

# Exploration of the superlattice thermal conductivity design space

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Molecular dynamics (MD) simulations are used to predict the thermal conductivity of model Lennard-Jones superlattices with species that differ only in mass. The cross-plane thermal conductivity is predicted using a nonequilibrium, steady-state approach (i.e., the direct method), and the in-plane thermal conductivity is predicted using the equilibrium, Green-Kubo method. The superlattice unit cell design is varied with the goals of (i) minimizing the cross-plane thermal conductivity and (ii) maximizing the in-plane to cross-plane thermal conductivity ratio, characteristics desirable for application. The cross-plane thermal conductivity design space for superlattices with a mass ratio of two is shown in Fig. 1. Lattice dynamics calculations are presented to explain some of the predicted thermal conductivity trends, and preliminary work into the thermal conductivity prediction of Si/Ge superlattices is also presented.

Superlattices have potential as materials in thermoelectric energy conversion applications because the cross-plane thermal conductivity can be reduced while maintaining good electron transport properties, resulting in high values of the thermoelectric figure-of-merit. These structures can also have a highly anisotropic thermal conductivity tensor, making them attractive in heat transfer applications since they can be used to simultaneously insulate a device in one direction and channel heat from it in another. The design and development of superlattices for these applications are dependent on obtaining an understanding of the thermal transport behavior in these structures.

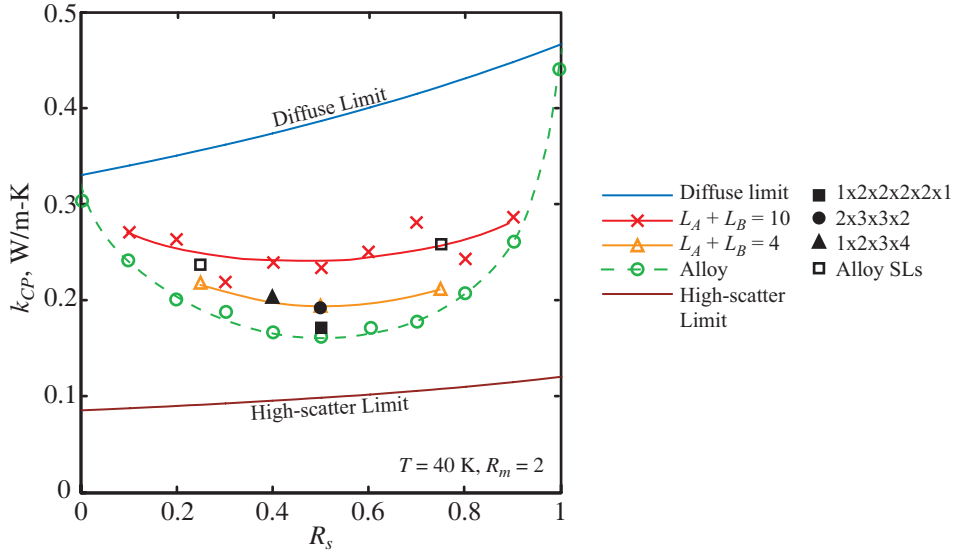


Figure 1: Cross-plane thermal conductivity ( $k_{CP}$ ) design space for model Lennard-Jones superlattices with species that differ only in mass. The predicted superlattice thermal conductivities are all between the diffuse and alloy limits, and the predicted minimum  $k_{CP}$  is observed for a superlattice with a complex unit cell design.

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