L-N Yang, N Yang, and B Li, Extreme Low Thermal Conductivity in Nanoscale 3D Si Phononic Crystal with Spherical Pores, *Nano Letters* **14**, 1734 Published on 21 Feb (2014). dx.doi.org/10.1021/nl403750s

   2. L-N Yang, N Yang, and B Li, Reduction of Thermal Conductivity by Nanoscale 3D Phononic Crystal, *Scientific Report* **3**, 1143, published on 31 January 2013

b. Manuscript submitted but not yet published

L-N Yang, J Chen, N Yang, and B Li, Manipulating Graphene Thermal Conductivity by Phononic