Heat transport across a SiGe nanowire axial junction: interface thermal resistance and thermal rectification

Riccardo Rurali[1], Xavier Cartoixà[2], and Luciano Colombo[3]

rrurali@icmab.es

[1]Institut de Ciència de Materials de Barcelona (ICMAB–CSIC) Campus de Bellterra, 08193 Bellaterra, Barcelona, Spain
[2]Departament d'Enginyeria Electrònica, Universitat Autònoma de Barcelona, 08193 Bellaterra, Barcelona, Spain
[3]Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, I-09042 Monserrato (Ca), Italy

Semiconducting nanowires (NWs) have attracted a growing interest in recent years and are recognized as important building blocks for emerging applications in nanoelectronics [1-3]. The understanding of thermal transport has lately acquired a great importance as well, because NWs have been proposed to be a pathway for the engineering of efficient thermoelectric materials.

Here we study thermal transport in SiGe nanowires across a Si/Ge axial interface by means of nonequilibrium molecular dynamics simulations. We calculate the interface thermal resistance (ITR) of realistic models of axial SiGe heterojunctions, whose morphology depends strongly on the different experimental conditions [4-7]. We also investigate if these asymmetric junctions can yield thermal resistances that depend on the applied thermal gradient, i.e. thermal rectification. We find that diffuse interfaces result in larger ITR, while sharp junctions yield a small, but non-negligible thermal rectification, favoring heat transport from Si to Ge. These results can be tracked back to the different temperature dependence of the thermal conductivity of Si and Ge NWs, thus indicating that rectification derives from properties of the pristine NWs and can be tuned by the morphology of the interface. Curvature of the flat interface provides an additional modulation on both the ITR and the thermal rectification. These results shade a light on the atomic scale nature of the ITR and the observed thermal rectification is promising for the engineering of nanoscale phononic devices.

References

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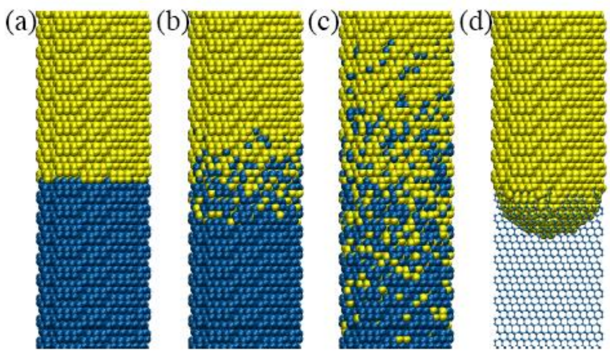

Figure 1. SiGe axial heterojunctions studied in this work. (a) atomically sharp, flat interface; (b,c) diffuse interface where the chemical composition switches from Si to Ge within a region of 5 and 15 nm; (d) curved interface. Light yellow spheres and dark blue spheres represent Si and Ge atoms, respectively. A ball-stick model is used for Ge in panel (d) to show the hemispherical shape of the interface.

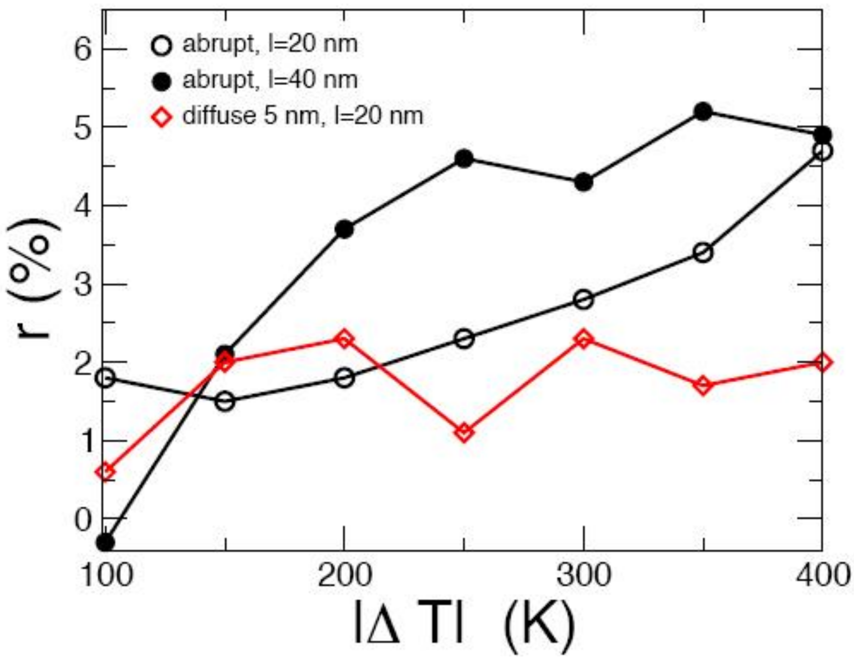

Figure 2. Heat rectification r as a function of |ΔT| in a 20 nm SiGe NW with an abrupt (empty black circles) and a diffuse interface, δl = 5 nm (empty red diamonds) and in a 40 nm SiGe NW with an abrupt interface (filled black circles). Notice that in the case of diffuse junctions, due to random nature of the alloy region, one should in principle average the results over several different configurations.