Alejandro R. Goñi
goni@icmab.es
ICREA,
Passeig Lluís Companys 23,
08010 Barcelona, Spain
Institut de Ciència de Materials de Barcelona-CSIC,
Esfera UAB, 08193 Bellaterra, Spain

Tailoring Thermal Transport in GeSi/Si Multilayered Nanostructures

The manipulation of phonons similarly to what is currently achieved with electrons and photons is the ultimate goal for the realization of a new generation of devices for thermal management applications. Good thermoelectric performance, for instance, requires materials with low thermal conductivity. Different approaches are available to impair heat transport in a solid. Alloying is a simple yet effective means of decreasing thermal conductivity, because of the increase in high-frequency phonon scattering. The early realization of alloys in the isomorphic material system Si/Ge has resulted in high figures of merit ZT~0.65 at 1100 K. The incorporation of a high interface density in epitaxial heterostructures has been also recognized as another efficient approach to enhance boundary phonon scattering at low-frequencies with a corresponding decrease of thermal conductivity. Further nanostructuring of the materials is expected to push down thermal conductivity even more.

In this talk, I will present two examples of multilayer structures based on group-IV semiconductors, in which phonon transport is tailored by clever nanostructuring during the growth process of molecular beam epitaxy. On the one hand, I will show how thermal conductivity across a superlattice (SL) of self-assembled Ge/Si quantum dots (QDs) can be reduced by more than a factor of two just by playing with the vertical correlation between Ge dots. For that purpose we have used a seed layer of C or B to counteract stress memory between layers, leading to growth of vertically uncorrelated Ge QDs, rather than modifying the Si spacer thickness. We have found a striking correlation between the amount of vertical alignment of the Ge dots, as probed by Raman scattering by acoustic phonons, and the values of the cross-plane thermal conductivity measured by the 3ω-method.

On the other hand, I will present a novel approach for customizing thermal transport across multilayered structures, by fabricating $Si_{1-x}Ge_x$/Si SLs with well-defined compositional gradients across the SiGe layer from x=0 to 0.60 or from x=0.60 to 0, for example. We demonstrate that the asymmetry of the structure has a remarkable effect on heat flow propagation, as the thermal conductivity varies by an outstanding difference of around 40% depending if the heat flow is parallel or antiparallel to the concentration gradient. This asymmetry provides a new perspective for the design of thermal rectifiers. I would like to emphasize that we have followed this approach based on a recent theoretical development form a partner group, which effectively incorporates into the expression of the thermal conductivity the existence of spatial gradients appearing due to the compositional variations within the $Si_{1-x}Ge_x$ layers.