Phonon transport across Ge/GaAs heterojunctions by nonequilibrium molecular dynamics

T. Albrigi[1], R. Rurali[1] Institut de Ciència de Materials de Barcelona (ICMAB–CSIC)
Campus UAB, 08193 Bellaterra, Spain

Introduction

Thanks to their technological importance, the characterization of solid-state systems made of III-V semiconductor materials represents a well-assessed field of research in the scientific community. Within this context, we focused on the thermal transport properties of the **Ge/GaAs heterojunction** at the nanoscale, investigating their dependence on both geometrical and chemical defects, together with their tunable features. (Fig. 1, 2)

Theory

The figure of merit of our study is the concept of thermal boundary resistance - or **TBR**, and its pivotal role in engineering thermal transport and dissipation. Second to it, we are interested in the resulting non-linear behavior of the junction itself, thus allowing **thermal rectification** to take place. When we apply some thermal bias - and the system has reached the corresponding steady-state, a non-linear temperature profile appears, which exhibits a sharp temperature drop at the interface between the two materials (Fig. 3). The ratio with the heat flux then yields the basic definition of TBR. When we reverse the bias, the temperature profile doesn't become its mirror image to the interface, and the resulting TBR, as well as the conductivity of the whole system, is different from the forward-bias configuration. The **theoretical framework** to understand these phenomena counts various models, ranging from continuum to atomistic theories, all the way up to the Many Body one, none of which proved capable of explaining all of the data. [1]

Numerical simulation

We constructed a minimal interaction potential to model the physics at the interface and used **NEMD** to compute the TBR and a suitable rectification coefficient in several configurations. We have taken the parameters for Gallium Arsenide from Albe et al., whereas the parameters for Germanium, as well as the empirical rule to combine them with the previous ones, come from Tersoff [2] [3]. Then we varied the cell geometry, the average temperature, the thermal gradient applied, concentration mixing, and roughness of the interface; and calculated the dependence of the TBR and rectification coefficient on these quantities.

Results

The order of magnitude of our estimates shows fair agreement with the typical values found for other heterojunctions of the like kind [4]. We achieved a relative uncertainty of around 10% for the TBR at 180 nm x 8 nm², which we then used for probing into the other parameters. To a first approximation, different temperature gradients only affect the time needed to reach the steady state; we thus use a value of 1.65 K/nm in order to achieve a reasonable compromise between accuracy and a fast approach to the nonequilibrium steady-state. Mixing enhances the TBR by 0.15 K·m²/W per nanometer of the mixed zone, whereas interface roughness has a relatively minor impact. The temperature dependence of the TBR we obtained is about $T^{-1.6}$. The rectification coefficient crosses zero around 80 nm and stabilizes around 10% when we extrapolate it for the infinite system (Fig. 4, 5).

Acknowledgment

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References

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[3] J. Tersoff *Modeling solid state chemistry: interatomic potentials for multicomponent systems*, Physical Review B **39** (1989).
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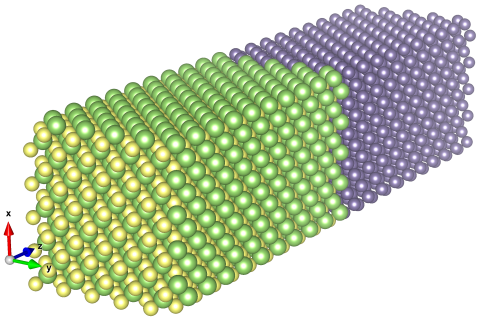

Fig. 1. Ge/GaAs junction with atomically flat interface

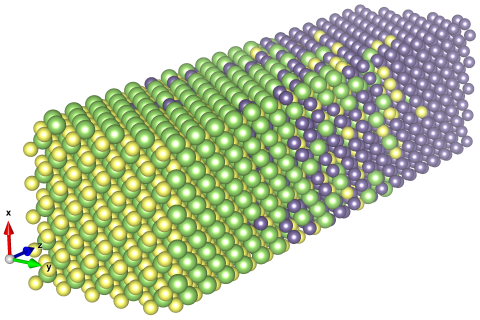

Fig. 2. Ge/GaAs junction with concentration mixing

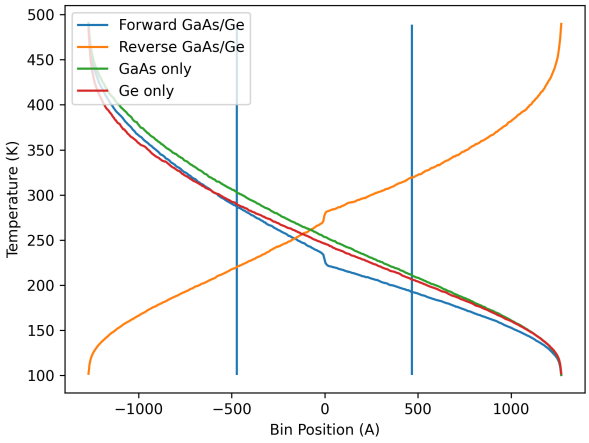

Fig. 3. Temperature profiles comparison for the 260nm x 8nm² cell

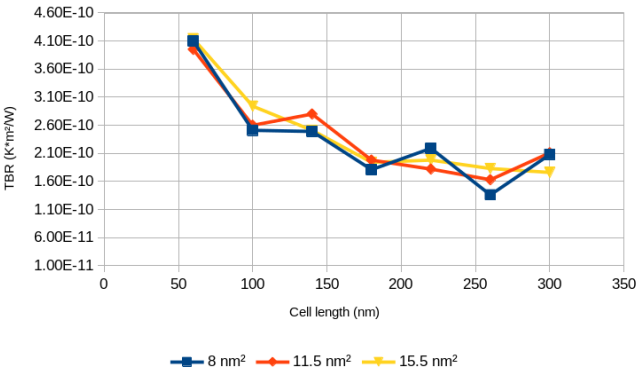

Fig. 4. Thermal boundary resistance dependence on cell length and cross section. A fixed thermal bias of 100K, centered at 300K, has been imposed in every simulation

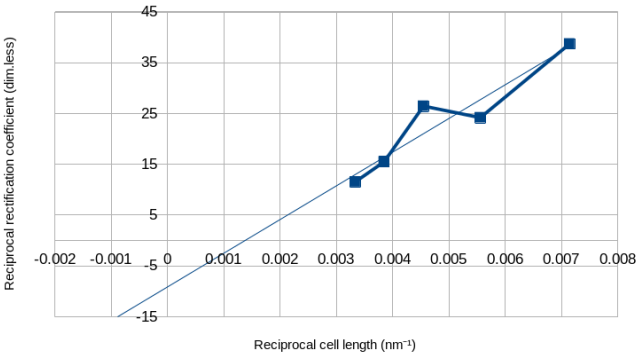

Fig. 5. Thermal rectification dependence on the cell lenght