

Effects of lattice dispersion and elastic anisotropy on the thermal properties of bcc metals

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Abstract. Two new parameters which take into account the effects of elastic anisotropy and phonon dispersion on lattice specific heat in the case of sodium and potassium have been evaluated. A new graded mesh method which uses a 162-direction approximation in (1/16) part of the Brillouin Zone (BZ) has been considered to evaluate the two parameters.

Keywords. Dispersion parameter; anisotropy parameters; Brillouin zone; graded mesh method; Gaussian-quadrature formula; specific heats.

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1. Introduction

The fundamental lattice dynamical models and their application to the study of the thermophysical properties of crystalline solids have been discussed in literature (Joshi and Rajgopal 1968; Rao 1979; Wallace 1972; Maradudin *et al* 1963). In the lattice dynamical model of Debye (1912), the medium is assumed to be dispersionless and that the crystal is elastically isotropic. A further assumption of the model is that the actual Brillouin zone is replaced by a sphere. The experimental neutron diffraction data (Bacon 1962; Dolling and Woods 1965) provided accurate information regarding the phonon dispersion relations and established the superiority of Born-Von-Karman (BVK) model (Blackman 1935, 1937).

An excellent review of Blackman's work on $\theta - T$ anomaly of two-dimensional and three-dimensional lattices has been given by Delaunay (1956) and Seitz (1940). The anomalous behaviour of $\theta - T$ curves gives a qualitative indication of the contribution of the combined effect of dispersion and anisotropy to the lattice specific heat of crystals.

It has become customary to present the low temperature specific heat results in terms of a single Debye temperature θ (Wallace 1972; Cochran 1973). Recently, instead of a $\theta - T$ plot, a quantitative study has been made regarding the effect of dispersion and anisotropy on the specific heat of some bcc and fcc metals (Tolpadi 1979; Singh and Tolpadi 1983).

In the present investigation a 162-direction approximation has been used in (1/16) part of the BZ for calculating the phonon frequencies by employing a nine-parameter lattice dynamical model of some bcc metals. The same 162-direction approximation has been used to develop a generalized Debye model of cubic crystals. This has enabled us to determine quantitatively both the effects of lattice dispersion and