ABSTRACT

In this thesis, the theoretical study of lattice dynamical properties is carried out for body centered cubic (bcc), face centered cubic (fcc) and hexagonal close packed (hcp) paramagnetic transition metals. The detailed band structure calculations are used in the non-interacting s- and d-band scheme to investigate the complete dielectric matrix. The lattice dynamical equations are obtained by inverting the dielectric matrix using factorization ansatz due to Sinha et al. Phonon frequencies, form factors, energy wavenumber characteristic functions and binding energies are studied.

The thesis consists of five chapters. In the first chapter, a brief account of literature on various models and the fundamental theories for the dielectric screening and the lattice dynamics of metals is reviewed. The resume of the present investigations is also presented there.

In the second chapter, the formalism of the dielectric screening for a transition metal is presented. Isotropic non-interacting band model is constructed for bcc transition metals, chromium and vanadium, with the help of the detailed band structure calculations considering three principal symmetry directions [100], [110], [111] and three off-symmetry directions [310], [311] and [221]. In chromium, it is found that the s-band and the three d-sub bands are partially filled and the other two d-sub bands are completely filled. In vanadium, the s-band and the two d-sub bands are partially filled, one d-sub band is completely...
filled and other two are completely empty. The number of electrons per atom to these d-sub bands are assigned in the ratio of the volume occupied by them. This model band structure is used to calculate the complete dielectric matrix $\varepsilon(q,G,G')$, which consists of both the intra- and interband parts, of chromium and vanadium for the electronic configurations $(3d)^5(4s)^1$ and $(3d)^4(4s)^1$, respectively. The plane wave approximation is used for the s-electrons and a simple tight-binding wavefunction and parabolic band approximation are used for the d-electrons. The calculations for the diagonal part of the dielectric matrix are performed for the field wavevector $q$ along the three principal symmetry directions [100], [110], and [111] and the anisotropy is found to be quite small. The diagonal part of the dielectric matrix, for paramagnetic chromium, is found comparable with the detailed calculations of Gupta and Sinha. In both the metals, the intraband part dominates for small values of wavevector while the interband part dominates for large values of the wavevector. The nondiagonal part, which gives rise to local field corrections, is found to be larger than the diagonal part for large values of the wavevector.

In chapter 3, a unified approach to the lattice dynamical study of transition metals, which takes into account the local field corrections, is presented. The inversion of the dielectric matrix is carried out using the factorization ansatz due to Sinha et al. and the explicit expressions for the dynamical matrix are obtained. The phonon dispersion relations for paramagnetic chromium are investigated. The direct ion-ion interaction contribution is evaluated using the
Ewald’s $e$-function transformation and the contribution due to the ion-ion exchange overlap potential is neglected because of small core size. In the evaluation of the ion-electron-ion interaction contribution, the bare ion potential is replaced by the Harrison simple metal model potential and the Animalu transition metal model potential (TMMP). The exchange and correlation corrections for the s-electrons are used due to Singwi et al. and for the d-electrons due to Lindgren et al. The agreement with the experimental values is reasonable except in the transverse branches in the [110] direction. Some anomalies in the phonon dispersion curves are also found. The form factor, the energy wavenumber characteristic function and the binding energy are also investigated in the simple metal like picture. The binding energy is in reasonably good agreement with the experimental value. Similar investigations are also carried out for vanadium using Animalu TMMP. The agreement of the calculated phonon frequencies with the experimental values is found reasonable except in the longitudinal branch in [100] direction and the transverse branch $T_\perp$ in the [110] direction. Some anomalies, which are observed experimentally, are also found in our calculations. The form factor, the energy wavenumber characteristic function and the binding energy are also investigated in the same manner as for chromium and the behaviour is found to be similar.

In chapter 4, the isotropic non-interacting band models, for nonrelativistic palladium and platinum, are constructed using the detailed band structure calculations along the principal symmetry
directions [100], [110] and [111]. The electronic configurations chosen are (4d)⁹.⁶ (5s)⁰.⁴ and (5d)⁹.⁶ (6s)⁰.⁴ for palladium and platinum, respectively. The various contributions to the dielectric matrix are evaluated numerically in the same way as in paramagnetic chromium and vanadium. The phonon frequencies are calculated by replacing the bare ion potential by the Animalu TMMP. The calculated phonon frequencies, in the longitudinal branches, are in good agreement with the experimental values while the transverse branches are lower than the experimental values. The anomalous behaviour is also found in our calculations. The form factor, the energy wavenumber characteristic function and the binding energy are also investigated for these metals as in the bcc metals. The binding energies are in poor agreement with the experimental values.

In the last chapter, the non-interacting band scheme is extended to the hcp transition metals. The isotropic non-interacting band models are constructed for scandium and yttrium using the detailed band structure calculations along the principal symmetry directions \( \Gamma A, \Gamma M \) and \( \Gamma K \). The electronic configurations chosen for scandium and yttrium are \((3d)^2 (4s)^1\) and \((4d)^2 (5s)^1\), respectively. The diagonal and the nondiagonal contributions to the dielectric matrix are calculated explicitly in the same way as in the bcc and the fcc metals. The phonon frequencies are investigated for both these metals using the Animalu TMMP. The calculated phonon dispersion relations are in reasonably good agreement with the experimental values. The acoustic isotropic behaviour is also found in our
calculated phonon dispersion relations which is consistent with the experimental observations. However, the Kohn anomalies are not found in our calculations explicitly.