This last chapter of the thesis summarizes briefly, the entire work of present study along with the important general conclusions emerging therefrom. Wherever possible this chapter also points the scope of the extension of the study for future work.

The present thesis is mainly aimed at the study of molecular dynamics, lattice dynamics and thermodynamics of some cubic metals based on pseudopotential formulation and second order perturbation theory. The principle advantage of this technique is that with its use it is possible to eliminate completely the core states and modify the external atomic potential in such a way that the valence wave functions are smooth and nodeless inside the core sphere and are matched with the same scattering properties at the sphere boundary. The pseudopotential method can be applicable to understand a very wide range of properties exhibited by metallic systems. This method has become even more important and useful in recent years after finding application in the study of disordered materials semiconductors and technologically important materials through computer simulation.

Before making any theoretical study of metallic properties a section of suitable form of model potential is essential. To fulfill this requirement in the present study we have proposed a local model.
pseudopotential, which is consistently applied to certain cubic metals in solid as well as liquid phase.

The cardinal point in such a formulation is the proper assumption of the bare ion potentials based on sound physical ground and its q-space version, which can lead to a well-behaved form factor. The proposed model potential represents the varying cancellation inside the core and outside the core it retains the Coulombic nature. This model potential is simple and convenient to use as it contains only one parameter.

The mode of determination of the parameter of the potential is very sensitive because it not only determines the core size but also the strength of cancellation inside the core for our proposed model potential. Earlier methods used to find the parameter through fitting procedure to some experimental results give good results for limited number of properties while they fail to give good estimations of other properties. For transferability of any model potential, it is also desirable that it should work for almost all the elements in the periodic table. This is possible if one determines the parameter from the information of periodic table. Instead of using single dependency if more number of information are used to determine parameter it works effectively for wide range of properties. Considering this idea we established a relation to determine the parameter of potential in
In another attempt to test the applicability of our proposed model potential we have also used zero pressure condition to determine the potential parameter. However, this method depends on the choice of local field correlation function. The parameter obtained through zero pressure condition is used for the study of molecular dynamics of Na.

The dielectric screening plays a very important role in the evaluation of self-consistent potential due to the screening of the electron gas and is fundamental for understanding the behaviour of metals. There are number of forms proposed so far to explain the exchange and correlation effects among the electrons. To see the effect of all these forms simultaneously is quite laborious. Also there are no criteria or theory available for the proper selection of screening functions. So in chapter 2, we gave the new criteria for the proper selection of screening function. We calculated the total energies using few selected screening functions by expanding and contracting the
system and plotted as the Energy- Volume relation. The screening function, which gives lowest energy, is then employed for the further computations. In our case it is seen that Taylor screening function gives the lowest energy for both Na and Al.

After characterizing the model potential the form factors were generated for bcc Na and fcc Al. It is found that both the form factors are independent of unnecessary oscillations and approaches $-\frac{2}{3} E_F$ value for the limit $q \to 0$. We then extended the study to check the validity and applicability of the proposed model potential in explaining various properties of cubic metals.

The study of MD technique coupled with an interaction potential that adequately describes the ion-ion interaction can be used to study the microscopic properties of a simple metal. This is unique technique, which provides a direct calculation of the anharmonic terms in the total system energy. In chapter 3 we calculated and presented these terms as a function of volume and temperature for the solid bcc sodium and fcc aluminium for 10% compression and 10% expansion. The results are displayed as equation of state points consisting of the system energies at given volume and temperature for both these metals. Our results are comparable to the work carried out by other people. We have also calculated the atomic distribution and pair correlation function for same metals at different temperatures.
The possibilities of future work using this technique are many. We have limited our study to the calculation of system energy using MD but it also possible to calculate system entropy using quasi harmonic theory at low temperatures for the solid. Ideal gas or hard sphere theories may be used at high temperature for the liquid. Once the entropy is known, the MD results may be used to obtain the free energies and thus the thermodynamics properties will be completely specified with these calculations. The phase change and melt regions may be determined from a comparison of free energies.

This technique also proves valuable because it may be extended to higher density and temperature regions. Such theoretical determination of equation of state and dynamic properties is applicable to many areas of current interest such as the study of shock-induced conditions.

In addition to total energy calculation the MD technique also allows the calculation of pressure through Virial theorem. Thus it is possible to generate equation of state points in pressure and temperature space. In this way one would be able to calculate the properties of materials at very high temperatures and pressures that are not easily accessible to experiment.
MD technique is also useful to study phase transition. Extending our calculation it is possible to reproduce the bcc-hcp martensitic phase transition in sodium as a dynamic process. This can be done by artificially changing a shape of the calculational volume during simulation. Thus such studies are feasible and indicates that such shape changes, which occur in nature will be necessary part of future studies.

The MD technique is not restricted to solid phase but it can be successfully applied to liquid state. There are many attempts to study the liquid behaviour of metals through simulation, which can be seen from our literature survey. The equation of state points generated by us for solid phase can be extended for liquid phase also. It is possible to calculate the mean square displacement, diffusion constant, specific heat, velocity correlation function, pair correlation function, structure factor and other related properties of liquid metals. Once the pair correlation function and structure factor at different temperatures are known many structure dependent properties can be evaluated. The melting of a system is studied through MD technique and hence melting temperature of a metal can be estimated.

The necessary literature survey made in chapter 3 supports future scope of further study.
The chapter 4 of the thesis reports the successful application of our model potential in the computation of lattice dynamics of sodium and aluminium. The work undertaken is about static and vibrational properties of cubic metals. Our calculations of the force constants, dynamical elastic constants, bulk modulus and other related properties as well as phonon dispersion curve on the basis of the real space sum method proved up to the mark. As interatomic potentials are long range in nature, the real space sum analysis for all the dynamical properties is carried out up to 33 shells in sodium and up to 37 shells in aluminium. The deviation from Cauchy relation, Cauchy ratio, Poisson ratio, Young's modulus, degree of elastic anisotropy and propagation velocity of elastic waves are also computed based on this study. We used the potential parameter from periodic table information along with Taylor screening function selected on the basis of minimum energy criteria. Our results are quite encouraging for sodium and aluminum. We have successfully employed our model potential to the calculation of lattice dynamics of transition metals as well as actinide metal thorium and the results are communicated in reputed journal. As a future scope of further study one can use the reciprocal sum method for complete analysis of lattice dynamics of this metals.

There are many attempts in developing the experimental techniques for obtaining the structure factor at different temperatures. On the theoretical side new theories are developing to study the
structure factor of liquid metals. There is keen interest in experimental as well as theoretical side to study the thermodynamic properties of liquid metals. In chapter 5 we have computed the internal energy excess entropy, enthalpy, Helmholtz free energy of cubic metals. We have also studied the temperature variations of these properties for some cubic metals using hard sphere reference theory for static structure factor. It is possible to estimate these properties using many other reference systems like OCP and CHS. As a most accurate procedure one can use structure factor for a given interaction potential derived from two machine simulation methods MC and MD.

At present the two more popular languages for numeric computations are Fortran and C. There are also some packages available e.g. Mathematica and SCI Lab for such computations. But there are an immense amount of scientific codes written in Fortran. Many of them are found as libraries or can be written as subroutine for solving a large variety of problems. The Fortran language is designed with a goal of easiness in coding and high performance in numerical applications. For these reasons all the programs developed during the present study are in F77/F90 programming language. The computations are carried out on Pentium-I, Pentium-2 and Pentium-3 machines at the laboratory of Condensed Matter Physics, Department of Physics, Sardar Patel University, Vallabhb Vidyanagar.