Study of the modal contributions to the heat flux to characterize the phonon transport regime in Si/Ge heterojunctions

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Heat management at the nanoscale is central to the design and optimization of thermoelectric [1] and nanoelectronic [2] devices. However, common macroscopic models such as heat Fourier's formalisms assuming local equilibrium is not relevant in complex nanostructures of characteristic lengths shorter than the phonon mean free path, in which the phonon transport can be strongly out of equilibrium, especially if thermal interfaces are involved.

Even if some analytical models have been developed to extend the validity of the Fourier's formalism [3], the particle Monte Carlo (MC) technique is an efficient and accurate numerical method to capture the out of equilibrium transport regime much beyond the linear approximation, even in complex real space geometries. This approach can naturally consider all phonon transport regimes from the diffusive to the fully ballistic regime.

In this work, phonon transmission across interfaces that are perpendicular to the heat flux has been implemented in our home made Full Band Monte Carlo simulator for phonons [4] by using a Full-band version of the Diffusive Mismatch Model (DMM).

First, the Knudsen number, commonly used to characterize the different transport regimes (diffusive, ballistic and intermediate) and defined as the ratio of the effective thermal conductivity $\kappa_{effective}$ to the ballistic one $\kappa_{ballistic}$, is plotted in Fig. 1 for homogenous Ge bars. This parameter appears strongly correlated to the spectral contributions of the thermal flux plotted in Fig 2. Then, single and double Si/Ge heterostructures shown in Fig. 3 were studied from the micrometer scale down to the nanometer scale. A typical temperature profile in a 300 nm-long double heterostructure is shown in Fig. 4. The total thermal conductance obtained for different heterostructures is plotted as a function of length in Fig 5.

Finally, the spatial evolution of the different spectral contributions to the thermal flux is plotted in Fig. 6. Used as a local indicator of the phonon transport regime and associated with the information provided by Figs. 2 and 3, this modal contribution and its deviation from bulk configuration indicate the occurrence and quantify the importance of out-of-equilibrium phonon transport around the interfaces.

[1] W. Liu, Q. et al., Acta Materialia, **87**, 57–376 (2015)

[2] IRDS report 2017, irds.ieee.org/images/files/pdf/2017/2017IRDS_MM.pdf

[3] B. Davier et al., arXiv, 2020.

[4] B. Davier et al., Journal of Physics: Condensed Matter, **30**, 495902 (2018)

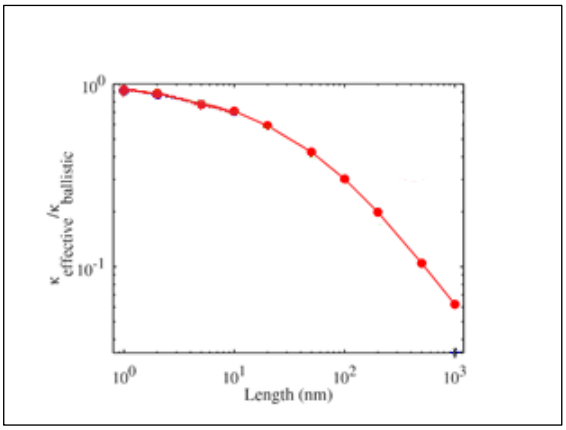

Fig.1:. The ratio $\kappa_{effective}/\kappa_{ballistic}$ as a function of the length L in Ge bars.

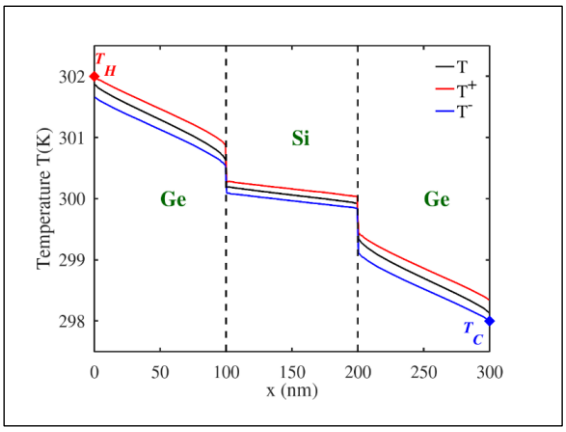

Fig.4: Temperature profiles in a Ge/Si/Ge double heterojunction. Hemispherical temperatures T+/T- are defined as the temperature of phonon sub-populations with a positive/negative velocity [3]

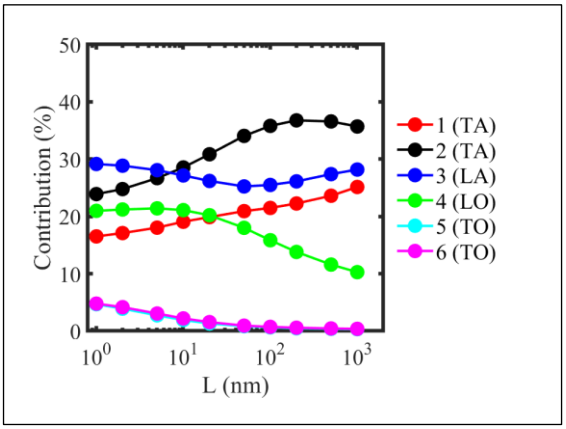

Fig.2: Modal contribution of phonons(for the 6 phonon modes) to the thermal flux as a function of the structure length in Ge bars

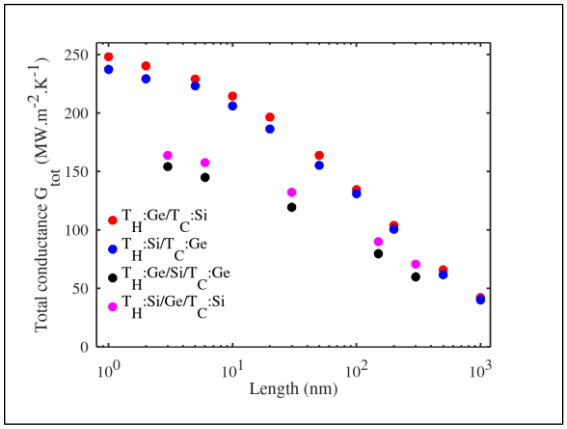

Fig.5: Total thermal conductance of simple and double heterojunctions for different device lengths

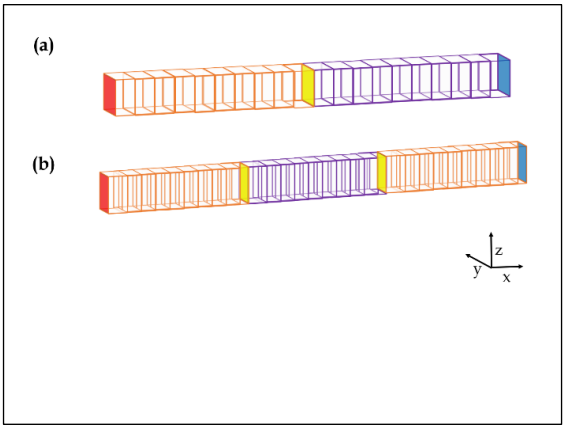

Fig.3: Heterogeneous nanostructures: (a) Simple heterojunction. (b) Double heterojunction. Red/blue faces are hot/cold thermostats. Transparent external faces: periodic boundaries. Yellow faces: DMM interfaces

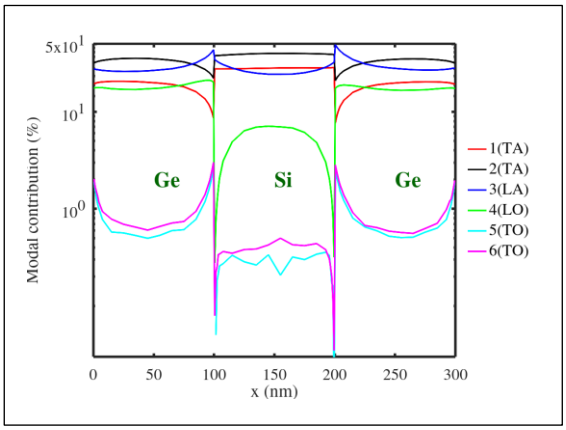

Fig.6: Variation of modal contribution to total thermal flux in 300 nm - long double heterojunction Ge/Si/Ge