CHAPTER - 1

Introduction

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1.1 Introduction

As is known, the properties of metals and its applications are very important to human life. Most of the properties of metals are determined by the valence electrons. Calculation of the physical properties of a metal requires the knowledge of the band electrons and interaction among ion cores. The total lattice potential could be calculated in principle, by solving the Schrödinger equation for a system of interacting nuclei and electrons that form the crystal. Thus, considerable effort has been made over the last couple of decades to understand the physical properties of matter in either liquid state or solid state. Integral equations, perturbation theory, molecular dynamics and Monte Carlo calculations are among the theories developed. However when they are to be applied in practical problems the knowledge of the intermolecular forces acting on the system among the particles of the system is necessary.

There have been various experimental investigations on the dynamic structure of liquid transition metals, their binary alloys and on bulk metallic glasses [1.1-1.10]. All elements of transition group as well as alloys made from simple metals have been studied using neutron scattering experiments [1.11-1.15]. Theoretical studies on these have also been attempted. In theoretical investigations the effective ion-ion potential in the liquid and solid transition metals can be handled through the pseudopotential and dielectric functions. Thus, this is a many body problem and is difficult to solve exactly. Hence it requires some unavoidable approximations like adiabatic or one-electron approximation [1.11-1.15].

The alkaline earth metals, transition metals and their binary alloys as well as bulk metallic glasses, in recent times, have been subjected to detailed study in the field of materials science, engineering, modern technology and industrial application due to many interesting properties exhibited by them [1.1-1.15]. The characteristic behaviour of alloys and metallic glasses generates manifold interest for experimentalists and theoreticians. For simple systems, the pseudopotential theory has been an effective medium to investigate various properties of alkaline earth metals and transition metals alloys (TM-
Alloys). Experimentalist and theoretician have shown interest in the bulk metallic glasses because they shown excellent combination of mechanical, chemical, magnetic and electrical properties.

It is found in the literature analysis that the concept of pseudopotential is well established in the theory of condensed matter, which helps us in understanding various properties including physical as well as chemical properties of crystalline and amorphous materials. The concept has emerged as a direct consequence of quantum mechanical scattering theory [1.11-1.18].

The method of pseudopotential is simple conceptually and computationally. The results properly generated by this method are comparable with those obtained from the first principle- all electron calculation. With certain approximations, fairly reliable analytical forms of interatomic interactions can be obtained. Via perturbation expansion, it directly provides the information of three body and four body forces in metals. It is interesting to note here that in spite of impressive success of pseudopotential theory in solving specific problems attempts of comprehensive studies to metallic complexes are surprisingly rare, even with a local pseudopotential and it still remains a problem of interest.

Looking to the simplicity of pseudopotential theory the aim of the present thesis entitled “STUDY OF CERTAIN PHYSICAL PROPERTIES OF SOME ALKALINE EARTH METALS, TRANSITION METALS, THEIR ALLOYS AND BULK METALLIC GLASSES USING PSEUDOPOTENTIAL THEORY” is to carry out the theoretical investigation of various properties of metals, their alloys and bulk metallic glasses. On the basis of pseudopotential theory very large numbers of successful applications are reported so far for the alkaline earth metals, transition metals and its alloys. But the compressive study for the metallic complexes are not reported, exhaustively, and hence the main emphasis is given to the binary and bulk metallic glasses systems.
The work reported in the present thesis is carried out with the following objectives:

- To investigate various structural properties, pair correlation functions, electrical transport properties, velocity auto correlation functions, phonon dispersion curve and elastic properties for alkaline earth and transition metals their liquid binaries and many bulk metallic glasses.

- To investigate total energy, pressure volume relations and Fermi surface distortion of solid solutions of metals and metallic complexes.

- Single parametric bare-ion local model pseudopotentials are identified and used. Two different types of model potentials, one in r-space and the other in q-space are selected for explaining electron-ion interactions in alkaline earth metals, transition metal and its alloys as well as bulk metallic glasses.

- To study the influence of various local field correction functions by employing six different local field correction functions in the aforementioned study.

- To infer the effect of the concentration dependence of the constituent elements and study the effect of temperature variation on the aforesaid properties in the binary alloys and bulk metallic glasses.

The structure related properties, electrical transport properties viz: electrical resistivity, thermo electrical power and thermal conductivity, phonon dispersion relation, auto correlation functions, power spectrum and mean square displacement are investigated for the liquid state of alkaline earth metal, transition metals and their alloys. The study also includes the computation of total energy, pressure volume relation and Fermi surface distortion for the bcc and fcc metals and their solid solutions.
The screening function due to Ichimaru-Utsumi [1.19], Farid et al. [1.20] and Sarkar et al. [1.21] are used to judge screening influence with reference to the more commonly employed dielectric functions of Taylor [1.22], Hubbard Sham [1.23, 1.24] and Hartree [1.10-1.12].

The investigators wish to emphasize that the present investigations will generate important set of data which will be used to both the experimentalists and theoretician working in this area.

The present work is purely computational in nature. The author has completed the literature survey up to the present date before starting the initial work. The initial work was more analytical in nature and it is mainly mathematical formulation of a single parametric local pseudopotential.

To fulfill the objective and scope of work in the present work, various forms of the model potentials have been formulated and tested on sound physical grounds. Then the two model potentials (one in r-space and other in q-space) are selected and characterized for its applications in numeric computations. The essential computer programs/codes are developed, indigenously. These programs are then executed for necessary calculations.

The results emerging from the computations are compared with other such available theoretical and experimental data, wherever possible. In absence of any experimental or theoretical comparison, the set of data will provide some base for other work in future.

The entire work of the present thesis entitled “Study of certain physical properties of some alkaline earth metals, transition metals, their alloys and bulk metallic glasses using pseudopotential theory.” is distributed over nine chapters, with the first chapter as an introduction. It also gives an outline of the whole thesis.
The concept of the pseudopotential is described in the second chapter of the thesis. This chapter deals with the general introduction of the pseudopotential theory and shows its capabilities as a tool for calculating and understanding various properties of matter. Two model potentials are identified in this chapter [1.25, 1.26]. The detailed characterization of the model potential and the determination of the parameter of the model potential are also presented. The effect of screening and the various forms of the local field correction functions considered in the present study are also discussed here. Hence, the analytical work regarding the selection of the two different model potentials gets completed in this chapter.

After characterizing two model potentials, it is then used to study some structural properties of metals and binary alloys. Chapter-3 is related to the structure factor of liquid metals and binary alloys. This structure factors have been computed using the approach of charged hard sphere (CHS) [1.27], one component plasma method (OCP) [1.28] and Percus-Yevick (PY) [1.29, 1.30]. These structure factors s(q), are then used for the computation of radial distribution function g(r), relative magnitude for structure factor s(q) and g(r), interatomic distance and co-ordination number for the liquid metals and binaries. A detailed study on electrical transport properties viz; electrical resistivity, thermo electrical power and thermal conductivity is done. Ziman’s formula along with the Ashcroft-Langreth partial structure factor is used to compute the electrical transport properties of binary alloys with different concentration of constituent elements and at different temperatures [1.31-1.33].

Chapter-4 is related to the phonon dispersion curves of liquid metals and their binary alloys. The well establish Hubbard Beeby approach [1.34,1.35] has been used to compute the phonon frequencies and elastic properties like bulk modulus B_T, Young modulus Y, Modulus of rigidity G, Debye temperature \( \theta_D \), Poisson ratio \( \xi \), longitudinal sound velocity \( V_l \) and transverse sound velocity \( V_t \) are computed.

In the 5th chapter, the computation of the velocity auto correlation function (VACF), power spectrum and the mean square displacement are reported for liquid
metals and binary alloys. The diffusive motion of the atoms in the liquid, which is always present, is described in terms of the linear growth of the mean square distance traveled by the vibrating atoms over a given time \[1.37, 1.38\].

Phonon dispersion curve using the Hubbard Beeby approach and different local field correction function for the bulk metallic glasses have not been found in literature survey. Chapter-6 is related to the detailed investigation of the phonon dispersion curves and elastic properties for bulk metallic glasses using the Hubbard Beeby approach with two model potentials and six different screening functions and the results are found to be good agreement with available experimental and theoretical results wherever available.

Chapter-7 is related to the investigations of the total crystal energy for the solid solution of BCC (Ba, Cr) and FCC (Al, Ca, Ni, Cu, Sr) and their alloys within the framework of the second order perturbation theory. It is in good agreement with available experimental or theoretical values of the total energy for pure components. Equation of State is also presented in this chapter.

The shape of the Fermi surface determines many electronic properties of metals and alloys. The detailed investigation on the shape of the Fermi surface distortion in transition-transition (BCC structure & FCC structure) binary alloys could be not found in literature survey. Hence in Chapter 8, the systematic theoretical investigation of the Fermi surface distortion of BCC Ba, and Cr and FCC Al, Ca, Ni, Cu and Sr metals and their alloys have been performed \[1.39-1.41\].

The final and concluding Chapter 9 of this thesis summarizes the entire work of the present investigation along with the important general conclusions. While giving proper shape to the thesis, however, the necessary discussion and comments are made at the appropriate point in every chapter. The scope of further study of the work is also described in the last chapter.
At the end of each chapter of this thesis important references have been listed. The necessary computer programs have been developed by us and tested for sufficient accuracy. Extra care has been taken for proper convergence of calculations. The necessary computation work is carried out in the condensed matter theory laboratory, Department of Physics, Sardar Patel University, Vallabh Vidyanagar.
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