Thermal conductivity of Si/SiGe and SiGe/SiGe superlattices

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The cross-plane thermal conductivity of four $Si/Si_{0.7}Ge_{0.3}$ superlattices and three $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices, with periods ranging from 45 to 300 and from 100 to 200 Å, respectively, were measured over a temperature range of 50 to 320 K. For the $Si/Si_{0.7}Ge_{0.3}$ superlattices, the thermal conductivity was found to decrease with a decrease in period thickness and, at a period thickness of 45 Å, it approached the alloy limit. For the $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ samples, no dependence on period thickness was found and all the data collapsed to the alloy value, indicating the dominance of alloy scattering. This difference in thermal conductivity behavior between the two superlattices was attributed to interfacial acoustic impedance mismatch, which is much larger for $Si/Si_{0.7}Ge_{0.3}$ than for $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$. The thermal conductivity increased slightly up to about 200 K, but was relatively independent of temperature from 200 to 320 K. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1455693]

The thermal conductivity of semiconductor superlattice films is of great importance for the performance of thermoelectric coolers and power converters as well as of optoelectronic devices. Low thermal conductivity materials are desired for thermoelectric elements in order to reduce the backflow of heat from the hot to cold junctions, while high conductivity materials are necessary for optoelectronic devices in order to dissipate heat. Recently, the thermal conductivity of several superlattice systems including GaAs/AlAs,[1–5] Si/Ge,[6,7] Si/SiGe,[8] and Bi_2Te_3/Sb_2Te_3 (Refs. 9 and 10) has been a topic of significant interest. Several of these studies have shown that the thermal conductivity of a superlattice can be lower than a corresponding value calculated from Fourier heat conduction theory using the constituent materials' bulk thermal conductivity. However, the causes for this dramatic reduction in thermal conductivity are not entirely clear, and a variety of mechanisms such as mismatch in acoustic impedance and phonon spectra, miniband formation, and interface scattering due to roughness and defects have been proposed as contributors. The primary goal of this work is to examine the role of the interface and acoustic impedance mismatch in the reduction of the thermal conductivity.

The superlattice samples were grown by molecular beam epitaxy (MBE) at HRL Laboratories, LLC, and complete details of the growth can be found elsewhere.[11] They were grown on Si substrates upon which a buffer layer was deposited to reduce strain and to ensure good growth conditions for the superlattice. Capping the superlattice were Si_xGe_{1-x} alloys doped appropriately to provide good ohmic contact. The thickness ratio of the two superlattice materials within each period was maintained at 2:1 and 1:1 for the $Si/Si_{0.7}Ge_{0.3}$ and $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices, respectively. Four $Si/Si_{0.7}Ge_{0.3}$ superlattices with period thicknesses of 300, 150, 75, and 45 Å were investigated along with three $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices with period thicknesses of 100, 150, and 200 Å. This comparison offers an opportunity to examine how the thermal conductivity may be influenced by alloy and defect scattering, miniband formation, tunneling, and phonon spectra acoustic impedance mismatch (AIM). The $AIM=(\rho V)_1/(\rho V)_2$ where ρ is the material density, V is the speed of sound, and subscripts 1 and 2 represent the adjacent layers. The AIM partially determines the fraction of phonons reflected at each interface.[12]

The thermal conductivity of the superlattices was measured using the 3-ω technique.[13] In short, the 3-ω method is an ac technique in which a thin metal line is patterned on the surface of the sample and is utilized as both a heater and a thermometer. Since the capping layers are electrically conducting, a thin insulating layer ($\sim$100 nm thick SiO_2) is deposited between the cap and metal heater line. Detailed explanations of the 3-ω technique[13,14] and the fabrication of the insulating layer and heater/thermometer lines on the samples[15] can be found elsewhere. The 3-ω measurement directly gives the total thermal resistance of the superlattice, buffer, cap, and insulating layer. The individual contributions of the buffer, cap, and insulating layers are measured separately and subtracted, leaving only the thermal conductivity of the superlattice. In order to confirm the suitability of assuming one-dimensional heat flow (cross-plane thermal conductivity), heater lines of varying widths (16, 20, and 25 μm)

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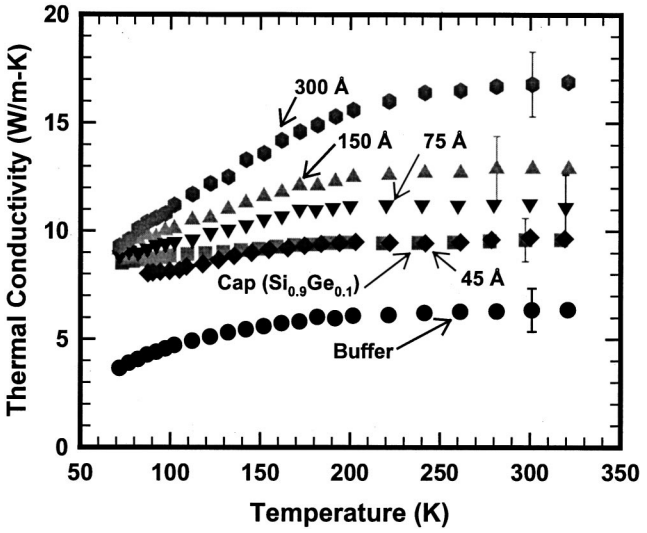

FIG. 1. Cross-plane thermal conductivity of four $Si/Si_{0.7}Ge_{0.3}$ superlattices. All superlattices are 3 μm thick and have a ratio of Si to $Si_{0.7}Ge_{0.3}$ of 2:1. The labels on the upper four curves refer to the period thickness. The curve labeled "Cap" is a 3.5 μm thick $Si_{0.9}Ge_{0.1}$ film, which has the same composition as the capping layers on the superlattices. The "Buffer" is a 1 μm thick $Si_{0.9}Ge_{0.1}$ film followed by a 1 μm thick $Si_{0.9}Ge_{0.1}/Si_{0.845}Ge_{0.15}C_{0.005}$ superlattice.

were tested. The difference among thermal conductivity values measured with lines of these widths was small, indicating that the lines were adequately wide to assume one-dimensional heat flow.

To assess the reliability of our data, we first measured the thermal conductivity of a 3.5 μm thick $Si_{0.9}Ge_{0.1}$ film that was boron doped with a carrier concentration of 5×10^{19} cm^{-3} (see Fig. 1). This measurement was then compared with data recently reported by Yonenaga *et al.*[16] for a similarly composed $Si_{0.9}Ge_{0.1}$ sample, also boron doped, only with a slightly higher carrier concentration of 8×10^{19} cm^{-3}. Our measured value of 9.6 W/m K for room temperature thermal conductivity compared favorably with their value of 9.35 W/m K, thus confirming the reliability of our measurements.

The number of interfaces present in a $Si/Si_{0.7}Ge_{0.3}$ superlattice strongly influences the thermal conductivity as demonstrated in Fig. 1. This plot was generated using the data from the 20 μm wide heater lines, which should be closely representative of the cross-plane thermal conductivity. For a decrease in period thickness (an increase in the number of interfaces per unit length), there was a corresponding decrease in the thermal conductivity. For the 45 Å period thickness, the thermal conductivity approached that of the $Si_{0.9}Ge_{0.1}$ alloy. It is noteworthy that for a $Si/Si_{0.7}Ge_{0.3}$ superlattice with a 2:1 thickness ratio, the overall ratio of Si to Ge is 9:1, which is the same ratio within the alloy. It is also worth noting that the thermal conductivity never fell below the value of the corresponding $Si_{0.9}Ge_{0.1}$ alloy. This is in contrast to the observations of Lee *et al.*[6] on superlattices of Si/Ge. Presumably, the larger AIM of the Si/Ge superlattices along with the presence of misfit dislocations and interface defects in their case increased phonon scattering. In our particular case, however, the superlattice acts as much like an alloy of its constituents as a layered structure. All superlattices show similar temperature dependence: a gradual increase in thermal conductivity with temperature up to about 200 K, and only a slight increase from 200 to 320 K.

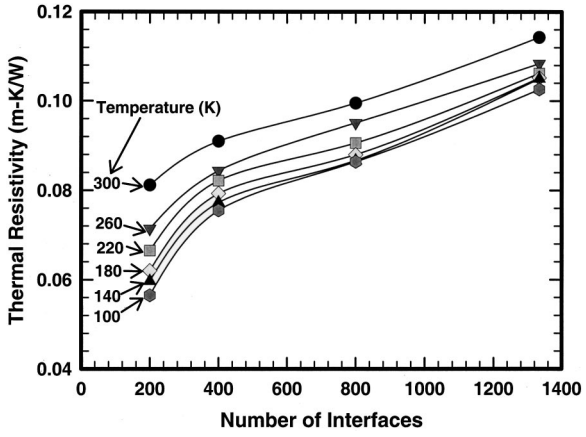

FIG. 2. Thermal resistivity of the four $Si/Si_{0.7}Ge_{0.3}$ superlattices as a function of the number of interfaces at six different temperatures (K). The resistivity decreases nearly linearly between 1334 and 400 interfaces, while it decreases slightly more between 400 and 200 interfaces.

Figure 2 shows a plot of the thermal resistivity of the superlattices as a function of the number of interfaces. The resistivity decreases nearly linearly from 1334 to 400 interfaces, and then drops off somewhat more rapidly between 400 and 200 interfaces. The linear portion seemingly indicates that the additional interfaces simply add a corresponding thermal boundary resistance to the superlattices. However, the reason for the deviation from linear behavior for long periods is unclear and may result from the interplay between competing thermal mechanisms. The overall trend towards lower thermal conductivity for shorter periods eliminates the possibility of miniband formation being a dominant mechanism for heat transport in these superlattices for the following reasons. When miniband formation occurs in the phonon dispersion relation, the number of locations in wavevector space where stop bands, or phonon band gaps, occur decreases with a decrease in period thickness, leading to fewer locations where there is a decrease in the phonon group velocity. Therefore, if miniband formation were domi-

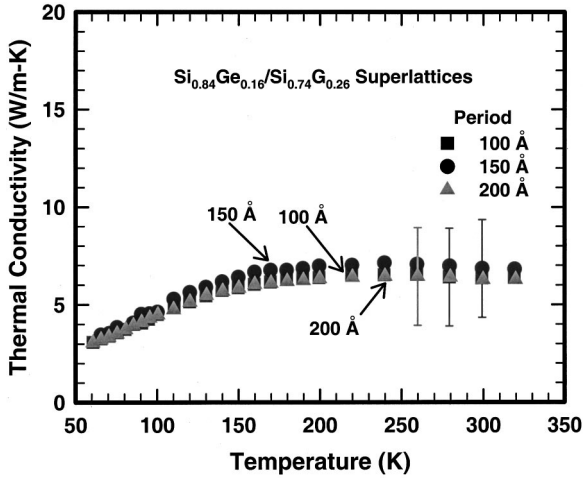

FIG. 3. Cross-plane thermal conductivity of three $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices. All superlattices are 3 μm thick and the labels on the curves refer to the period thickness. The high degree of uncertainty is only in regard to the absolute value of the thermal conductivity; all three samples have essentially the same conductivity.

nant, decreasing the thickness of the periods would actually result in an increase in the thermal conductivity.[17]

The thermal conductivity of the $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices measured with 25 μm heater lines is shown in Fig. 3. The main source of uncertainty in these data is due to the fact that a separate buffer sample was not available for measurement. Since the buffer layer consisted of a 0.95 μm thick layer of $Si_{0.8}Ge_{0.2}$ followed by a 3 μm thick graded SiGe film (graded from pure Si to $Si_{0.8}Ge_{0.2}$), we assumed that it acted thermally like a $Si_{0.9}Ge_{0.1}$ alloy that was measured previously. Nonetheless, the relative uncertainty among these three superlattices is not affected by this estimate. Unlike the Si/alloy samples, where the period thickness was significant with regard to the thermal conductivity, the alloy/alloy superlattice thermal conductivity was independent of the period thickness. We attribute this to the dissimilarity among the AIM of the superlattices. Using the data for the elastic constants of Si (Ref. 18) and Ge (Ref. 18) and a weighted average of data for the alloys,[19] and then averaging over all of the phonon modes and propagation directions, an estimate of an ''average'' AIM for each superlattice was obtained. The calculated average acoustic impedance mismatches were $\sim$1.15 and $\sim$1.03 for the $Si/Si_{0.7}Ge_{0.3}$ and $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices, respectively. From Figs. 1–3, we saw that the number of interfaces had a significant effect on the heat transport in the Si/alloy superlattices, while the alloy/alloy superlattices showed no such effect. If the AIM were dominant, then one would expect that, for the alloy/alloy superlattice, the number of interfaces would have little, if any, influence on the thermal conductivity. Rather, alloy scattering appears to be the dominant mechanism. Furthermore, in comparing Figs. 1 and 3, we see that the alloy/alloy superlattice exhibits a slightly lower thermal conductivity than the Si/alloy superlattices.

In summary, the cross-plane thermal conductivities of $Si/Si_{0.7}Ge_{0.3}$ and $Si_{0.84}Ge_{0.16}/Si_{0.76}Ge_{0.24}$ superlattices were examined and compared. For the Si/alloy superlattice, the role of the interface in affecting the thermal conductivity is important; however, for the alloy/alloy superlattice it is not. Taking advantage of both alloy scattering and the influence of the AIM, future investigation of a high AIM alloy/alloy superlattice could demonstrate the combined effect on the thermal behavior of these structures.

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