Resonant thermal transport in semiconductor barrier structures

P. Hyldgaard
Department of Applied Physics, Chalmers University of Technology, SE-41296 Göteborg, Sweden.
(Dated: January 18, 2004)

I report that thermal single-barrier (TSB) and thermal double-barrier (TDB) structures (formed, for example, by inserting one or two regions of a few Ge monolayers in Si) provide both a suppression of the phonon transport as well as a resonant-thermal-transport effect. I show that high-frequency phonons can experience a traditional double-barrier resonant tunneling in the TDB structures while the formation of Fabry-Perot resonances (at lower frequencies) causes quantum oscillations in the temperature variation of both the TSB and TDB thermal conductances $\sigma_{\text{TSB}}$ and $\sigma_{\text{TDB}}$.

PACS numbers: 66.70.+f, 42.25.Hz, 44.10.+i, 63.20.-e

The understanding of phonon transport in nanoscale heterostructured materials is in an exciting development motivated in part by the search to improve both thermo-electric and thermo-ionic cooling. The interest also derives from the observation that nanostructure phonons exhibit nanoscale-transport, confinement, and quantization effects similar to those observed for electrons and photons. A significant suppression is observed in the in-plane thermal conductivity of heterostructures and is explained by interface scattering as a phonon Knudsen-flow effect. Similarly, the perpendicular thermal conductivity $\kappa_{\text{SL}}$ of semiconductor superlattices shows a dramatic reduction (compared to the average bulk conductivities) that cannot be accounted for alone by the expected decrease in the effective superlattice-phonon lifetime $\tau_{\text{SL}}$. Instead, the strong reduction in $\kappa_{\text{SL}}/\tau_{\text{SL}}$ results from a pronounced miniband formation where the difference in materials hardness forces an increasing confinement of modes with a finite in-plane momentum to either the Si or Ge layers in the superlattice. Finally, the phonon quantum-point-contact effect in nanoscale dielectric wires shows that the phonon wave nature also directly affects the low-temperature phonon transport.

Here I extend the search for quantized thermal-transport effects in semiconductor nanostructures to finite temperatures. I focus on the phonon conduction across Si/few-Ge-monolayers/Si thermal single-barrier (TSB) and corresponding Si/Ge/Si/Ge/Si thermal double-barrier (TDB) heterostructures. I document (i) a strong suppression of the phonon-transport thermal conductances $\sigma_{\text{TSB}}$ and $\sigma_{\text{TDB}}$, (ii) a traditional type of double-barrier resonant tunneling for high-frequency phonons in the TDB structures, and (iii) that phonon Fabry-Perot resonances (at lower frequencies) produce a resonant-thermal-transport effect at finite temperatures in both the TSB and TDB structures (for sufficiently small Ge-barrier thicknesses). My focus is on the technology relevance rather than the low-temperature transport. Instead of the long-wavelength phonon analysis of Ref. [12], I therefore present a phonon-model calculation of the (resonant) thermal transport which remains applicable at finite frequencies, includes the phase-space limitations imposed by total-internal reflection, and describes the important effect of increasing misalignment of the Si-/Ge-phonon dynamics as the in-plane momentum $q$ increases. The prediction (iii) bridges the concept of thermal-transport quantization effects from the previous focus on low-temperature phonon transmission to the finite-temperature nanostructure heat conduction for which I show that oscillations persist up to temperatures $\Theta \approx 50$ K.

To emphasize the potential technological relevance I first report a simple estimate for the thermal-conductance suppression in two examples of TSB and TDB structures, Fig. 1, formed as a Si/triple-Ge-monolayer/Si and as a Si/2Ge/3Si/2Ge/Si semiconductor heterostructure, respectively. I predict below a strong...
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\[ M \]

\[ F \]

\[ K \]

are polarized and propagating in the perpendicular \( \hat{z} \) direction is well described within such a one-dimensional description than the co-called effective conductance \( G_{\text{SL}} = \kappa_{\text{SL}}(d)/(d/2) \) \( \sim 10^4 \text{W/Kcm}^2 \) extracted \( \text{from measurements at (} \Theta = 200 \text{K) of the thermal conductivity } \kappa_{\text{SL}}(d) \text{ in Si/Ge superlattices with a nanoscale periodicity } d. \) The estimate \( \text{shows that repeating the TSB or TDB formation every 50 nm would be needed if the limit } \sigma_{\text{TSB}} \lesssim G_{\text{SL}} \text{ applies}. \)

The TSB and TDB structures also give rise to a resonant-thermal-transport effect which is observable at finite temperatures (\( \Theta \lesssim 50 \) K). Fig. 1 shows a schematics of the phonon model which I here solve to calculate the phonon tunneling and the resulting thermal conductance across both a single interface and across the repeated interfaces in the TSB and TDB structures. I assume a shared silicon (germanium) lattice constant \( a \), the atomic masses \( M_{\text{Si(Ge)}} \), and intra-silicon (intra-germanium) force constants \( F_{p,\text{Si(Ge)}} \) and inter-layer coupling constant \( K_F \equiv (F_{p,\text{Si}}F_{p,\text{Ge}})^{1/2} \) specified by the materials sound velocities \( v \). The tunneling \( v \) of phonon modes that are polarized and propagating in the perpendicular \( \hat{z} \)-direction is well described within such a one-dimensional lattice model. I refer to our previous investigation of superlattice thermal transport \( v \) for a description of how I include the effects of a finite in-plane momentum within a simple-cubic model by adding in-plane force constants \( F_{t,\text{Si(Ge)}} \) and corresponding characteristic frequencies \( \Omega_{t,\text{Si(Ge)}} = (4F_{t,\text{Si(Ge)}}/M_{\text{Si(Ge)}})^{1/2} \); Fig. 1 of Ref. \( v \). The set of force constants \( F_{t,\text{Si(Ge)}} \) also specifies the phonon-transport contributions from \( \xi_{q,\hat{q}} \) \( \equiv \tilde{\xi}, \tilde{\gamma} \)-polarized heterostructure phonons \( \| \) and these modes are, of course, also included in the transport calculation. Below I limit the formal discussion to the contributions from \( \xi_{q,\hat{q}} \) \( \equiv \tilde{\xi}, \tilde{\gamma} \)-polarized heterostructure phonons \( \| \) across the heterostructure interfaces in this phonon-transport model study.

To clarify the nature and measurability of the high-frequency resonant tunneling, I summarize the model calculations of the phonon dynamics at general in-plane momentum \( q \). The figure reports a comparison of \( T_K(\omega, \alpha_{\hat{q}}=0) \) and \( T_{\text{DB}}(\omega, \alpha_{\hat{q}}=0) \) and identifies the onset (vertical dashed-dotted line) when incoming Si phonons become attenuated in Ge. The TDB structure is seen to support a traditional type of double-barrier resonant tunneling above this limit (when the Ge-layers represent actual barriers) but also multiple Fabry-Perot resonances (at lower frequencies) when incoming phonons experience a partial transmission at each of the individual Si/Ge interfaces. Note that the TDBs (and TSBs) naturally become completely transparent as \( \omega \rightarrow 0 \).

To clarify the nature and measurability of the high-frequency resonant tunneling, I summarize the model calculations of the phonon dynamics at general in-plane momentum \( q \). I note that bulk silicon (germanium) phonon propagation at a given \( \omega_{\hat{q}} \) requires that the frequency square exceeds \( \omega_{\text{Si(Ge)},\text{min}}^2(\alpha_{\hat{q}}) \equiv \Omega_{t,\text{Si(Ge)}}(\alpha_{\hat{q}}/2) \) but remains bounded by \( \omega_{\text{Si(Ge)},\text{max}}^2(\alpha_{\hat{q}}) \equiv \Omega_{t,\text{Si(Ge)}}^2(\alpha_{\hat{q}}/2) + \Omega_{t,\text{Si(Ge)}}^2 \). The finite silicon/germanium acoustic mismatch ensures that \( \omega_{\text{Si(min/max)}}(\alpha_{\hat{q}}) > \omega_{\text{Ge(min/max)}}(\alpha_{\hat{q}}) \). Phonon propagation (i.e., absence of attenuation) in both silicon and germa-
niurn layers thus effectively requires that
\[ \omega_{\text{Si,min}}^2(a_q) < \omega^2 < \omega_{\text{Ge,max}}^2(a_q), \] (2)
since this is the condition for an incoming silicon phonon to avoid total internal reflection at an individual Si/Ge interface (as formulated in the present model study). The condition (2) is a severe phase-space restriction which, for example, becomes impossible to satisfy at \( a_q > 2 \) in Si/Ge structures \( ^{17} \). For incoming Si phonons with a frequency \( \omega \) above the onset of Ge attenuation, the model study yields a strong exponential decay \( 1/\gamma \) oncoming silicon phonon

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\( \sigma_{\text{K,TSB,TDB}} = \sum_m \int \frac{d^2 q}{2\pi} \frac{h \omega}{T_{\text{K,TSB,TDB}}(\omega; a_q)} \left( \frac{dN}{d\Theta} \right) m \) \] (3)

by summing up the contributions at different modes \( m = \xi_x, \xi_y, \xi_z \) and in-plane momenta \( q \). In the result (3), \( \omega_{\text{min}} \) and \( \omega_{\text{max}} \) are the corresponding frequency-integration limits \( \omega_{\text{Si,min}}(a_q) \) and \( \omega_{\text{Si}(Ge,max)}(a_q) \). I stress that the condition (2) must be absolutely satisfied to obtain a transport contribution to the interface conductance \( \sigma_{\text{K}} \) and effectively satisfied for the TSB and TDB conductances \( \sigma_{\text{TSB,TDB}} \) (however, all TSB and TDB-transport contributions are retained in the calculations reported here).

The top panel of Fig. 3 illustrates the general validity of the “classical” thermal-conductance approximation, Eq. (1), and documents the additional temperature variation produced by the low-energy Fabry-Perot resonances. The panel shows that the thermal-barrier conductance \( \sigma_{\text{TSB}} \) (solid curve) at all temperatures is comparable to and generally smaller than the individual Si/Ge-interface conductance \( \sigma_{\text{K}} \) (dotted curve).

The insert compares the corresponding phonon transmission probability \( T_{\text{TSB}}(\omega) \) (calculated for Si/3Ge/Si at \( q \) = 0) and the single-Si/Ge-interface transmission (dotted curve). The insert motivates the estimate (1) by emphasizing that (a) the thermal single-barrier transport is effectively restricted to incoming Si modes that satisfy the condition (2) (exactly as was found for the TDB transport, Fig. 2) and (b) the single-interface transmission (dotted curve) approximates the average thermal-barrier transmission

\[ \langle T_{\text{TSB}}(\omega) \rangle \sim \langle T_{\text{K}}(\omega) \rangle \approx \frac{T_{\text{Si/Ge}}^0}{Z_{\text{Si}} + Z_{\text{Ge}}}, \] (4)
specified by the differences in acoustic impedances, \( Z_{\text{Ge}}/Z_{\text{Si}} \approx 1.5 \); \( T_{\text{Si/Ge}}^0 \approx 0.95 \). The observations (a) and (b) complete the argument (proof) for the “classical” thermal-conductance estimate (1).

The bottom panel of Fig. 3 documents that the phonon Fabry-Perot resonances refine the classical estimate (1).
I have investigated the phonon transport perpendicular to the interfaces of (silicon/triple-
germanium-layer/silicon) thermal single-barrier (TSB) and corresponding thermal double-barrier (TDB) 
structures. I document a strong suppression of the finite-
temperature heterostructure thermal conductances $\sigma_{TSB}$ and $\sigma_{TDB}$ which approximately are limited by the conductance $\sigma_K$ of an individual Si/Ge interface. In addition, I predict quantum oscillations in the thermal-conductance ratios $\sigma_{TSB}/\sigma_K$ and $\sigma_{TDB}/\sigma_K$ which arise from phonon Fabry-Perot resonances trapped in the central barrier or double-barrier region, respectively.

Discussions with G. D. Mahan are gratefully acknowledged. This work was supported by the Swedish Foundation for Strategic Research (SSF) through ATOMICS.