PREFACE

During my study at M.Sc. level, I got interested towards theoretical physics. The first step towards this direction was my M.Phil. programme, in which I had selected theoretical solid state physics as a specialization and submitted my dissertation entitled "An empirical form factor for the alkali metals." I first started thinking about pseudopotential during this time. I knew virtually nothing about the pseudopotential theory at the time and my understanding of various properties of condensed matter was distinctly limited. The M.Phil. programme had given me the boost to go for further research work. As a result, to day, I am able to submit my Ph.D. thesis entitled "Study of some physical properties related to metallic density by pseudopotential theory."

The present thesis is aimed to serve following objectives:

(i) To establish a very simple empirical form of a bare-ion local pseudopotential,

(ii) To see the applicability of proposed empirical form factor in explaining various physical properties of some simple metals,

(iii) To investigate the validity of the model potential in the reproduction of various properties of some liquid metals,

(iv) To see the potentiality of the developed model in the study of simple binary alloys and metallic glasses,

(v) To infer the varying contributions of different local field correction functions in the aforesaid study.
To fulfill these objectives, the thesis is structured in seven chapters with very vast literature citations at the end.

The first chapter is very preliminary and introductory in nature, as it does normally, gives the overview of the work carried out in the present journey.

The conceptual aspects and the background on which the pseudopotential theory has grown up are narrated briefly in the second chapter. This chapter provides general features of the theory which are very essential, useful and equally important for concrete foundation in the progressive staircase of the pseudopotential formalism.

The third chapter deals with the construction and characterization of the model potential. Here, instead of proposing a bare-ion model potential in the r-space, single parametric empirical model potential is developed directly in the q-space. The parameter of the potential is determined from the well established $q = q_0$ value. Five different dielectric functions are used to see the relative influence of the exchange and correlation in the screening.

The computation of the pair potentials, interatomic force constants, dynamical elastic constants, dynamical bulk modulus, Cauchy relation, Young's modulus, Poisson's ratio, propagation of elastic waves, phonon dispersion curves, total crystal energy per atom, distortion in the Fermi surface, Fermi energy, monovacancy resistivity and susceptibility of some simple metals are presented in the fourth chapter of the thesis.
Chapter five covers the study of electrical resistivity, thermoelectric power, thermal conductivity, temperature dependence of these properties, electron dispersion curves, Fermi energy, susceptibility, Knight-shift and temperature coefficient of Knight-shift of some simple liquid metals.

The application of our model potential in the computation of total crystal energy, the effective pair potentials, pair correlation functions and phonon frequencies of some simple binary alloys and metallic glasses is worked out successfully in the chapter six of the thesis.

Present thesis includes 63 Tables and 146 Figures, in all, pertaining to various properties investigated. A positive effort is made to put exhaustive comparison with other such theoretical findings and experimental data, wherever possible. Important conclusions and comments, emerging from the investigations, are put forward in the text where it was felt appropriate. In addition, the general summary and conclusions are made very briefly in the last chapter.

Utmost care is taken in writing the thesis, so that it becomes useful document and serves as an important citation. The 364 references cited were required to give academic shape to the thesis.

Of course, this is my second step in the process of higher learning, but not the last. The experiences which I gained during this journey have opened new directions of visualizing various scientific aspects. This passage of time has motivated and provided enough boost for further riding.

(P. N. GAJJAR)