# The contribution of surfaces and interfaces to the crystal thermal conductivity

M. Kazan, P. Masri

Abstract:

This review provides theoretical understanding of the role of the surface and interface in the thermal conductivity of solids. An attempt is made to collect the various methods used in the analysis of experiments. The adequacy and range of validity of these methods are evaluated, and suggestions are made concerning possible theoretical and experimental investigations which seem desirable. A major part of the paper is devoted to the description of the surface vibrational modes, the surface thermal conductivity, the interaction of defects with crystal surfaces, and the phonon scattering from crystal surfaces. First, a review is made of the general form of the interatomic potential energy and lattice vibrations. Certain aspects related to the three- and four-phonon processes are discussed. Then, the heat current is calculated in the presence of scattering processes described by a relaxation time, and a general formalism for the lattice thermal conductivity is derived. A special consideration is given to the effect of boundary scattering and boundary thermal conductance. In the first sections, despite the consideration of boundary scattering, the calculation of the thermal conductivity is carried out with adopting of the cyclic boundary conditions. Such a treatment, while mathematically convenient, eliminates the possibility of studying the dynamical properties of atoms in the neighborhood of a free surface of a real crystal because the crystal structure in the surface layers may differ from the structures in the bulk of the crystal. The forces acting on atoms in the surface layers will be different from the forces acting on atoms in the bulk since an atom in the surface layers has fewer nearest neighbors, next-nearest neighbors, etc., than an atom in the interior of a crystal. Therefore, one would expect that the dynamical properties and the resultant thermal conductivity are different for atoms in the surface layers of a crystal than for atoms in the bulk of the crystal. Moreover, when crystal size becomes small enough that the ratio of surface to volume is not negligible, the modification of the frequency distribution function of the crystal by the presence of free surfaces, which is the addition of a contribution from an essentially two-dimensional crystal, will alter the temperature dependence of thermal conductivity and give rise to distinct size effects on the thermal conductivity. Furthermore, selection rules governing physical properties in crystals, which have their origins in symmetry properties, translational and rotational, of an infinitely extended crystal, can be relaxed for finite crystals or for atoms in the surface layers of crystals for which these symmetry properties no longer hold. Thus, one would expect to find that the thermal conductivity of a thin film or small particle will show specific features that do not appear for the case of bulk material. In order to present theoretical understanding of the effect of size

and surface contribution to the lattice thermal conductivity, we present in the last sections a theoretical lattice dynamical discussion of the thermal conductivity in which the modification of the lattice vibration by the presence of free boundary surfaces play a dominant role.