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Designing SiGe superlattices and alloys for minimum thermal conductivity JIHUI NIE, PAWEL KEBLINSKI, Rensselaer Polytech Inst — We use equilibrium molecular dynamics simulations to study the thermal conductivity of SiGe alloys to design the structures for minimum thermal conductivity, which is desired, e.g., for better thermoelectric properties or thermal barriers coatings. We explore how a combination of layered/superlattice structures with a degree of random alloying is capable of effective scattering of both low frequency (long wavelength) and high frequency (short wavelength) phonons thus greatly reducing thermal conductivity. We will discuss strategies towards guided search for arrangements of alloy constituents that minimizes thermal conductivity.

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