Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Thermal conductivity of silicon nanowires: interplay between core defects and surface roughness YUPING HE, GIULIA GALLI, UC Davis — Recent experiments [1] suggested that the thermal conductivity (κ) of Si nanowires may be reduced by about two orders of magnitude compared to that of bulk Si (κ_{bulk}), making them attractive materials for thermoelectric applications. Size reduction plays an important role [2] in determining such reduction but it does not fully account for recent measurements [1]. We investigated κ in wires with 15 nm diameter (comparable to experimental sizes) using large scale molecular dynamics simulations. We show that, unlike the case of thin [3] (2-3 nm diameter) rods, the presence of an amorphous layer at the surface accounts only for a decrease by a factor of 4 in κ with respect to that of wires with smooth surfaces. It is the combined effect of defects in the core and rippled surfaces that enables a decrease up to a factor of 90 with respect to κ_{bulk}. Work supported by DOE/SciDAC-e.

[1] A.I. Hochbaum et al., Nature 451, 163 (2008); A. I. Boukai et al., Nature, 451, 168 (2008).
[2] D.Li et al. APL 2003.
[3] D. Donadio and G. Galli, Phys. Rev. Lett. 102, 195901 (2009).

Yuping He
UC Davis

Date submitted: 01 Dec 2011 Electronic form version 1.4