Thermal Transport in SiGe Alloy-based Nanowires and Superlattices for Thermoelectric Applications

Zlatan Aksamija[a] and Irena Knezevic[b]

[a] *Electrical and Computer Engineering, University of Massachusetts-Amherst, USA, zlatana@engin.umass.edu*
[b] *Electrical and Computer Engineering, University of Wisconsin-Madison, USA.*

Silicon-germanium (SiGe)[1] nanowires and $Si/Si_{1-x}Ge_x$ superlattices[2] show promise for application as efficient thermoelectrics because of their low thermal conductivity, below that of bulk $Si_{1-x}Ge_x$ alloys (Fig. 1). Addition of quantum dots at the interface between layers of the SL has also been shown to decrease thermal conductivity[3,4]. Lattice thermal conductivity in nanowires is dominated by partially diffuse scattering at the boundaries, while in superlattices it is dominated by scattering from the rough interfaces between layers, even at room temperature[5]. Therefore, boundary and interface properties, such as roughness, orientation, and composition, are expected to play a significant role in thermal transport and they offer additional degrees of freedom to control the thermal conductivity in semiconductor nanostructures.

We demonstrate the sensitivity of the lattice thermal conductivity in SiGe nanostructures to the properties of their boundaries and interfaces, based on solving the phonon Boltzmann transport equation under the relaxation time approximation. Previous calculations relied on treating the interface scattering with an empirical specularity parameter, which is then adjusted to fit measured data. In this work, in order to accurately treat phonon scattering from a series of rough interfaces with a given rms roughness height (Δ), we employ a *momentum-dependent* specularity parameter $p(\mathbf{q})$ that is the fraction of specular reflections to the total number of reflections from a rough boundary ($0<p(\mathbf{q})<1$). $p(\mathbf{q})$ is obtained from the momentum-dependent specularity parameter for a single boundary or interface[6] $p(\mathbf{q})=\exp(-4\pi^2\Delta^2q^2\cos^2\theta)$ by averaging this specularity parameter over the distribution of roughness heights on the surface of a nanowire or the many interfaces present between the successive layers in a superlattice.

Diffuse boundary scattering usually gives a phonon a lifetime that is proportional to the smallest distance between the boundaries; however, in the case of SiGe alloy-based nanostructures, strong alloy scattering due to the difference in mass between the Si and Ge atoms plays a significant role (Figure 1). We show that, in the calculation of the total phonon lifetime, there is a competition between surface roughness and internal scattering mechanisms which include Umklapp phonon-phonon, impurity, and isotope scattering. The expressions for τ_{phonon} and $\tau_{isotope}$ were previously shown in Ref. 6. The full thermal conductivity tensor $\kappa^{\alpha\beta}$ of a nanowire is computed as a sum over all phonon momenta and branches. In the case of a superlattice, the two alternating layers are combined in series for cross-plane transport through the SL, and in parallel for in-plane transport along the plane of the interfaces. Results for 4 nm SiGe SLs (Fig. 2) show a strong anisotropy of thermal conductivity due to the directional dependence of the phonon velocity and boundary scattering [7]. The computed values of κ show excellent agreement with the measurements on $Si_{1-x}Ge_x$ SLs [2] (Fig. 3 and Fig. 4) at both high and low temperatures.

1.Lee, S.-M., Cahill, D. G. & Venkatasubramanian, R. Thermal conductivity of Si–Ge superlattices. *Appl. Phys. Lett.* **70**, 2957-2959 (1997).
2.Huxtable, S. T. *et al.* Thermal conductivity of Si/SiGe and SiGe/SiGe superlattices. *Appl. Phys. Lett.* **80**, 1737-1739 (2002).

3.Lee, M. L. & Venkatasubramanian, R. Effect of nanodot areal density and period on thermal conductivity in SiGe/Si nanodot superlattices. *Appl. Phys. Lett.* **92**, 053112 (2008).
4. Pernot, G. *et al.* Precise control of thermal conductivity at the nanoscale through individual phonon-scattering barriers. *Nat. Mater.* **9**, 491–495 (2010).
5. Chen, G. Thermal conductivity and ballistic-phonon transport in the cross-plane direction of superlattices. *Phys. Rev. B* **57**, 14958–14973 (1998).
6. Aksamija, Z. & Knezevic, I. Anisotropy and boundary scattering in the lattice thermal conductivity of silicon nanomembranes. *Phys. Rev. B* **82**, 045319 (2010).
7. Liu, W. L., Borca-Tasciuc, T., Chen, G., Liu, J. L. & Wang, K. L. Anisotropic Thermal Conductivity of Ge Quantum-Dot and Symmetrically Strained Si/Ge Superlattices. *Journal of Nanoscience and Nanotechnology* **1**, 39-42(4) (2001).

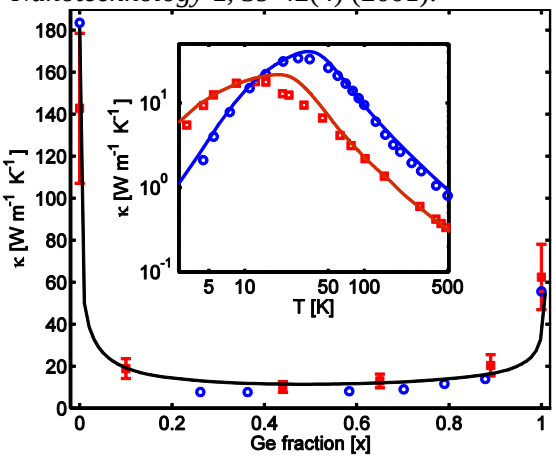

Figure 1. Thermal conductivity of bulk SiGe alloys, showing a strong variation of thermal conductivity with the germanium proportion x due to mass difference between Si and Ge.

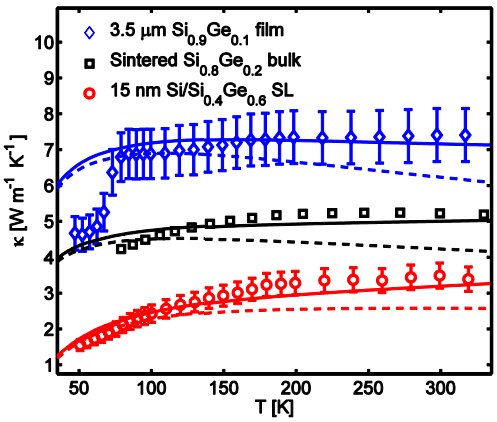

Figure 3. Thermal conductivity of a 3.5 um $Si_{0.9}Ge_{0.1}$ alloy film (black) and a 15 nm period thickness $Si/Si_{0.4}Ge_{0.6}$ alloy superlattice (red). Dashed lines indicate lattice thermal conductivity, while solid lines include the electronic contribution.

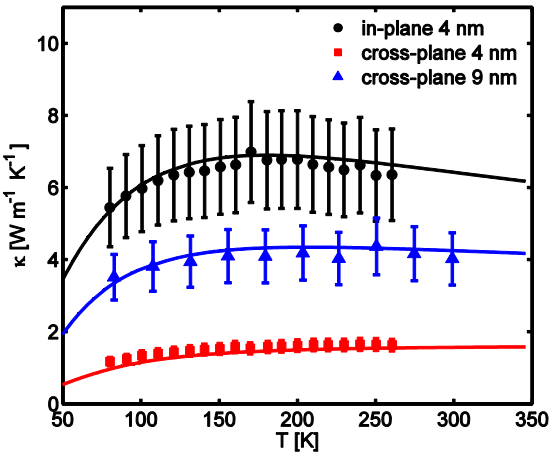

Figure 2. Thermal conductivity of a 9 nm period Si/Ge superlattice in the cross-plane direction (blue diamonds), and a 4 nm period Si/Ge superlattice in both the in-plane (black circles) and cross-plane directions (red squares).

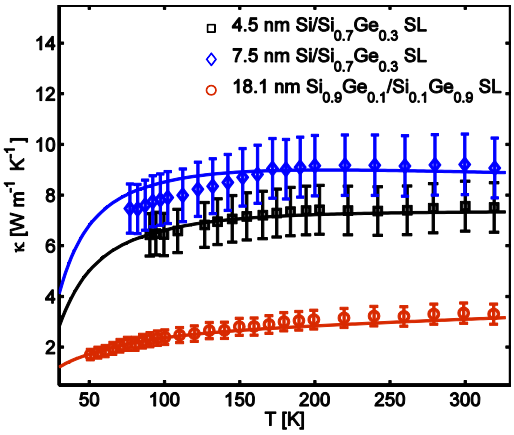

Figure 4.Cross-plane thermal conductivity of $Si_{1-x}Ge_x/Si_{1-y}Ge_y$ superlattices showing strong decrease due to combined effect of alloying and interface scattering.