This thesis consists of the theoretical studies of the charge perturbation and the electric field gradients (EFGs) in the dilute alloys of copper and aluminium. These studies are presented in the five chapters.

In the first chapter we give a brief account of the literature on various models and fundamental theories for the charge perturbation, EFGs and change in density of states. The resume of the present investigations is also presented there.

In chapter 2 we start with the generalities for evaluating EFG and asymmetry parameter $\eta$. The basic approaches of Blandin and Frisch (1960) and Kohn and Vosko (1960) are used to evaluate the valence effect contribution to EFG. The Alfred and Van Ostenburg (1967) charge density which includes the contribution of preasymptotic region is used. The size effect contribution is evaluated in the elastic continuum model for the matrix proposed by Sagalyn and Alexander (1977). The two contributions are added according to symmetry requirements. The formalism is used to investigate the EFGs and $\eta$ for non-magnetic dilute alloys of copper and aluminium. It is found that the valence effect alone cannot explain the observed EFGs and $\eta$. The size effect contribution is found dominating in CuIn, CuGa, CuGe, CuAg, CuCd, CuIn and CuSn alloys while the valence effect contribution
is larger than the size effect contribution for CuSb. In aluminum alloys the size effect is found larger in AlMg, AlSi, AlCu, AlZn, AlGa, AlAg and AlCd while for AlMg, the valence effect contribution is larger than the size effect contribution at 1NN. At 2NN the size effect contribution is larger than the valence effect contribution in AlMg, AlSi and AlGa alloys whereas reverse is the case in AlCu, AlZn, AlGa, AlAg and AlCd. The calculated values for $E_{IG}$'s and $\eta$'s are found in good agreement with the experimental values for almost all the alloys. The results are also compared with the other available theoretical results. An attempt is also made to correlate the magnitudes of $E_{IG}$'s and $\eta$ with the magnitudes of the impurity effective charges which are estimated with consideration of the bound state and size effect.

In chapter 3, we developed the formalism where the valences effect contribution to $E_{IG}$ is evaluated using the charge perturbation obtained in transition metal model potential (TMMP) theory. The explicit expressions for the $E_{IG}$'s due to the free electron and the depletion hole parts of charge density are obtained adopting both the Kohn and Vosko (KV) and Segalyn and Alexander (SA) models for the impurity perturbed region. The necessary modifications are introduced to evaluate the integrals involved therein. The Bloch character of the conduction electron wave function and the core polarization is explicitly incorporated in the evaluation of depletion hole contribution, therefore core enhancement factor $\alpha$ is eliminated. The components of free electron and depletion hole contributions are added. The formalism for
the size effect contribution is retained the same as in chapter 2. Only the size effect parameter \( \lambda \) is introduced to explain EFG(q) and \( \eta \). The magnitude of depletion hole contribution is found to be larger than the free electron contribution. Except for CuGe and CuSn, these contributions are found of opposite sign at 1NN. At 2NN these are additive except for CuSb. Overall, the valence effect contribution is found to be smaller than the size effect contribution. The calculated values of q and \( \eta \) are found in good agreement with the experimental values. The effective hardness of fourth row impurities is found larger than that of the fifth row impurities.

In chapter 4, the transition metal model potential theory of chapter 3 is extended for Al alloys by putting \( l = 2 \) component equal to zero. This becomes equivalent to a non-local model potential theory for Al dilute alloys, which is utilized to evaluate the free electron and depletion hole contribution to the EFG. The explicit expressions are obtained. The size effect contribution due to SA is added and the results for the EFG and \( \eta \) are explained. Although the non-locality of model potential greatly modifies the valence effect contribution, the valence effect alone does not explain observed EFG and \( \eta \). The size effect contribution is again found larger than the valence effect contribution. The calculated and experimental values of EFG and \( \eta \) are found in good agreement for almost all the alloys and these are found
to be correlated with the magnitude of effective charges on impurities. A comparison of the EFG and $\eta$ for Cu and Al alloys is also presented in this chapter.

In chapter 5 the pseudo Green's formalism is developed in an over complete set of basis functions. The $d$-band effects are included through the non-local effective impurity potential. The formalism leads to an exact expression for the change in density of states caused by the introduction of an impurity. The $d$-band contribution to the density of states is calculated for dilute Cu and Ag alloys using a simple model for the electronic structure of $d$-band metals. It is found that the $d$-band contribution is responsible for the resonances and antiresonances in the density of states. A systematic study of the effects of the impurity potential, $d$-resonance width and $d$-band energy on the density of states is carried out. The repulsive potential scatters the $d$ states towards the higher energy which may lead to bound and virtual bound states in the vicinity of Fermi level, while attractive potential scatters the $d$-states towards the lower energy which may lead to bound and virtual bound states towards the bottom of the conduction band. It is also predicted that the bound and virtual bound states are more probable in dilute alloys of Cu and Ag having narrow $d$-bands. The positions of virtual bound states in CuAl, CuCo and AgNi alloys are found at 0.514, 0.54 and 0.40 Ryd respectively which are in agreement with available theoretical and experimental informations.