Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Kapitza resistance at segregated boundaries in β-SiC NIPUN GOEL, EDMUND WEBB III, ALPARSLAN OZTEKIN, JEFFREY RICKMAN, SUDHAKAR NETI, Lehigh University — Silicon Carbide is a candidate material for high-temperature thermoelectric applications for harvesting waste heat associated with exhaust from automotive and furnaces as well hot surfaces in solar towers and power electronics. However, for SiC to be a viable thermoelectric material, its thermoelectric figure of merit must be improved significantly. In this talk we examine the role of grain-boundary segregation on phononic thermal transport, an important factor in determining the figure of merit, via non-equilibrium molecular dynamics simulations. In particular, we consider the role of dopant concentration and dopant/matrix interactions on the enhancement of the Kapitza resistance of symmetric tilt grain boundaries. We find that the calculated resistance depends on the segregation profile, with increases of more than a factor of 50 (relative to an unsegregated boundary) at the highest dopant concentrations. Finally, we relate the calculated phonon density of states to changes in the Kapitza resistance.

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Date submitted: 31 Oct 2015 Electronic form version 1.4