

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Atomistic simulations of thermal transport in Si and SiGe based materials: From bulk to nanostructures¹ IVANA SAVIC, Department of Chemistry, UC Davis, USA, NATALIO MINGO, LITEN, CEA-Grenoble, France, DAVIDE DONADIO, Department of Chemistry, UC Davis, USA, GIULIA GALLI, Department of Chemistry and Department of Physics, UC Davis, USA — It has been recently proposed that Si and SiGe based nanostructured materials may exhibit low thermal conductivity and overall promising properties for thermoelectric applications. Hence there is a considerable interest in developing accurate theoretical and computational methods which can help interpret recent measurements, identify the physical origin of the reduced thermal conductivity, as well as shed light on the interplay between disorder and nanostructuring in determining a high figure of merit. In this work, we investigate the capability of an atomistic Green's function method [1] to describe phonon transport in several types of Si and SiGe based systems: amorphous Si, SiGe alloys, planar and nanodot Si/SiGe multilayers. We compare our results with experimental data [2,3], and with the findings of molecular dynamics simulations and calculations based on the Boltzmann transport equation. [1] I. Savic, N. Mingo, and D. A. Stewart, Phys. Rev. Lett. 101, 165502 (2008). [2] S.-M. Lee, D. G. Cahill, and R. Venkatasubramanian, Appl. Phys. Lett. 70, 2957 (1997). [3] G. Pernot et al., submitted.

¹Work supported by DOE-SciDAC, DE-FC02-06ER25794.

Giulia Galli
Department of Chemistry and Department of Physics, UC Davis

Date submitted: 20 Nov 2009

Electronic form version 1.4