# Calculation of the lattice thermal conductivity in granular crystals

M. Kazan and S. Volz

Abstract:

This paper provides a general model for the lattice thermal conductivity in granular crystals. The key development presented in this model is that the contribution of surface phonons to the thermal conductivity and the interplay between phonon anharmonic scattering and phonon scattering by boundaries are considered explicitly. Exact Boltzmann equation including spatial dependence of phonon distribution function is solved to yield expressions for the rates at which phonons scatter by the grain boundaries in the presence of intrinsic phonon scattering mechanisms. The intrinsic phonon scattering rates are calculated from Fermi's golden rule, and the vibration parameters of the model are derived as functions of temperature and crystallographic directions by using a lattice dynamics approach. The accuracy of the model is demonstrated with reference to experimental measurements regarding the effects of surface orientation and isotope composition on the thermal conductivity in single crystals, and the effect of grains size and shape on the thermal conductivity tensor in granular crystals.  [http://dx.doi.org/10.1063/1.4866362]