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**Toward Thermal Wavelength Scale Two-and Three-Dimensional Phononic Crystals**

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**Final Report**

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## Towards Thermal Wavelength Scale Two-and-Three Dimensional Photonic Crystals

Contract/Grant #: FA9550-12-1-0073

Reporting Period (since last report submission): April 1, 2015 to December 31, 2015

Final Reporting Period: April 1, 2012 to December 31, 2015

Paul Braun (PI), David Cahill and Sanjiv Sinha (co-PIs)

During the last period of performance, the team investigated the effect of patterning two-dimensional arrays of holes in thin-film silicon on its thermoelectric figure of merit, the anisotropic thermal conductivity of nanoscale graphite layers and the changes in the thermal conductivity of a prototypical perovskite oxide, SrTiO<sub>3</sub>, with off-stoichiometric compositions.

In the Si work, we investigated the effect of patterning two-dimensional array of holes in thin-film silicon on its thermoelectric figure of merit. Distinct from previous work, we measured all three properties (electrical conductivity, thermal conductivity and the Seebeck coefficient) on the same sample at different doping. We were able to successfully fabricate *n*-type samples with low electrical resistivity down to few mΩ-cm. In the bulk, the thermoelectric power factor peaks at  $\sim 4 \times 10^{19} \text{ cm}^{-3}$ . In “holey” silicon, we have measured the power factor in the vicinity of such doping to be approximately one half of that in the bulk, contrary to previous reports that there is no degradation in the power factor. Combined with a thermal conductivity reduced to  $\sim 10 \text{ W/mK}$  at 300 K, we find the overall enhancement in *ZT* to be modest compared to bulk silicon. We will report these findings in a manuscript under preparation [1]. We are further investigating frequency dependence in the scattering of acoustic phonons from holes in such 2-dimensional periodic arrays and are completing this now.

We studied the anisotropic thermal conductivity of nanoscale graphite layers deposited by chemical vapor deposition on Ni substrates at relatively low temperatures between 825 and 900 °C [2]. Graphite layers have potential as heat spreaders for flexible electronics. The in-plane thermal conductivity varies with deposition temperature between 650 and 1000  $\text{W m}^{-1} \text{K}^{-1}$ , and is 30-50% of the in-plane thermal conductivity of HOPG. The reduced thermal conductivity in comparison to HOPG is attributed to a combination of grain boundaries and structural disorder. We developed a figure-of-merit for a flexible heat-spreader and find that the figure-of-merit for CVD graphite is a factor of 2 larger than the figure-of-merit for Au.

We also studied, in collaboration with colleagues at Cornell University, the changes in the thermal conductivity of a prototypical perovskite oxide, SrTiO<sub>3</sub>, produced by microstructures induced by off-stoichiometric compositions [3]. Epitaxial layers were grown by reactive molecular-beam epitaxy and characterized by transmission electron microscopy. Both point defects and planar defects decrease the longitudinal thermal conductivity with the greatest decrease observed for films containing planar defects oriented perpendicular to the direction of heat flow. The longitudinal thermal

conductivity can be modified by as much as 80%—from  $11.5 \text{ W m}^{-1} \text{ K}^{-1}$  for stoichiometric homoepitaxial  $\text{SrTiO}_3$  to  $2 \text{ W m}^{-1} \text{ K}^{-1}$  for strontium-rich films—by incorporating  $(\text{SrO})_2$  Ruddlesden-Popper planar defects.

#### References

1. J. Ma, K.V. Valavala, J.S. Sadhu, H. Tian, and S. Sinha, “Effect of patterning holes on  $ZT$  in  $n$ -type silicon near optimal doping”, In preparation.
2. Qiye Zheng, Paul V. Braun, and David G. Cahill, “Thermal conductivity of graphite thin films grown by low temperature chemical vapor deposition on Ni (111),” submitted for publication.
3. Charles M. Brooks, Richard B. Wilson, Anna Schäfer, Julia A. Mundy, Megan E. Holtz, David A. Muller, Jürgen Schubert, David G. Cahill, and Darrell G. Schlom, "Tuning thermal conductivity in homoepitaxial  $\text{SrTiO}_3$  films via defects," *Appl. Phys. Lett.* **107**, 051902 (2015).

1.

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Towards Thermal Wavelength Scale Two-and-Three Dimensional Photonic Crystals

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**Principal Investigator Name****The full name of the principal investigator on the grant or contract.**

Prof. Paul V Braun

**Program Manager****The AFOSR Program Manager currently assigned to the award**

Dr. John Luginsland

**Reporting Period Start Date**

04/01/2012

**Reporting Period End Date**

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**Abstract**

The team investigated the effect of patterning two-dimensional arrays of holes in thin-film silicon on its thermoelectric figure of merit, the anisotropic thermal conductivity of nanoscale graphite layers and the changes in the thermal conductivity of a prototypical perovskite oxide, SrTiO<sub>3</sub>, with off-stoichiometric compositions. In the Si work, we find the overall enhancement in ZT for holey Si to be modest compared to bulk silicon. Distinct from previous work, we measured all three properties (electrical conductivity, thermal conductivity and the Seebeck coefficient) on the same sample at different doping. We were able to successfully fabricate n-type samples with low electrical resistivity down to few mΩ-cm. In "holey" silicon, we have measured the power factor in the vicinity of such doping to be approximately one half of that in the bulk, contrary to previous reports that there is no degradation in the power factor. In the carbon work, we studied the deposited by chemical vapor deposition on Ni substrates at relatively low temperatures between 825 and 900 °C. The in-plane thermal conductivity varies with deposition temperature between 650 and 1000 W m<sup>-1</sup> K<sup>-1</sup>, and is 30-50% of the in-plane thermal conductivity of HOPG. The reduced thermal conductivity in comparison to HOPG is attributed to a combination of grain boundaries and structural disorder. We developed a figure-of-merit for a flexible heat-spreader and find that the figure-of-merit for CVD graphite is a factor of 2 larger than that for Au. Finally, in the perovskite work, we find the longitudinal thermal conductivity can be modified by as much as 80%—from 11.5W m<sup>-1</sup> K<sup>-1</sup> for

stoichiometric homoepitaxial SrTiO<sub>3</sub> to 2W m-1 K-1 for strontium-rich films—by incorporating (SrO)<sub>2</sub> Ruddlesden-Popper planar defects.

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### **Archival Publications (published) during reporting period:**

1. J. Ma, B.R. Parajuli, M.G. Ghossoub, A. Mihi, J. Sadhu, P.V. Braun and S. Sinha, "Coherent Phonon-Grain Boundary Scattering in Silicon Inverse Opals," Nano Letters, 13, 618-624 (2013). DOI: 10.1021/nl304190s
2. P.K. Singh, M.H. Seong and S. Sinha, "Detailed Consideration of the Electron-Phonon Thermal Conductance at Metal-Dielectric Interfaces," Applied Physics Letters, 102, 181906 (2013). DOI: 10.1063/1.4804383
3. J. Ma, J.S. Sadhu, D. Ganta, H. Tian, and S. Sinha, "Thermal transport in 2- and 3-dimensional periodic 'holey' nanostructures," AIP Advances 4, 124502 (2014). DOI: 10.1063/1.4904073
4. R.B. Wilson and D.G. Cahill, "Anisotropic failure of Fourier's law in Si and MgO and the importance of temperature-profile extrema," Nature Commun., 5, 5075 (2014). DOI: 10.1038/ncomms6075
5. J. Liu, G.-M. Choi, and D.G. Cahill, "Measurement of the anisotropic thermal conductivity of molybdenum disulfide by the time-resolved magneto-optic Kerr effect," J. Appl. Phys. 116, 233107 (2014). DOI: 10.1063/1.4904513
6. R.B. Wilson and D.G. Cahill, "Limits to Fourier theory in high thermal conductivity single crystals," Appl. Phys. Lett. 107, 203112 (2015). DOI: 10.1063/1.4935987
7. C.M. Brooks, R.B. Wilson, A. Schäfer, J.A. Mundy, M.E. Holtz, D.A. Muller, J. Schubert, D.G. Cahill, and D.G. Schlom, "Tuning thermal conductivity in homoepitaxial SrTiO<sub>3</sub> films via defects," Appl. Phys. Lett., 107, 051902 (2015). DOI: 10.1063/1.4927200
8. Q. Zheng, P.V. Braun, and D.G. Cahill, "Thermal conductivity of graphite thin films grown by low temperature chemical vapor deposition on Ni (111)," submitted for publication.
9. J. Ma, K.V. Valavala, J.S. Sadhu, H. Tian, and S. Sinha, "Effect of patterning holes on ZT in n-type silicon near optimal doping," in preparation.
10. H. Tian, J.S. Sadhu, J. Ma, D. Ganta, and S. Sinha, "Multiple scattering of phonons in mesoporous silicon from low temperature measurements," in preparation.

11. H. Tian, J.S. Sadhu, J. Ma, D. Ganta, and S. Sinha, "Characterization of free carrier concentration after ex-situ doping of mesoporous silicon", in preparation.

**Changes in research objectives (if any):**

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**Extensions granted or milestones slipped, if any:**

No-cost extension granted on March 31, 2015.

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**Laboratory Task Manager**

**Program Officer**

**Research Objectives**

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Supplies			
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