Lattice thermal conductivity and interface thermal resistance in SiGe nanosystems

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SiGe nanosystems (namely, nanocomposites and superlattices) are investigated by means of non-equilibrium molecular dynamics (NEMD) simulations as for their thermal transport properties.

We focus on the structure-property relationship governing both thermal conductivity and resistance. More specifically, we investigate how they depend on nanoscale features like: granulometry and stoichiometry in nanocomposites [1], or interface structure and superperiodicity in superlattices [2].

The resulting picture will emerge from large-scale simulations taking full profit from the reduced computational workload of the specific NEMD approach [3] we developed and implemented for the above systems.

References:

[1] C. Melis, L. Colombo, Phys. Rev. Lett. 112, 065901 (2014)
[2] M. Puligheddu, R. Dettori, K. Han, C. Melis, L. Colombo, submitted for publication (2014)
[3] C. Melis, R. Dettori, S. Vandermeulen, L. Colombo, Eur. Phys. J. B 87, 96 (2014)