

Behavior of Thermal Transport Properties of Disordered Alloys: A Theoretical Study

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We shall present a formulation for the calculation of configuration averaged lattice thermal conductivity and thermal diffusivity in disordered binary alloys. The formulation is based on the augmented space theorem, introduced by one of us [1], combined with a generalized Feynman diagrammatic technique. The diagrammatic approach simplifies the problem of including effects of disorder correction to a great extent. A Kubo-Green formula for the thermal transport in solids will be introduced which relates the thermal conductivity to the (heat) current-current correlation function. We show that disorder scattering renormalizes both the phonon propagators as well as the heat currents in the Kubo formula. A mode dependent diffusivity $D(n)$ and then a total thermal diffusivity averaged over different modes will be defined. Numerical results on the lattice thermal conductivity show that the contribution of disorder corrections to the heat current is rather small. The temperature dependence of lattice conductivity $K(T)$ looks reasonable, which rises smoothly from zero to a T -independent final or saturated value reflecting the experimental data. A quadratic T -dependence in the low temperature regime has also been extracted. The concentration dependence of K appears to justify the notion of minimum thermal conductivity as verified by Kittel, Slack and others. Each harmonic mode has an intrinsic (harmonic) diffusivity. A numerical estimate of this quantity gives an idea about the location of mobility edge, fraction of delocalized states etc. The analysis of the numerical results on thermal diffusivity for two different alloys indicates that "the more dominant the force constant disorder is the more delocalized the vibrational modes will be."

[1] *J. Phys. C.* **6**, L205 (1973).