Theoretical study of thermal properties of polytypic interfaces

B. Davier[1,2], J. Larroque[1], T. kaewmaraya[1], L. Chaput[3], Y. Chalopin[2], P. Dollfus[1], S. Volz[2], J. Saint-Martin[1]

1 Institut d'Electronique Fondamentale, CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France
2 Laboratoire d'Energétique Moléculaire et Macroscopique, Combustion, CNRS, CentraleSupélec, Université Paris-Saclay, Chatenay Malabry, France
3 Laboratoire d'Energétique et de Mécanique Théorique et Appliquée (LEMTA), Université de Lorraine, CNRS : UMR7563

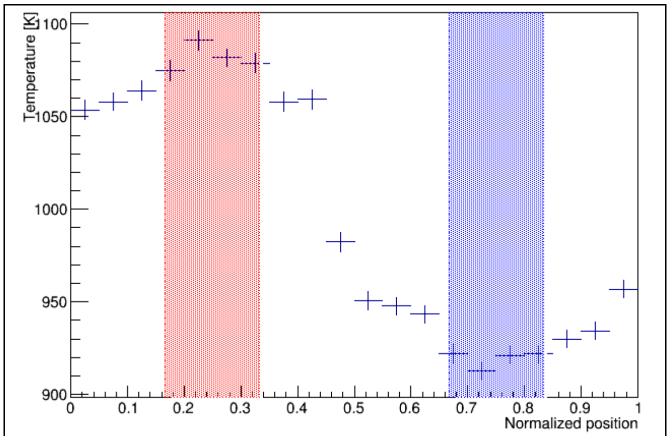

Figure 1. Steady state temperature profile along the cross plane direction in a cubic (100) Si/Ge interface. Colored areas represent the thermostats. The interfaces are at positions 0 and 0.5.

Interfaces can be used to design nanostructures with low thermal conductance to achieve optimized thermoelectric performance.

In this work, interfaces made of stacked hexagonal and cubic phases of both Si and Ge, that have been recently fabricated [1], were investigated.

To model the interface resistance, both Acoustic mismatch model and diffusive models based on a Full band approach have been derived. They are based on phonon dispersions computed via semi-empirical approaches that have been compared with ab-initio results. In parallel, Molecular Dynamics (MD) simulations have been performed to provide a complementary approach. In the future, the interface transmission computed via the previous approaches will be integrated in a particle Monte-Carlo simulator of phonon transport. This multi scale approach will allow an accurate modeling of the polytypic nanowires at the device level.

In figure 1, a non-equilibrium MD method was used: a temperature difference was imposed between the two materials. We calculated the interfacial thermal conductance from the injected heat flux and the temperature drop observed at the interface. We found a value of 237 GW/m²K for a cubic Si/Ge interface, which is consistent with previous results of 294 GW/m²K obtained with an Acoustic Mismatch Model [2].

1. L. Vincent, G. Patriarche, G. Hallais, C. Renard, C. Gardès, D. Troadec, and D. Bouchier, "Novel Heterostructured Ge Nanowires Based on Polytype Transformation," Nano Lett., vol. 14, no. 8, pp. 4828–4836, Aug. 2014.
2. D. Singh, J. Y. Murthy, and T. S. Fisher, J. Heat Transf., vol. 133, no. 12, p. 122401, 2011.