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Thermal conductivity of silicon-germanium alloys and superlattices from first-principles JIVTESH GARG, NICOLA BONINI, NICOLA MARZARI, Massachusetts Institute of Technology — Thermoelectric materials will become commercially viable for converting heat into electricity and for refrigeration once their figure of merit (ZT) is improved. One key approach to increase performance is to reduce thermal conductivity - e.g. in alloys it is lower than the binary endpoints due to increased scattering induced by strain and disorder. Understanding the thermal conductivity of complex materials is also important in other applications from reducing hot-spot temperatures in electronic chips to better thermal-insulation materials. Here, we have calculated the thermal conductivity of silicon-germanium alloys using ab-initio density functional perturbation theory. The electronic structure of the alloy is studied with the virtual crystal approximation and the single mode relaxation time approximation; perturbation theory up to the third order provides phonon lifetimes, and disorder effects are taken into account by ensemble averages over configurations with random mass disorder. We find that first-principles calculations lead to excellent qualitative agreement with experiments. The thermal conductivity of Si/Ge superlattices has been measured to be lower than Si/Ge alloys. Here we present the first principle calculations of the thermal conductivity of Si/Ge superlattices as a function of layer thickness.

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