THERMAL PROPERTIES OF BINARY ALLOYS

By

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CERTIFICATE

This is to certify that the thesis,"THERMAL PROPERTIES OF BINARY ALLOYS", submitted for the award of the degree of 'DOCTOR OF PHILOSOPHY' to Indian Institute of Technology,Delhi is a bonafide work carried out by Ms Sadhana Garg under our supervision and no part of this thesis has been submitted for any other degree.

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ABSTRACT

The challenge of producing unusal materials of technological use has attracted the scientists and technologists to a great extent in the recent past. An important class of such materials is alloys which hold promise in a variety of applications, owing to their versatile structure and properties. An alloy is a metallic solid or liquid formed from the combination of two or more elements. These days alloys of various compositions and properties are prepared that find applications ranging from home-appliances to outer-space. Both theoretical and experimental investigations of electronic, magnetic, lattice-dynamical and electrical properties have added a great deal to our understanding of these materials. The knowledge of the nature of interatomic interactions in alloys is of interest as it leads to an understanding of their vibrational, elastic, electrical, thermal and various other physical properties. Therefore, it is of great importance to understand the lattice-dynamic properties of alloys.

The present thesis deals with the thermal properties that include phonon dispersion relations, phonon density of states, specific heat, Debye temperature and elastic constants of disordered binary alloys. On the basis of atomic arrangement the binary alloys $A_{1-x}\ B_x$ can be divided into two broad categories: (1) ordered, and (2) disordered alloys. An ordered alloy is the

one in which the atoms A and B have a regular periodic arrangement with respect to one another, whereas in disordered binary alloys the distribution of atoms A and B in the lattice is random and is such that the concentration of A is (1-x) and that of B is x. The disordered binary alloys, Ta-W, Cr-W, Fe-Aℓ, Ni-Cr, In-Tℓ, Fe-Ni, Fe-Pd are considered at length in the present thesis. It is observed that all these alloys exhibit only one set of phonon frequencies for all the studied concentrations. Due to their disordered nature it is assumed that the alloy is a perfect crystal in which the lattice sites are occupied by virtual atoms, that have mass equal to the configurational average of the masses of atoms A and B. The lattice constant is also assumed be an average of the lattice constants of the constituent members. In most of the cases the force constants of the alloys are calculated by the linear relation $\alpha_{alloy} = (1-x)\alpha_A + x\alpha_B$. The central and the angular force constants of the end members A and B (α_A and α_B) are evaluated in their original structures using the measured elastic constants. The obtained phonon dispersion relations, phonon spectrum, Debye temperature are compared with available experimental data. The results are also compared with the ones reported by other theoretical groups.

The study of $Rb_{1-x}K_x$ alloys that exhibit local mode behaviour is also undertaken. The experimental data suggest that the clustering of atoms plays an important role in such binary alloys. In the present work the effect of clustering is accounted in terms of a non-randomness parameter λ. The dynamical matrix

is accordingly modified to account for the clustering effect. The short-range interatomic forces (both central and angular) are considered upto three nearest neighbours. The angular forces are calculated using deLaunay's approach. It is observed that this model is able to successfully explain the local mode behaviour in the binary alloys.

The resistivity of some partially filled d-band transition metals is also calculated and is reported at the end of this thesis.

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