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Thermal boundary resistance in Si/Ge interfaces determined by approach-to-equilibrium simulations MARCELLO PULIGHEDDU[1], KONSTANZE HAHN, CLAUDIO MELIS, LUCIANO COLOMBO, Department of Physics, University of Cagliari, Italy — Nanostructured materials hold great promises as efficient thermoelectrics. In such materials, the propagation of phonons is hindered by the internal interfaces (grain boundaries), leading to a reduced overall thermal conductivity and, therefore, to a larger figure of merit. Any further improvement in this field does, however, require a better fundamental understanding of the specific interface effects on thermal transport. In the present work we use approach-to-equilibrium molecular dynamics simulations (AEMD) [1] to investigate the interfacial thermal resistance (ITR) of Si/Ge interfaces, occurring in very promising nanostructured SiGe alloys [2]. We discuss how ITR depends on the thickness of the interface layer, as well as on its composition. Furthermore, the effect of the heat flux direction has been investigated at ambient temperature showing lower ITR for thermal transport from Si to Ge than vice versa. This feature is discussed in connection to possible rectification effects.
Reference: [1] C. Melis, R. Dettori, S. Vandermeulen, L. Colombo, Eur. Phys. J. B 87, 96 (2014) [2] C. Melis and L. Colombo, Phys. Rev. Lett. 112, 065901 (2014)

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