A MODEL TO STUDY THE LATTICE DYNAMICS OF HEXAGONAL METALS

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" न हि ज्ञानेन सदृशं पवित्रमिह विद्यते "

गीता -4/38

"There is nothing in this world so purifying as Knowledge"

Gita - 4/38

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ABSTRACT

In the present work, a model has been proposed for the lattice dynamical studies of hexagonal close-packed metals which takes into account central forces and electron-ion interaction. In order to incorporate electron-ion interaction, the compressive strain produced in the electron gas by thermal motion of ions, has been averaged over the actual shape of the Wigner-Seitz cell of the hcp lattice. It is important to point out that several workers (e.g. Gupta and Dayal, Bose, Tripathi and Gupta) in this field have followed Sharma and Joshi approximation of replacing the Wigner-Seitz cell by a sphere of equivalent volume. This is not very much justified for, according to Wilson, 'In the Wigner-Seitz method, the assumption that the elementary cell can be replaced by a sphere makes the energy a function of atomic volume only and not of the type of the crystal structure.' Sharan and Bajpai approximated the atomic polyhedron to an ellipsoid of equivalent volume. Later on, Verma and Upadhyaya made minor correction in their expressions and worked on hcp metals. Our expressions for electron-ion interaction are free from the approximations used by the above authors and produce better results on application to various hcp metals.

Besides this, the author has also investigated the lattice dynamics, atomic and electrical properties of strontium and calcium based on the force constant and pseudopotential approaches.

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