CHAPTER 5

PSEUDO-GREEN’S FUNCTION THEORY FOR DILUTE ALLOYS OF d-BAND METALS

In chapter 3 we developed the transition metal model potential theory to evaluate the change in charge distribution due to an impurity. The Bloch character is explicitly incorporated and the results of the EPG and asymmetry parameter in dilute alloys of Cu are explained satisfactorily. The calculations are extended for dilute alloys of Al in chapter 4.

In recent years, there has been a considerable amount of experimental work devoted to the study of transitional impurities in transition metal and noble metal hosts (Milson 1970, Beaglehole and Erlbach 1972, Shevchik and Goldman 1974). The initial theoretical work on these transitional impurity systems was that of Friedel (1958, 1963) who argued that the localized d-electrons of transitional impurities would interact with the degenerate conduction electrons of the host metal to form resonance broadened virtual bound states. Friedel’s simple theoretical treatment did not yield the quantitative results in any particular case. Several attempts have been made to provide a more rigorous and sophisticated treatment of these impurity systems. The most popular of these has been the coherent potential approximation (Seven 1967, 1969; Valicky et al. 1968, 1970; Pant and Joshi 1970, Levin and Ehrenreich 1971, Stocks et al. 1971). This approximation scheme interpolates well between the weak and strong scattering limits and is appropriate to the entire concentration range.
Later Lasseter and Sovan (1973) considered the dilute alloy systems in which the interactions between the impurities are assumed to be negligible. Representing the host metal as a system of muffin-tin potential they have derived an exact expression for the change in density of states on alloying. The details of the host band structure and impurity potential are incorporated.

An alternative approach to the dilute transitional impurity problem is that of Riedinger (1971). In this scheme one derives an exact solution of the Dyson equation for a single impurity in terms of the overcomplete basis set of OPWs and localized d atomic orbitals (Sholl and Smith 1977). While the host metal band structure is rigorously included in this treatment, the impurity potential is generally assumed to be strongly localized and of the screened Coulomb form. To simplify the treatment of host band structure effects Moriarty (1972) developed a general one-electron pseudo-Green's function formalism as an extension of the true Green's function technique of Anderson. Pseudo Green's function equations are derived in an arbitrary, overcomplete basis representation for a general non-Hermitian pseudo-Hamiltonian. The flexibility in the choice of both the basis set and the pseudopotential makes the method useful for treating variety of physical systems. Formal calculations of the pseudo Green's function and the density of states are considered for simple metals as well as for d-band metals.

In this chapter we develop the pseudo-Green's function formalism for dilute alloys of d-band metals. The
d-band effects are included through the non-local impurity effective potential. An exact expression for the change in density of states caused by the introduction of an impurity is obtained. The d-band contribution to the density of states is calculated for dilute copper alloys using a simple model for the electronic structure of the d-band metals. A systematic investigation is carried out for dilute alloys of copper and silver. It is found that the d-band contribution is responsible for the resonances and antiresonances in the density of states. 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 the 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.

The plan of this chapter is as follows: The pseudo-Green's function formalism for charge perturbation around impurities is developed in section 5.1. The evaluation of density of states for d-band metals is carried out in section 5.2. The calculations and results for Cu and Ag alloys are presented in section 5.3 and these are concluded in section 5.4.

5.1 Pseudo Green's Function Formalism

The introduction of a simple metal impurity in a pure d-band metal gives rise to a self-consistent impurity potential \( U'(r) \) which is determined using the Friedel sum rule. In these matrices the s or p-type conduction electrons screen the impurity uniformly through the scattering process.
while the quasi bound $d$-electrons screen the impurity by forming a bound state or a virtual bound state (da Silva et al. 1971). The position and the strength of the bound states will depend upon impurity characteristics. For example, in the case of a repulsive impurity potential the scattered quasi-bound $d$-states may pile up at the top of the $d$-band or a $d$-bound state above it. In both cases, because of $s$-$d$ mixing (impurity induced or through the hybridization potential) an enhancement of the $d$-character is found at the Fermi level.

The Schrödinger equation for a matrix with impurity is,

$$ H^+ |\psi^+\rangle = (H + U') |\psi^+\rangle = E^+ |\psi^+\rangle. \quad (5.1) $$

$E^+$ and $|\psi^+\rangle$ are the perturbed energy eigenvalues and the scattered eigenstates. $H$ is Hamiltonian for a pure system.

From Eq. (5.1) the time independent one-electron Green's function may be defined as,

$$ (E + i\delta - H_U') G^+ = 1, \quad (5.2) $$

where

$$ G^+ = \sum_k \frac{|\psi^+_k\rangle <\psi^+_k|}{E + i\delta - E^+_k}. \quad (5.3) $$

$E^+_k$ is the perturbed energy eigenvalue corresponding to the scattered state $|\psi^+_k\rangle$. Let $|\gamma\rangle$ represent the overcomplete set of basis functions for the impure system. Following Anderson (1961, 1967) the DOS $f^+(E)$ for a metal with impurity becomes

$$ f^+(E) = -\frac{1}{\pi} \text{Im} \sum_{\gamma} G^+_{\gamma\gamma}, \quad (5.4) $$
and the Green's function satisfies the equation
\[ E \sum_{\gamma''} S_{\gamma\gamma''} G^{+}_{\gamma''} - \sum_{\gamma''} (H_{\gamma\gamma''} + U_{\gamma''}) G^{+}_{\gamma''} = S_{\gamma\gamma'}, \quad (5.5) \]
where \( S_{\gamma\gamma'} = <\gamma'|\gamma'> \). In an overcomplete set \( G^{+}_{\gamma\gamma'} \neq \langle\gamma'|G^{+}|\gamma'> \).
In Eq.(5.5) and in the following discussion \( E+i\epsilon \) is replaced by \( E \). We adopt pseudopotential approach to evaluate the Green's function and the DOS defined by Eqs.(5.4) and (5.5).

For the substitutional alloys with simple and noble metals as the host, da Silva et al. (1971) gave self-consistent scattering mechanism and transformed Eq.(5.1) into a pseudopotential equation,
\[ H |\phi^{+}\rangle = (H + U_{\text{off}}) |\phi^{+}\rangle = E |\phi^{+}\rangle, \quad (5.6) \]
where \( H_{\text{PS}} \) is pseudo-Hamiltonian for the host, \( |\phi^{+}\rangle \) is the scattered pseudo-wavefunction and \( U_{\text{off}} \) is nonlocal effective impurity potential. The main difference in the simple metal and noble metal pseudopotential equations is provided by the definition of \( U_{\text{off}} \). In the simple metals \( U_{\text{off}} \) is the reduced (dressed) impurity potential while in the noble metals it contains, in addition, the \( d\)-band effects like \( d-d \) scattering and \( s-d \) mixing. Assuming the scattering mechanism of da Silva et al. (1971) given by Eq.(5.6), the pseudo-Green's function (PGF) \( G^{+}_{\text{PS}} \) for the impurity problem is defined as,
\[ (E-H^{+}_{\text{PS}}) G^{+}_{\text{PS}} = (E-H^{+}_{\text{PS}} - U_{\text{off}}) G^{+}_{\text{PS}} = 1. \quad (5.7) \]
For a complete set of pseudo-wavefunctions \( |\phi^{+}_{n}\rangle \) the PGFs satisfy the coupled equations,
It can readily be shown that the PGFs which satisfy Eq. (5.8) are given as,

\[ g_{nn'}^{\text{PS}} = \frac{\delta_{nn'}}{E - E_n^{\text{PS}}} \]  

(5.9)

where \( E_n^{\text{PS}} \) is the energy eigenvalue of \( H_n^{\text{PS}} \) for the \( n \)th state.

We adopt the method due to Moriarty (1970, 1972) to generalize Eq. (5.8) for an overcomplete set of basis functions (Rivier and Zitkova 1971). Since \([\phi_n^+]\) forms a complete set there exists a transformation from \([\phi_n^+]\) to the overcomplete set \([\xi^+_q]\) and vice versa given as,

\[ \xi_q^+ = \sum_{n} U_{n q}^+ \phi_n^+ \]  

(5.10)

and

\[ \phi_n^+ = \sum_{q} V_{q n}^+ \xi_q^+ \]  

(5.11)

where

\[ \sum_{q} U_{n q}^+ V_{q n}^+ = \delta_{nn'} \]  

(5.12)

It can be shown that for valence and core states \( U_{n q}^+ \xi_q^+ \) are unique but \( V_{q n}^+ \xi_q^+ \), in general, where \( \xi_q^+ \) constitute an overcomplete set, are not unique (Moriarty 1970, 1972). With the help of Eqs. (5.10) to (5.12) it is straightforward to show that the trace of the PGFs remains invariant both in the complete and overcomplete representations (Moriarty 1972). Therefore Eq. (5.8) can directly be generalized for an overcomplete set as,
which is the principal result of this text and is valid for any basis set, complete or overcomplete. If we substitute $U_{\text{eff}} \xi' \xi'' = 0$ and $G^{+PS} \xi' \xi'' = G^{PS} \xi' \xi''$, the Eq. (5.13) reduces to the PGF equation for pure metals given by Moriarty (1970, 1972). Further more if we put $U_{\text{eff}} \xi' \xi'' = 0$ and substitute exact Hamiltonian $H$ for the pseudo-Hamiltonian $H^{PS}$ of the pure metal, we get Anderson result (1961, 1967). The main novelty of Eq. (5.13) is that it includes the overlap effects in the overcomplete basis. Rivier and Zitkova (1971) have emphasized the importance of overlap effects in some alloys like RhCo, RhFe and RhMn. Therefore Eq. (5.13) is general and allows us to derive exact analytical expressions for the PGFs and the DOS.

\[ \rho(E) = -\frac{1}{\pi} \text{Im} \sum_{\xi} G^{+PS} \xi' \xi'' \] (5.14)

for an impure system.

5.1.1 Application to simple metal alloys

The pseudo-Hamiltonian $H^{PS}$ for a simple metal is given as,

\[ H^{PS} = T + W = T + \sum_{c} \left[ U_{c} \phi_{c} \phi_{c} \right] \] (5.15)

where $\phi_{c}$ is the core state and $\theta$ is an arbitrary operator.

In the above equation the summation is over the core states of the crystal. The pseudopotential $W$ is weak. As the simple metal atom is added as an impurity, the plane waves, which form a complete orthonormal set, are scattered by the impurity and the basis set, comprising of scattered plane waves, is
given as

\[ | \vec{K} > = | k > + \frac{f(k, k')}{n} | k' >, \]  
(5.16)

where \( f(k, k') \) is the scattering amplitude. The scattered wavefunctions \( | \vec{K} > \), although form a complete set but are neither orthogonal nor normalized. Eq.(5.13) for a simple metal impurity system becomes

\[ E \sum_{K''} \sum_{K'''} G^{PS}_{KK''} C_{KK''}^{PS} G^{PS}_{KK'''}, \sum_{K''} \sum_{K'''} G^{PS}_{KK''} C_{KK''}^{PS} = \sum_{K''} \sum_{K'''} G^{PS}_{KK''} C_{KK''}^{PS} = S_{KK'}, \]  
(5.17)

where \( C_{KK'} = h^2 k^2 / 2m \) is the free electron energy of the scattered waves. Using the standard perturbation theory, Eq.(5.17) can be solved for \( G^{PS}_{KK'} \), which is given as

\[ G^{PS}_{KK'} = \frac{\delta_{KK'} \Xi_{KK'}}{E_{KK'} - (E - E_{KK'})}, \]  
(5.18)

where

\[ \Xi_{KK'} = \Xi_1^{(1)} + \Xi_2^{(2)} + \Xi_3^{(3)}, \]  
(5.19a)

and

\[ \Xi_1^{(1)} = W_{KK'}^{+} + \frac{W_{KK'}^{+} W_{KK'}^{+}}{E - E_{KK'}}, \]  
(5.19b)

\[ \Xi_2^{(2)} = U_{KK'}^{+} + \frac{U_{KK'}^{+} U_{KK'}^{+}}{E - E_{KK'}}, \]  
(5.19c)

\[ \Xi_3^{(3)} = \frac{W_{KK'}^{+} U_{KK'}^{+}}{E - E_{KK'}}, \]  
(5.19d)

\[ W_{KK'}^{+} = \Xi_{KK'}^{1}, W_{KK'}^{+} = \Xi_{KK'}^{1}, W_{KK'}^{+} = \Xi_{KK'}^{1}, W_{KK'}^{+} = \Xi_{KK'}^{1}, \]  
(5.20)
and are normalized pseudopotential and effective impurity potential. From Eqs. (5.14) and (5.18) the change in the DOS becomes

$$\delta \rho(\varepsilon) = \sum_{K} \delta(\varepsilon - \varepsilon_{K} - \varepsilon_{K'}) - \sum_{K} \delta(\varepsilon - \varepsilon_{K} + \varepsilon_{K'}) . \ (5.21)$$

The quantity\( \Sigma_{KK'}^{(1)} \), called proper self-energy, differs from \( \Sigma_{KK'} \) only by the omission of all the diagonal terms involved in the summations in Eqs. (5.19). The terms \( \Sigma_{KK'}^{(1)} \), \( \Sigma_{KK'}^{(2)} \) and \( \Sigma_{KK'}^{(3)} \), given by Eq. (5.19) correspond to host-host, impurity-impurity and host-impurity interaction contributions to all orders. These contributions are analogous to the change in DOS due to (i) change in the free electron charge density, (ii) change in orthogonalization charge density and (iii) change in interference charge density, respectively, as obtained by da Silva et al. (1971). The contributions \( \Sigma_{KK'}^{(2)} \) and \( \Sigma_{KK'}^{(3)} \) are quite small at large distances (as \( U_{\text{eff}} \) is negligible in this region), but may be significant in the vicinity of the impurity.

5.1.2 Application to d-band metal alloys

In the d-band metals conduction electrons have both s- and d-characters. Therefore in the pseudopotential theory the d-band metal with impurity has the conduction states comprising of the scattered plane waves \( |K\rangle \) and the atomic d-states \( |d\rangle \). For such a system the Green's function equations are written, from Eq. (5.13), by putting \( \varepsilon_{d} = \varepsilon_{K} \) and \( d \) given as follows,
Using the standard perturbation theory we solve Eqs. (5.22) for \( G_{K,K'}^{+} \) and \( G_{d,d'}^{+} \), incorporating the interference Green's functions \( G_{Kd}^{+} \) and \( G_{dK}^{+} \) in the same way as did by Moriarty (1972) and we get

\[
G_{d,d'}^{+} = A(d^{+}) / \mathcal{D}^{+}(E)
\]  

and

\[
G_{K,K'}^{+} = \sum_{K''} \frac{S_{K''}^{-1} S_{K'''}^{-1}}{E - \mathcal{E}_{K'''}} + \sum_{K''} \frac{S_{K''}^{-1} T_{K''''}^{-1} S_{K''''}^{-1}}{(E - \mathcal{E}_{K'''}) (E - \mathcal{E}_{K''''})} + \frac{1}{\mathcal{D}^{+}(E)}
\]

Here \( H_{\text{PS}} = E = V \). The dash over the summation sign denotes that the diagonal terms in the sum are omitted.

The \( |\mathbf{k}\rangle \) and \( |d\rangle \) states both contribute towards the DOS \( \rho(E) \), therefore we can write

\[
\rho^{+}(E) = -\frac{1}{\pi} \text{Im} \left( \sum_{K} G_{K}^{+} + \sum_{d} G_{d}^{+} \right).
\]  

(5.23)
where

\[ D^+(\omega) = \det \left[ - (V_{dd'} + U_{dd'}^{\text{eff}} + \Lambda_{dd'}^+ + \Lambda_{dd'}^{\text{imp}}) \right], \]  

\[ f^+_{dd'} = S_{dd'} \sum_{K, K'} \frac{(V_{Kd} + U_{Kd}^{\text{eff}}) S_{dK'} S_{dK'}}{E - E_{K'}}. \]

\[ + \sum_{K', K'', K'''} \frac{(V_{Kd} + U_{Kd}^{\text{eff}}) S_{dK''} S_{dK'''}}{(E - E_{K''}) (E - E_{K'''}).} \]  

\[ \left( \frac{\partial}{\partial \omega} \right) f^+_{dd'} = \sum_{K, K'} \frac{(V_{Kd} + U_{Kd}^{\text{eff}}) S_{dK'} S_{dK'}}{E - E_{K'}}. \]

\[ \left( \frac{\partial}{\partial \omega} \right) \left( \frac{\partial}{\partial \omega} \right) f^+_{dd'} = \sum_{K, K'} \frac{(V_{Kd} + U_{Kd}^{\text{eff}}) S_{dK'} S_{dK'}}{E - E_{K'}}. \]

\[ \left( \frac{\partial}{\partial \omega} \right) \Lambda_{dd'} = \sum_{K, K'} \frac{(V_{Kd} + U_{Kd}^{\text{eff}}) S_{dK'} S_{dK'}}{E - E_{K'}}. \]

Because of the five-fold degeneracy of the d-bands \( D^+ (\omega) \) and \( A(\alpha^+ \beta) \) are determinants of order 5N, where N is the number of scattering centres per unit volume, \( A(\alpha^+ \beta) \) and \( A(\alpha^+ \beta) \) are obtained by replacing the \( \beta \)-th column of \( D^+ (\omega) \) by \( f^+_{d\beta} \) and \( g^+_{d\beta} \) respectively. \( T_{KK'} \) is the transpose of \( T_{KK'} \). The quantities \( f^+_{dd'} \) and \( \Lambda^+_{dd'} \) contain the physical effects arising from the \( \alpha-d \) hybridization in a pure d-band metal described by \( V_{dK} \) or \( V_{dK} \) and the impurity induced \( \alpha-d \) hybridization described by \( V_{dK} \) or \( V_{dK} \).
Later on it will be shown that $\Gamma_{dd}^+$ is related to $\text{d}$-resonance width and $\text{d}$-band energy of the impure system. Using Eqs. (5.24) and (5.25) in Eq. (5.23) the DOS for an impure $\text{d}$-band metal is written as,

$$
\rho^+(E) = \frac{1}{\pi} \text{Im} \left[ \frac{\Sigma_{K,K'}^1}{K,K'} + \frac{\Sigma_{K,K'}^1}{K,K',K''} \left( \frac{1}{E - \varepsilon_{K}^1}(E - \varepsilon_{K''}^1) \right) \right] + \frac{1}{\pi} \text{Re} \left[ \frac{\Sigma_{K,K'}^1}{K,K'} \right].
$$

Substituting $\text{U}_{\text{eff}}^{\text{dd}} = 0$ and replacing $|K>$ by $|k>$ one gets quantities $\Gamma_{dd}^+$, $\Lambda_{dd}^+$, $f_{dd}^+$, $\varepsilon_{dd}^+$, $D^+(E)$ and $\Sigma_{KK}^{(1)}$ for a pure $\text{d}$-band metal corresponding to the quantities $\Gamma_{dd'}^+$, $\Lambda_{dd'}^+$, $f_{dd'}^+$, $\varepsilon_{dd'}^+$, $D^+(E)$ and $\Sigma_{KK'}^{(1)}$, respectively. With the above substitution one easily gets the PGEs and the DOS $\rho(E)$ for the pure metal, the same as obtained by Moriarty (1972). This gives the change in electronic DOS for a $\text{d}$-band metal alloy as,

$$
\delta \rho(E) = \frac{1}{\pi} \left[ \left( \frac{\Sigma_{K,K'}^1}{K,K'} - \frac{\Sigma_{K,K'}^1}{K,K'} \right) \frac{1}{E - \varepsilon_{K}^1} \right] + \left( \frac{\Sigma_{K,K'}^1}{K,K'} \right)^2 \frac{1}{E - \varepsilon_{K}^1}.
$$
which is an exact expression. The only infinite series which appear in the expression for change in DOS (charge perturbation) are \( Z_{K,k}^\to \) and \( Z_{K,k}^{(1)} \).

We write \( \rho'(E) \) in a more physically transparent form by expanding the determinant \( \Delta \) around the \( d \)th column using Laplace's development. It can be shown that, in the local pseudopotential approximation for the host, the contribution to \( \delta \rho'(E) \) attributed by terms in the last three brackets of Eq. (5.32) can be written as \( \frac{d}{dE} \ln \left( \frac{D^+(E)}{D(E)} \right) \). Therefore,

\[
\delta \rho'(E) = -\frac{1}{\pi} \text{Im} \left[ \left( \frac{S_{KK}^{-1}}{E - E_{K}^*} \frac{S_{KK}^{-1}}{E - E_{K}^*} \right) - \frac{1}{E - E_{K}^*} \right]
\]

\[
+ \left( \frac{S_{KK}^{-1}}{E - E_{K}^*} \frac{S_{KK}^{-1}}{E - E_{K}^*} \right) - \frac{1}{E - E_{K}^*} \right] \]

\[
\Sigma \frac{d}{dE} \ln \left( \frac{S_{KK}^{-1}}{E - E_{K}^*} \frac{S_{KK}^{-1}}{E - E_{K}^*} \right) - \Lambda_+ \]
In Eq. (5.32) the terms in the first curly bracket arise from the scattering of plane waves due to the presence of the impurity and the terms in the second curly bracket are the corrections to the first term which arise due to the modification of the self-energy which include multiple $s$-scattering terms. The last two terms are due to $d$-scattering: the last but one term arises from the single $d$-scattering and the last term arises from multiple $d$-scattering. The $d$-band contribution contains the terms $V_{kd}$ (or $V_{kd'}$), $U_{dd}^{\text{eff}}$ (or $U_{dd'}^{\text{eff}}$) and $U_{dd'}^{\text{eff}}$. The terms $V_{kd}$ and $U_{dd}^{\text{eff}}$ represent the $s$-$d$ hybridization in a pure metal and the impurity induced $s$-$d$ hybridization, respectively. The impurity induced $d$-$d$ scattering represented by the matrix elements $U_{dd'}^{\text{eff}}$ may be responsible for piling up of the $d$-states near the top of the $d$-band or at the bottom of the $d$-band depending upon the characteristics of the impurity (Friedel 1958, da Silva 1971). This may give rise to bound states or virtual bound states at the respective positions.

5.2 Evaluation of Density of States for $d$-band Metal Alloys

The Eq. (5.2) can be solved for the true Green's function $G^+(\mathbf{r},\mathbf{r}',\mathbf{E})$ in the direct space. The integration over $\mathbf{r}$-space
leads to the well known expression for the DOS of impure system as,

$$\rho^+ (E) = \rho_o^+ (E) + \frac{2}{\pi} \frac{E}{1} (21 + 1) \frac{d}{dE} \delta' + \text{Oscillatory terms} \quad (5.34)$$

where $\rho_o^+ (E)$ is the free electron DOS and $\delta'_1$ is the phase shift for the $l$th component of the angular momentum. Similarly one can solve for the Groan's function $G(\mathbf{r}, \mathbf{r}', \mathbf{E})$ for the pure system. Therefore the change in the DOS caused by the introduction of the impurity is written as,

$$\delta \rho^+ (E) = \delta \rho_o^+ (E) + \frac{2}{\pi} \frac{E}{1} (21 + 1) \frac{d}{dE} (\Delta \delta_1) + \text{Oscillatory terms,} \quad (5.35)$$

where $\Delta \delta_1 = \delta'_1 - \delta_1$ is the change in the phase shift resulting due to the scattering from the impurity. Here it is to be noted that Eq. (5.35) is valid only for dilute alloys.

To have correspondence between Eqs. (5.33) and (5.35) we write the free electron contribution to $\delta \rho^+ (E)$ in the PGF formalism as

$$\delta \rho_o^+ (E) = \delta \rho_o^+ (E) + \delta \rho_o'' (E), \quad (5.36)$$

where

$$\delta \rho_o^+ (E) = -\frac{1}{\pi} \text{Im} \left\{ \sum_{\mathbf{K}, \mathbf{K}'} \frac{S^{-1}_{\mathbf{KK}'} \Sigma_{\mathbf{K} K'}}{2E - \Sigma_{\mathbf{K} K'}} - \frac{1}{E - \xi_{\mathbf{K}}^F} \right\}, \quad (5.37)$$

$$\delta \rho_o'' (E) = -\frac{1}{\pi} \text{Im} \left\{ \sum_{\mathbf{K}, \mathbf{K}' \mathbf{K}''} \frac{S^{-1}_{\mathbf{KK}'} \Sigma_{\mathbf{K} K''} \Sigma_{\mathbf{K}'' K}}{2E - \Sigma_{\mathbf{K} K''} \Sigma_{\mathbf{K}'' K} - \xi_{\mathbf{K}}^F} - \frac{\Sigma_{\mathbf{KK}''}}{2E - \xi_{\mathbf{K}}^F \xi_{\mathbf{K}''}^F} \right\}. \quad (5.38)$$

$\delta \rho_o'' (E)$ gives the multiple scattering contribution to $\delta \rho_o^+ (E)$.
The third term in Eq. (5.33) represents the contribution to $\delta f(E)$ arising from the single $d$-resonant scattering. The $l=2$ phase shift in the impure system for a single scatterer is defined as,

$$\delta_2 = \tan^{-1}\left[\frac{-\text{Im} \gamma_{dd}^+}{\text{Re} \gamma_{dd}^+ - E}ight].$$

(5.39)

Comparing Eq. (5.39) with the standard resonance formula,

$$\delta_2 = \tan^{-1}\left(\frac{\frac{1}{2} \frac{W_i}{E_d - E}}{1}ight),$$

(5.40)

we find the $d$-resonance width $W^i_d$ and the $d$-band energy $E^i_d$ of the impure system as

$$\frac{1}{2} W^i_d = -\text{Im} \gamma_{dd}^+ (E^i_d),$$

(5.41)

and

$$E^i_d = \text{Re} \gamma_{dd}^+ (E^i_d) + \text{Re} \gamma_{dd}^+ (E^i_d).$$

(5.42)

Substituting $U_{\text{eff}} = 0$ and replacing $\gamma_{dd}^+$ by $\gamma_{dd}^+$ one finds the phase shift $\delta_2$ for the pure system as,

$$\delta_2 = \tan^{-1}\left(\frac{\frac{1}{2} \frac{W_i}{E_d - E}}{1}\right)$$

(5.43)

where

$$E_d = \text{Re} \gamma_{dd}^+ (E_d),$$

(5.44)

$$\frac{1}{2} W_d = -\text{Im} \gamma_{dd}^+ (E_d).$$

(5.45)
$W_d$ and $E_d$ are the $d$-resonance width and the $d$-band energy for the pure system. This result is the same as obtained by Morairty (1972). Using Eqs. (5.36) to (5.45), the Eq. (5.33) for a single $d$-resonant scattering (neglecting the last term of Eq. (5.33)) becomes

$$
\delta \langle \Omega \rangle = \delta \langle \Omega \rangle + \frac{10}{\pi} \frac{d}{dE} \left( \Delta \delta \right) + \frac{d}{d\omega} \left[ \left( 1 - \frac{\Lambda^{dd}}{E - \frac{H_{ff}}{dd} - \Gamma^{dd}} \right) \right],
$$

(5.46)

The factor of 10 in the second term of Eq. (5.46) is the $d$-band multiplicity factor. The first two terms of Eq. (5.46) are similar to the first two terms of Eq. (5.35) and the last term of Eq. (5.46) is a multiple scattering term and may exhibit oscillatory behaviour. Therefore the expression for $\delta \langle \Omega \rangle$ obtained on the PGO approach is similar to that obtained through the true Green's function formalism. The quantity $\Lambda^{dd}$ contains three contributions, $\Lambda^{hh}$, the host-host interactions, $\Lambda^{ih}$, the impurity-host interactions and $\Lambda^{ii}$ the impurity-impurity interactions. Therefore we can write

$$
\Lambda^{+}_{dd} = \Lambda^{+hh}_{dd} + \Lambda^{+ih}_{dd} + \Lambda^{+ii}_{dd}.
$$

(5.47)

For dilute alloys the impurity-impurity interactions (represented by $\Lambda^{(2)}_{ii}$ and $\Lambda^{+ii}_{dd}$) are negligible. Moreover in the $d$-band metals all the phase shifts, except $l = 2$, are slowly varying.

For dilute alloys the impurity-impurity interactions (represented by $\Lambda^{(2)}_{ii}$ and $\Lambda^{+ii}_{dd}$) are negligible. Moreover in the $d$-band metals all the phase shifts, except $l = 2$, are slowly varying.
functions of energy and hence their contribution towards \( \delta \rho (E) \) may be negligible. The magnitude of the multiple scattering contribution in Eq. (5.36) is also quite small, therefore the change in DOS may be written as

\[
\delta \rho (E) = \delta \rho_o (E) + \frac{10}{\pi} \frac{d}{dE} (\Delta \delta_2).
\]

This is the exact result due to Anderson (1961, 1967) in the limit \( W \rightarrow 0 \).

In a dilute alloy of d-band metal there are \( N \) d-resonant scatterers. The first two terms of Eq. (5.33) are unaffected except that the sum over all the \( 5N \) d-states instead of only five is performed. The last term of Eq. (5.33) represents the contribution from the interference between the different d-resonant scatterers and may cause broadening in d-band DOS. The exact evaluation of all the terms in Eq. (5.33) is extremely difficult. However to extract new features introduced by the theory at least qualitatively, we make few simplifications. Following Moriarty (1972) and the arguments of Anderson (1961, 1967) we assume \( W = 0 \). This is equivalent to assuming a constant pseudopotential for the s- and d-conduction electrons. Again we assume that impurity-impurity interaction is negligible. This simplifies Eq. (5.33) as,

\[
\delta \rho (E) = \delta \rho_o (E) + \delta \rho_d (E),
\]

where

\[
\delta \rho_d (E) = \rho^{+}_d (E) - \rho^{+}_d (E) = \delta \rho^+_1 \delta \rho^+_2 \delta \rho^+_3
\]
\begin{align}
\delta \Phi_{1}(E) &= \frac{10N}{\pi} \left[ \frac{1}{2} \frac{\psi_{d}^{2}}{E_{d}^{2}} - \frac{1}{2} \frac{\psi_{d}^{2}}{E_{d}^{2}} \right], \quad (5.51) \\
\delta \Phi_{2}(E) &= \frac{1}{2} \frac{10N}{\pi} \left[ \frac{S^{2} \left( \frac{1}{2} \psi_{d}^{2} \right)^{3} \left[ 3 \left( E - E_{d}^{i} \right)^{2} - \left( \frac{1}{2} \psi_{d}^{i} \right)^{2} \right]} \right]^{3} \\
&\quad - \frac{S^{2} \left( \frac{1}{2} \psi_{d}^{2} \right)^{3} \left[ 3 \left( E - E_{d}^{i} \right)^{2} - \left( \frac{1}{2} \psi_{d}^{i} \right)^{2} \right]} \left[ \left( E - E_{d}^{i} \right)^{2} + \left( \frac{1}{2} \psi_{d}^{i} \right)^{2} \right]^{3}, \quad (5.52) \\
\delta \Phi_{3}(E) &= \frac{1}{2} \frac{10N}{\pi} \left( \frac{1}{2} \psi_{d}^{2} \right)^{2} \left| \frac{\psi_{dd}^{i}}{dd} \right|^{2} \frac{3 \left( E - E_{d}^{i} \right)^{2} - \left( \frac{1}{2} \psi_{d}^{i} \right)^{2}} \left[ \left( E - E_{d}^{i} \right)^{2} + \left( \frac{1}{2} \psi_{d}^{i} \right)^{2} \right]^{3} \quad (5.53)
\end{align}

In the above equations we retain only the first term in the expansion of logarithm function in the last term of Eq. (5.33). Further we substitute \( V_{dd}^{i} + V_{dd}^{i} = -iS \left( \frac{1}{2} \psi_{d}^{i} \right) \) and \( V_{dd}^{i} + V_{dd}^{i} = -iS \left( \frac{1}{2} \psi_{d}^{i} \right) \). In Eq. (5.49), \( \delta \Phi_{1}(E) \) is the contribution purely due to \( s \)-electrons and \( \delta \Phi_{2}(E) \) is the contribution purely due to \( d \)-electrons. From Eqs. (5.49) to (5.53) it is evident that if we know \( \psi_{dd}^{i}, \psi_{dd}^{i}, \psi_{dd}^{i} \) and \( S' \) for an impure system, \( \delta \Phi(E) \) can be evaluated using the corresponding values of the pure system.

The effective impurity potential for a \( d \)-band metal alloy as defined by da Silva et al. (1971) is given as,

\[ u^{\text{eff}}(E) = U'(1 - \sum_{d} \alpha > \alpha |d > d|) + \sum_{d} \frac{\omega_{d}^{i} |d > d|}{E_{d} - E} \left( E - E_{d} - U' \right) |d > d| U'(1 - \sum_{d} \alpha > \alpha |) \]

\[ + \sum_{d} \frac{\omega_{d}^{i} |d > d|}{E - E_{d}} \]
\[ F(E) = \frac{1}{E - E_d}, \quad \tilde{U}' = \langle d|U'|d \rangle. \]  

where \( \alpha \) are the core states. Here it is assumed that the self-consistent impurity potential is localized, i.e., \( \langle d|U'|d'\rangle = \tilde{U}' \) is independent of \( |d\rangle \) and \( |d'\rangle \) states (da Silva et al. 1971). \( \Delta \) is hybridization potential as defined by Harrison (1969) and is given as,

\[ \Delta|d\rangle = \delta V|d\rangle - \langle d|\delta V|\alpha \rangle |\alpha \rangle, \]  

where \( \delta V \) is the difference between the actual self-consistent potential \( U \) of the pure crystal and the atomic potential \( U_a \).

The last term of Eq.\((5.54)\) represents the multiple \( d-d \) scattering contribution (higher order term) and is expected to be small in comparison with the single scattering contribution. For simplicity we neglect higher order terms thereby reducing Eq.\((5.54)\) to

\[ U_{\text{eff}}^{d-d} = \tilde{U}' (1 - \frac{\langle \alpha|\alpha \rangle}{d} - \frac{\langle d|d\rangle}{E_d - E} + \sum_{d'} \frac{\langle \alpha|\alpha \rangle}{d'} \frac{d|d\rangle}{E_d - E}) \]

\[ + \sum_{d'} \frac{d|d\rangle}{E_d - E} |\Delta' + U'| \frac{d|d\rangle}{E_d - E} (1 - \frac{\langle \alpha|\alpha \rangle}{d}) \]  

\[ = \tilde{U}' + |\tilde{U}'|^2 \sum_{d'} \frac{1}{E_d - E_{d'}}. \]

Using Eqs.\((5.55)\) and \((5.56)\) in Eq.\((5.57)\) we find

\[ U_{\text{dd}}^{\text{eff}} = \langle d|U_{\text{dd}}^{\text{eff}}|d \rangle \]

\[ = -\tilde{U}' + |\tilde{U}'|^2 \sum_{d'} \frac{1}{E_{d'} - E_{d'}}. \]
In obtaining Eq. (5.58) it is assumed that $\delta V$ is spherically symmetric so that $\langle d | \Delta | d' \rangle = 0$ as argued by Harrison (1969, 1970). Also the variation of $\Delta$ over the core states is neglected (Harrison 1969, 1970) by virtue of which $\langle d | \Delta | d \rangle = 0$. Considering other approximations involved, this simplification may not cause serious error.

It is evident from Eq. (5.58) that $U_{dd}^\text{eff}(E)$ diverges at $E = E_d$. Anisalu (1974) discussed that the expression $1/(E - E_d)$ is valid for the energy band calculations but for the scattering problem it is represented as $1/(E - E_d + i \frac{1}{2} \nu_d)$. Following Anderson (1961) the divergence can be avoided by replacing $\sum 1/(E - E_d)$ by

$$
\frac{C \left( \frac{1}{2} \nu_{d'} \right)}{(E - E_d')^2 + \left( \frac{1}{2} \nu_{d'} \right)^2},
$$

where the constant $C = \frac{\pi}{k_d \Omega / \pi^2}$ is the DOS at $E_d = k_d^2 \nu_d^2 / 2$. Therefore Eq. (5.58) for $U_{dd}^\text{eff}$ is simplified as

$$
U_{dd}^\text{eff} = -U' + \left( U' \right)^2 \frac{C \left( \frac{1}{2} \nu_{d} \right)}{(E - E_d')^2 + \left( \frac{1}{2} \nu_{d} \right)^2}.
$$

### 5.3 Calculations and Results

#### 5.3.1 The variation in $\delta_b^\alpha(\tilde{E})$ with $\tilde{U}', \nu_{d}^\alpha$ and $E_d^\alpha$

We now present the numerical results for the DOS for dilute alloys of copper and the change in the DOS in the alloy formation. Moriarty (1972) showed that in the pure Copper metal...
s-electron contribution to the DOS is smooth and much smaller as compared to the d-electron contribution. Smith (1978) also found the small contribution of the s-electrons in the regions of resonances and anti-resonances. He concluded that resonances and anti-resonances arise almost solely from the strong hybridization of the quasi-localised d-electrons and the s-electrons as predicted by Friedel (1958, 1963). According to the above findings, the basic quantity of interest is the d-electron DOS, which may give rise to bound or virtual bound states. Fig. 5.1 shows the d-electron DOS $\tilde{\rho}_d(E)$ for pure copper with the same parameters as those used by Moriarty (1972), i.e., $E_d = 0.5$ Ry, $\frac{1}{2} W_d = 0.05$ Ry and $S = 0.75$. The single d-scattering term gives a resonance at $E = E_d$ while the multiple scattering term gives an anti-resonance at the same energy value. These two contributions cancel each other around $E_d$ and create two overlapping peaks in $\tilde{\rho}_d(E)$ as is evident from Fig. 5.1.

In the case of an alloy the exact values of the self-consistent potential $\tilde{U}'$, the band width $W_d^i$ and the d-band energy $E_d^i$ are not known. Therefore we choose the values of these parameters at variance of about 20 percent which may be quite near to any realistic physical system. Fig. 5.2 shows the d-electron DOS $\tilde{\rho}_d^i(E)$ for copper alloy with $E_d^i = 0.6$ Ry, $\frac{1}{2} W_d^i = 0.06$ Ry, $S' = 1.0$ and for different values of repulsive and attractive $\tilde{U}'$. We find that $\tilde{\rho}_d^i(E)$ shows two distinct peaks around $E_d^i$ with a dip at $E = E_d^i$. This dip is very sensitive to $\tilde{U}'$ and increases rapidly with the increase
Beyond a critical value of $\tilde{U}'$ (attractive or repulsive) the $\int d(E)$ becomes negative in a small region around $E_d^{\pm}$ which may lead to instability of the system. This may also explain the non-solubility of certain impurities in certain matrices such as Ag in Ni and Au in Ni (Pearson 1958). We also note that the peak separation and peak heights, which denote the piling of the $d$-states in two distinct bands around $E_d^{\pm}$, go on increasing with the increase of $\tilde{U}'$. This may lead to the formation of bound or virtual bound states. This conclusion is consistent with Friedel (1958) and the calculations of Swietendik (1972) that by introducing Ag in Pd the partially filled $d$-band of Pd is filled by the impurity valence electrons.

For the repulsive $\tilde{U}'$ the peak height of resonance, at the higher value of $E$ is larger as compared to the peak height of resonance at lower value of $E$. This shows that the repulsive potential scatters the $d$-states towards the higher energy value thereby enhancing the $d$-character near the Fermi level. This may lead to virtual bound state in the vicinity of the Fermi level or a bound state above the Fermi level under favourable situations. For the attractive $\tilde{U}'$ the peak height of resonance at the lower value of $E$ is larger than that at the higher value of $E$. The antiresonance at $E = E_d^{\pm}$ is slightly deeper than that obtained for the repulsive potential $\tilde{U}'$ with the same magnitude. Therefore in the case of attractive $\tilde{U}'$ the $d$-states are scattered towards the lower energy values and may lead to a bound or virtual bound state near the bottom of the conduction band.
\( \delta \rho_d^i (E) \) for the copper alloy with \( E_d^i = 0.6 \) Ry, \( \frac{1}{2} \nu_d^i = 0.65 \) Ry and \( S' = 1.0 \) is shown in Fig. 5.3 for the two repulsive potentials \( U' = 0.05 \) Ry and \( 0.10 \) Ry. For the repulsive and attractive potentials of equal magnitude, the resonances and antiresonances are at the same positions but differ in magnitude at the most by 10%. For example for an attractive potential \( U' = -0.1 \) Ry, the height of the peak at \( E = 0.5 \) Ry is increased while the height of the peak at \( E = 0.65 \) Ry is decreased as compared with the corresponding curve for \( U' = 0.1 \) Ry. For the clarity of the diagram \( \delta \rho_d^i (E) \) for \( U' = 0.05 \) Ry and \( -0.10 \) Ry are not shown in Fig. 5.3. The different contributions to \( \delta \rho_d^i (E) \), i.e. \( \delta \rho_1 (E) \) and \( \delta \rho_2 (E) \) and \( \delta \rho_3 (E) \), are also separately shown in Fig. 5.4 for \( E_d^i = 0.6 \) Ry, \( \frac{1}{2} \nu_d^i = 0.06 \) Ry \( S' = 1.0 \) and \( U' = 0.10 \) Ry. \( \delta \rho_1 \) is negative below \( E = 0.55 \) Ry and exhibit an antiresonance at \( E = 0.5 \) Ry while it is positive for energy higher than \( E = 0.55 \) Ry and exhibit a resonance at \( E = 0.61 \) Ry. This concludes that the single \( \delta \) resonant scattering piles up the states near the Fermi energy thereby decreasing the DOS at lower energies, i.e., near the bottom of the d band. The multiple scattering contribution \( \delta \rho_1^i + \delta \rho_2^i \), shown in Fig. 5.4 in the present formalism is similar, at least qualitatively, to the change in the \( \delta \)-electron DOS for CuNi alloy obtained by Smith (1978). The antiresonance in \( \delta \rho_1^i + \delta \rho_2^i \) occurs at \( E = 0.475 \) Ry which is near to the copper absorption edge observed at \( E \approx 0.488 \) Ry and a virtual bound state at \( E = 0.64 \) Ry.
to have the bound and virtual bound states in the dilute alloys of narrow d-band. The variation of $\delta\rho_d(E)$ with $E_d^i$ is shown in Fig. 5.6 for the fixed values of $U'$, $\frac{1}{2} W_d^i$ and $S'$. For $E_d^i = 0.5$ Ry ($= E_d$) there are two resonances around $E_d^i$ and an antiresonance at $E_d^i$. The two resonances are of approximately equal magnitudes and almost symmetrical about the antiresonance. For $E_d^i = 0.4$ Ry ($< E_d$) and $0.6$ Ry ($> E_d$) two resonances and two antiresonances are observed. For $E_d^i = 0.4$ Ry, the resonance at the lower energy value is much more stronger than that occurring at the higher energy while for $E_d^i = 0.6$ Ry the resonance at higher energy is more dominating. It shows that with the increase in the d-band energy, in the formation of an alloy, the d states are scattered towards the Fermi energy while with the decrease in the d-band energy the d-states are scattered towards the bottom of the conduction band. The similar conclusions were also drawn for the repulsive and attractive impurity potentials. From the study of the effects of the nature of the impurity potential and the variation of d-band energy it appears that in the case of an attractive impurity potential the d-band energy of the alloy is lowered while for the repulsive impurity potential the d-band energy is enhanced.

5.3.2 Change in density of states for CuNi, CuCo and AgNi alloys.

We calculated $\delta f(E)$ for CuNi, CuCo and AgNi alloys as the relevant parameters were available to us. These parameters are given in Table 5.1. The Ni and Co impurities in
Cu and Ni impurity in Ag are repulsive, therefore $U$ is taken as positive. It is found that the major contribution to $\delta P(E)$ arises from $\delta P_1(E)$ and $\delta P_2(E)$. $\delta P_3(E)$ is found to be quite small as $U_{dd}$ is small. Comparing $\delta P_1(E)$ and $\delta P_2(E)$, $\delta P_1(E)$ is found larger than $\delta P_2(E)$, which emphasises that the leading contribution to $\delta P_d(E)$ is from the single $d$-scattering.

The results for $\delta P_d(E)$ as a function $E$ are shown in Figs. 5.7, 5.8 and 5.9 for CuNi, CuCo and AgNi alloys respectively. The results for all the alloys have the same systematics. It is evident that the repulsive potential scatters the $d$-states towards the higher energy and virtual bound states are formed near the Fermi energy. If the splitting of the peaks is ignored, the shape of the virtual bound state is Lorentzian at $E = E_d^i$, which is consistent with the calculations of Podloucky et al. (1980) and Neiminen and Puska (1980). The maximum value of $\delta P_d(E)$ is near $E = E_d^i$.

$\delta P_d(E)$ for CuNi is found to be maximum at $E = 0.514$ Ry ($\approx E_d^i$) and it is minimum at $E = 0.36$ Ry. The value of $\delta P_d(\text{max})$ is about 9 states / ev. Smith (1978) and Dederichs and Zeller (1981) reported this value about 10-12 states / ev. Experimental data is not available to us for a ready comparison. For CuCo alloys, $\delta P_d(\text{max}) = 2.5$ states/ev at $E = 0.54$ Ry, Dederichs and Zeller (1981) found $\delta P_d(\text{max}) = 1$ state/ev at $E = 0.53$ Ry. Therefore the position of virtual bound in both the calculations agree. However, the peak value is found
larger in our calculations than in the calculations of Dederichs and Zeller. For AgNi alloy $\delta P_d^{(\text{max})} = 6.5 \text{ states/ev}$ at $E = 0.4 \text{ Ry}$, Podloucky et al. (1980) found $\delta P_d^{(\text{max})} = 6-8 \text{ states/ev}$ at $E = 0.39 \text{ Ry}$. Therefore the two calculations yield almost similar results.

5.4 Conclusions

The pseudo Green's function formalism for the dilute alloys of the d-band metals is developed adopting the impurity scattering mechanism due to da Silva et al. (1971). The exact expression for the change in density of states is obtained, however its numerical evaluation is found to be a difficult task. The calculations for DOS for dilute alloys of copper and silver are carried out. It is found that the s-electron part is quite small and does not contribute substantially towards the structural features of the DOS. The d-band contribution to the change in the DOS $\delta P_d^{(\text{max})}$ is found dominating and is responsible for resonances and antiresonances. The single d-resonance contribution to the DOS (i.e., $P_d^{(3)}$ or $P_d^{(\pi)}$) gives rise to resonance while the multiple d-scattering contribution is oscillatory and consists of both resonances and antiresonances. The combined effect of $\delta P_1^{(2)}(E)$ and $\delta P_2^{(2)}(E)$ is analogous to the results obtained by Smith (1978). $\delta P_3^{(2)}(E)$, which explicitly depends upon $U_{dd}^{\text{off}}$, is quite important in the vicinity of $E_{\text{d}}^d$. This term separates and sharpens the two peaks around $E_{\text{d}}^{d}$ and gives some information about the non-solubility of certain impurities in d-band matrices. It
is also noteworthy that the present PGF formalism describes explicitly the effect of the variation of $\frac{1}{2} V_\sigma$, $E_\sigma^i$, and $\Gamma_\sigma^j$ (repulsive or attractive) on the charge perturbation around the impurity. With the increase in the $\sigma$-band width the peak heights go on decreasing while the separation goes on increasing. With the increase in the $\sigma$-band energy the piling of the $\sigma$-states increases towards the higher energy and the reverse is the case with the decrease of the $\sigma$-band energy. The repulsive impurity potential scatters the $\sigma$-states towards the higher energy which may lead to the formation of the bound or virtual bound states in the vicinity of the Fermi energy. The attractive impurity potential scatters the $\sigma$-states towards the lower energy values which may form bound or virtual bound states towards the bottom of the conduction band. Our calculations confirm the predictions of Friedel and Anderson.
### Physical parameters for CuNi, CuCo and AgNi alloys

<table>
<thead>
<tr>
<th>Alloy</th>
<th>( \frac{1}{2} W_d ) (eV)</th>
<th>( E_d ) (eV)</th>
<th>( \ln a_d ) (eV)</th>
<th>( E_p ) (eV)</th>
<th>( \Omega ) (a.u.)</th>
<th>( m )</th>
<th>( S )</th>
<th>( S' )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuNi</td>
<td>0.1176(^{b,c})</td>
<td>0.414(^{b,c})</td>
<td>0.0470(^d)</td>
<td>0.514(^d)</td>
<td>0.005</td>
<td>0.5685</td>
<td>79.4</td>
<td>1.0</td>
</tr>
<tr>
<td>CuCo</td>
<td>0.1176(^{b,c})</td>
<td>0.414(^{b,c})</td>
<td>0.0470(^d)</td>
<td>0.516(^d)</td>
<td>0.005</td>
<td>0.5685</td>
<td>79.4</td>
<td>1.0</td>
</tr>
<tr>
<td>AgNi</td>
<td>0.1237(^{b,c})</td>
<td>0.156(^{b,c})</td>
<td>0.0243(^d)</td>
<td>0.400(^d)</td>
<td>0.005</td>
<td>0.450</td>
<td>114.6</td>
<td>1.0</td>
</tr>
</tbody>
</table>

\(^a\) D. Beaglehole (1976)  
\(^b\) G. Das Sashibala (1973)  
\(^c\) M.M. Traum and N. V. Smith (1974)  
\(^d\) Podloucky et al (1980)
FIGURE CAPTIONS

Fig. 5.1 The solid line shows $\rho_d(E)$ versus $E$ for pure copper metal with $E_d = 0.5$ Ry, $\frac{1}{2} \nu_d = 0.05$ Ry and $S = 0.75$. The dashed lines 1 and 2 present the single $\sigma$-scattering and multiple $\sigma$-scattering contributions, respectively, to $\rho_d(E)$.

Fig. 5.2 $\rho_d^+(E)$ versus $E$ for the copper alloys with repulsive and attractive impurity potentials taking $E_d^i = 0.6$ Ry, $\frac{1}{2} E_d^i = 0.06$ Ry and $S' = 1.0$.

Fig. 5.3 For copper alloys with $E_d^i = 0.6$ Ry, $\frac{1}{2} E_d^i = 0.06$ Ry and $S' = 1.0$, $\delta \rho_d(E)$ is plotted against $E$ for the repulsive impurity potential $E' = 0.05$ and $0.10$ Ry.

Fig. 5.4 The contributions $\delta \rho_1$, $\delta \rho_2$, $\delta \rho_3$ and $\delta \rho_1^+ + \delta \rho_2^+$ to the $\sigma$-electron DOS versus $E$ are shown for the copper alloy with $E_d^i = 0.6$ Ry, $\frac{1}{2} E_d^i = 0.06$ Ry, $S' = 1.0$ and $E' = 0.1$ Ry.

Fig. 5.5 For the copper alloy with $E_d^i = 0.6$ Ry, $E' = 0.1$ Ry and $S' = 1.0$, $\delta \rho_d(E)$ versus $E$ is shown for $\frac{1}{2} E_d^i = 0.04$, $0.05$ and $0.06$ Ry.

Fig. 5.6 $\delta \rho_d(E)$ versus $E$ for $E_d^i = 0.4, 0.5$ and $0.6$ Ry assuming $E' = 0.1$ Ry, $\frac{1}{2} E_d^i = 0.06$ Ry and $S' = 1.0$.

Fig. 5.7 $\delta \rho_d(E)$ versus $E$ for CuNi alloys.

Fig. 5.8 $\delta \rho_d(E)$ versus $E$ for CuCo alloys.

Fig. 5.9 $\delta \rho_d(E)$ versus $E$ for NiNi alloys.
Fig. 5.1

\[ E_d = 0.5 \text{ Ry} \]
\[ \frac{1}{2} W_d = 0.05 \text{ Ry} \]
\[ S = 0.75 \]
Fig. 5.2
Fig. 5.3

$E^i_d = 0.6 \text{ Ry}$

$\frac{1}{2} W^i_d = 0.06 \text{ Ry}$

$S' = 1.0$

$\tilde{U}' = 0.1 \text{ Ry}$

$\bar{U}' = 0.05 \text{ Ry}$

$\delta \rho_d(E) \text{ (N STATES/ev)}$
\begin{align*}
E_d & = 0.6 \text{ Ry} \\
\frac{1}{2}W_d & = 0.06 \text{ Ry} \\
S' & = 1.0 \\
\bar{U}' & = 0.1 \text{ Ry}
\end{align*}

Fig. 5.4
Fig. 5.5

\[ E_d = 0.6 \text{ Ry} \]
\[ \bar{U} = 0.1 \text{ Ry} \]
\[ S = 1.0 \]

\[ \delta \rho_d(E) \text{ (N STATES/eV)} \]

\[ E \text{ (Ry)} \]

\[ \frac{1}{2} w_d = 0.04 \text{ Ry} \]
\[ \frac{1}{2} w_d = 0.05 \text{ Ry} \]
\[ \frac{1}{2} w_d = 0.06 \text{ Ry} \]
\( \frac{1}{2} W_d^i = 0.06 \text{ Ry} \)
\( U' = 0.1 \text{ Ry} \)
\( S' = 1.0 \)

\( E_d^i = 0.4 \text{ Ry} \)
\( E_d^i = 0.6 \text{ Ry} \)

\( E_d^i = 0.5 \text{ Ry} \)

Fig. 5.6
Fig. 5.7

$\rho_{d}^{p}(N \text{ STAES/ev})$

$E (\text{RY})$

$E_F$
Fig. 5.8

$\delta\rho_d (\text{N STATES/eV})$

$E \text{ (Ry)}$

$\text{CuCo}$

$E_F$
\[ \delta \rho_d (N \text{ STATES/eV}) \]

E (Ry)

\[ \text{AgNi} \]

\[ E_F \]

Fig. 5.9