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The coherent-potential approximation in the tight-binding linearized-muffin-tin-orbital formalism for a single-band model of a solid

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Abstract. We have developed a model of a random alloy based on a simplified single-(s-type)-band model of a solid introduced by Andersen to demonstrate the screening of orbitals in the LMTO formalism. To this model we have applied the coherent-potential approximation in the LMTOs put forward by Kudrnovsky *et al.* The electronic densities of states calculated showed interesting features similar to those found in realistic calculations, for all types of disorder considered, namely purely diagonal, both diagonal and off-diagonal, and purely off-diagonal.

1. Introduction

During the last decade or so the linearized band method for the muffin-tin orbital (MTO) description, namely the linearized-muffin-tin-orbital (LMTO) method, has become an efficient first-principles band-structure method (Andersen and Jepsen 1977, Skriver 1984, Andersen *et al* 1985, 1986, 1987, Skriver and Rosengaard 1991, Andersen 1992). A tight-binding (TB) scheme may be constructed in this formalism where we shall see later that the Hamiltonian is expressed in terms of, firstly, the potential function which describes the scattering properties of the atoms and which is a function of parameters specifying the band centre (resonance energy), band width and band shape and secondly, the structure factor matrix which is dependent on the geometry. The original infinite-range MTOs can be linearly transformed or in other words screened by MTOs from neighbouring sites, thus leading to short-ranged MTOs and a TB type of description.

A simple single-(s-type)-band model with a spherical Brillouin zone was introduced by Andersen (1992). We have developed a simple model of a substitutional binary random alloy based on this model by choosing random band positions and random band widths which are analogous to site energies and hopping in the Anderson TB model and applied to it the coherent-potential approximation (CPA) in the TB LMTO formalism developed by Kudrnovsky and co-workers (1985, 1990). Indeed the numerical results obtained for the density of states (DOS) show many features similar to that found by Kudrnovsky and co-workers (1985, 1990) for realistic systems. We have presented the calculations for both wide (i.e. free-electron-type) bands and narrow (i.e. d-type) bands in transition metals and the effects of randomness in both band positions and band widths show many distinct features in the alloy DOS. In addition we have also discussed the novel band shape disorder within the framework of our model.

2. Formalism

2.1. Hamiltonian and Green function in the TB LMTO formalism

In the following we discuss briefly the TB LMTO atomic sphere approximation (ASA) mainly to introduce notation and basic equations. A screened MTO set may be obtained by linearly combining the envelopes of the conventional MTOs into a short-ranged basis set. The energy-independent MTO in such a screened representation is given by

$$\chi_{RL}^\alpha(r_R) = \phi_{RL}(r_R) + \sum_{R'L'} \dot{\phi}_{RL}^\alpha(r_R) h_{R'L',RL}^\alpha + K_{RL}^{\alpha,i}(r_R) \quad (1)$$

in the $\kappa^2 = 0$ envelope set used by Andersen *et al* (1986). In (1),

$$\dot{\phi}_{RL}^\alpha(r_R) = \dot{\phi}_{RL}(r_R) + \phi_{RL}(r_R) o_{RL}^\alpha. \quad (2)$$

The symbol α here represents the elements of the diagonal matrix $[\alpha_{RL}]$ defining the MTO representation and its meaning will be clearer later. Here $\phi_{RL}(r_R) = \phi_{RL}(|r_R|)Y_L(r_R)$ where $r_R = r - R$, $r_R = r_R/|r_R|$ is the solution of the scalar relativistic Schrödinger equation for the spherically averaged one-electron solid state potential $V_R(r_R)$ determined within the density-functional theory and calculated at a suitable energy. $\dot{\phi}_{RL}(r_R)$ is the energy derivative at the same energy. o_{RL}^α is the overlap of ϕ_{RL} and $\dot{\phi}_{RL}^\alpha$; $o_{RL}^\alpha = \langle \phi_{RL} | \dot{\phi}_{RL}^\alpha \rangle$. The matrix $h_{R'L',RL}^\alpha$ is chosen in such a way that the wavefunction is continuous and differentiable at each sphere boundary. Its explicit form is

$$h_{R'L',RL}^\alpha = (c_{RL}^\alpha - E_{VRL})\delta_{R'R}\delta_{L'L'} + (\Delta_{R'L'}^\alpha)^{1/2} S_{R'L',RL}^\alpha (\Delta_{RL}^\alpha)^{1/2}. \quad (3)$$

The c^α , Δ^α , o^α are the so-called potential parameters which are expressible in terms of the potential function $P^\alpha(E)$ in the α -representation as previously mentioned (Andersen *et al* 1986). $S_{R'L',RL}^\alpha$ are the matrix elements of the structure constant matrix. The potential function in the screened representation α and the conventional potential functions $P_{RL}^0(E)$ are connected by

$$P_{RL}^\alpha(E) = P_{RL}^0(E)[1 - \alpha_{RL} P_{RL}^0(E)]^{-1}. \quad (4)$$

$P_{RL}^0(E)$ are directly proportional to the cotangents of the phase shifts related to the solid state potential potentials $V_R(r_R)$ in a sphere at R and can be parameterized over a broad range of energies in terms of the potential parameters, the band centre C_{RL} , the band width Δ_{RL} and the band distortion γ_{RL} of the pure RL bands:

$$P_{RL}^0(E) = \frac{E - C_{RL}}{\Delta_{RL} + \gamma_{RL}(E - C_{RL})}. \quad (5)$$

The potential parameters C , Δ and γ via P^α and P^0 characterize the scattering properties of atoms on the lattice sites. The simple relation between potential functions of the two screened representations is given by

$$P_{RL}^\alpha(E) = P_{RL}^\beta(E)[1 - (\alpha_{RL} - \beta_{RL})P_{RL}^\beta(E)]^{-1}. \quad (6)$$

As noted earlier, the geometry of the lattice enters through the structure constant matrix S^α which is in turn expressed via the canonical structure constant (Andersen *et al* 1985, 1986) S^0 as

$$S_{RL,R'L'}^\alpha = [S^0(1 - \alpha S^0)^{-1}]_{RL,R'L'}. \quad (7)$$

The elements $S_{RL,R'L'}^0$ depends only on R/w and R'/w , where R and R' are atomic positions and w is the average Wigner-Seitz (WS) radius. $S_{RL,R'L'}^0$ decay as $(w/d)^{l+l'+1}$ where $d = |R - R'|$, and is thus long ranged for low l -values. The screen structure matrix elements decay as $\exp(-\lambda_{ll'}^\alpha d/w)$ with $\lambda_{ll'}^\alpha$ dependent on the choice of the representation α .

Two screened representations are of particular importance.

(i) The orthogonal or γ -representation has $\alpha_{RL} = \gamma_l$, the band distortion parameter in which the MTO set is orthonormal (if one neglects some small terms (Andersen *et al* 1986)).

(ii) The most localized β -representation has screening parameters given by $\beta_s = 0.3485$, $\beta_p = 0.0530$ and $\beta_d = 0.0107$ yielding the fastest and almost monotonic decay in real space. \mathbf{S}^β almost vanishes beyond the second-nearest neighbour for close-packed lattices and consequently the X_{RL}^β are highly localized in space. If in (5) we set $\alpha \equiv \beta$ and $\beta \equiv \gamma$ representation-wise we obtain two very useful equations in this work:

$$P_{RL}^\beta(E) = \frac{E - C_{RL}}{\Delta_{RL} + (\gamma_{RL} - \beta_{RL})(E - C_{RL})} \quad (8)$$

$$\dot{P}_{RL}^\beta(E) = \frac{\Delta_{RL}}{[\Delta_{RL} + (\gamma_{RL} - \beta_{RL})(E - C_{RL})]^2} \quad (9)$$

Indeed this description is appropriate for a TB type of description. We shall now introduce the expressions for the Hamiltonian and one-electron Green function (GF) in this representation. In the ASA, the MT spheres are replaced by slightly overlapping space-filling WS spheres so that the interstitial region is left out. The Hamiltonian $H_{RL,R'L'}^\beta \equiv \langle \chi_{RL}^\beta | -\nabla^2 + V(r) | \chi_{R'L'}^\beta \rangle$ and overlap $O_{RL,R'L'}^\beta = \langle \chi_{RL}^\beta | \chi_{R'L'}^\beta \rangle$ in the ASA are obtained

$$O^\beta = (1 + h^\beta o^\beta)(o^\beta h^\beta + 1) \quad (10)$$

$$H^\beta = h^\beta(1 + o^\beta h^\beta) + (1 + h^\beta o^\beta)E_v(o^\beta h^\beta + 1) \quad (11)$$

with the contribution from the interstitial part being omitted. The quantity of prime interest for a model of random alloys is the one-electron GF as any quantity of interest may be determined from it.

To introduce the $G_{RL,R'L'}^\beta(z)$ where $z = E + i0^+$ (0^+ is a small positive quantity giving a small imaginary part to the argument), we first introduce the GF in the γ -representation:

$$G_{RL,R'L'}^\gamma(z) = (z\hat{1} - H^\gamma)_{RL,R'L'}^{-1} = \Delta_{RL}^{-1/2} [(P^\gamma(z) - S^\gamma)^{-1}]_{RL,R'L'} \Delta_{R'L'}^{-1/2}. \quad (12)$$

Here $\hat{1}$ is the unit operator, z is the energy in the complex plane and $P^\gamma(z) = (z - C)/\Delta$ is the potential function in the MTO representation γ . Using the simple relation between GFs of various MTO representations in the ASA, $G(z)$ in the β -representation is

$$G_{RL,R'L'}^\beta(z) = \lambda_{RL}^\beta(z) \delta_{RR'} \delta_{LL'} + \mu_{RL}^\beta g_{RL,R'L'}^\beta(z) \mu_{R'L'}^\beta \quad (13)$$

$$g_{RL,R'L'}^\beta(z) = ([P^\beta - S^\beta]^{-1})_{RL,R'L'} \quad (14)$$

$$\lambda_{RL}^\beta = (\gamma_{RL} - \alpha_{RL}) \mu_{RL}^\beta(z) / \Delta_{RL}^{1/2} \quad (15)$$

$$\mu_{RL}^\beta(z) = [P_{RL}^\beta(z)]^{1/2} = \Delta_{RL}^{1/2} / [\Delta_{RL} + (\gamma_{RL} - \alpha_{RL})(z - C_{RL})]. \quad (16)$$

2.2. Coherent potential approximation in the TB LMTO ASA

In the above the quantities $P_L^\beta(z)$, $\lambda_L^\beta(z)$, $\mu_L^\beta(z)$, etc, are site-diagonal quantities and in the case of a binary substitutional alloys they randomly assume the values characteristic of the two constituents with probabilities proportional to the concentrations of the respective constituents.

Kudrnovsky and co-workers (1985, 1990) performed the configuration averaging of the GF in the β -representation (equation (13)) within the CPA. The expression for the coherent potential function $P_L^\beta(z)$ is obtained from a pair of coupled CPA equations as

$$P_L^\beta(z) = \langle P_L^\beta(z) \rangle + [P_L^{\beta,A}(z) - P_L^\beta(z)]\phi_L^\beta(z)[P_L^{\beta,B}(z) - P_L^\beta(z)] \quad (17)$$

$$\phi_L^\beta(z) = \frac{1}{N} \sum ([P^\beta(z) - S^\beta(k)]^{-1})_{LL'}. \quad (18)$$

$S_{LL'}^\beta(k)$ is the Bloch transform of $S_{RL,R'L'}^\beta$. For the random alloy,

$$\phi_L^\beta(z) = \sum_Q c^Q \phi_L^{\beta,Q}(z) \quad (19)$$

where $Q \equiv A, B$ (say) are the constituents of the binary alloy, and the summation in (19) is a summation over the constituents with c^Q being the concentration of the constituent. Also

$$\phi_L^{\beta,Q}(z) = \phi_L^\beta(z)(1 + [P_L^{\beta,Q}(z) - P_L^\beta(z)]\phi_L^\beta(z))^{-1}. \quad (20)$$

The configuration-averaged GF is given by

$$\langle G \rangle_{RL,RL} = \sum_Q c^Q \dot{P}^{\beta,Q}(z)\phi_L^{\beta,Q}(z). \quad (21)$$

From (21) the alloy density of states is obtained by the standard formula $-(1/\pi) \text{Im}(\langle G \rangle)$; the component DOS for each alloy is thus obtainable as

$$-(1/\pi) \text{Im}[\dot{P}_L^{\beta,Q}(z)\phi_L^{\beta,Q}(z)] \quad \text{for } Q \equiv A \text{ or } B. \quad (22)$$

We note from (8) and (9) that $P_L(E)$ and $P_L^\beta(E)$ have poles at the energies $\epsilon_L = C_L - \Delta_L/(\gamma_L - \beta_L)$ and at these energies the expression for the DOS will be singular and constitute spurious δ -functions. One has to take care when making CPA calculations to have these poles outside the bands.

2.3. The spherical solid model and s-type screening

To illustrate the idea of screening of MTOS, Andersen introduced a simple single-(s-type-)band model of a solid with sites on a lattice with translations T and the same background phase shifts for all sites. The screening is done up to the s level, i.e. with monopoles only. By Bloch summation of bare structure constants we obtain in the k -space

$$S(\kappa^2, k) = - \sum_{T=0} \frac{\exp(ik \cdot T) 2kw \cos(\kappa T)}{\kappa T} \quad (23)$$

$$= - \frac{6}{wz} \sum_G (|k + G|^2 - \kappa^2)^{-1}. \quad (24)$$

A simplifying assumption is made by considering the Brillouin zone (BZ) to be spherically symmetric, whence it becomes a sphere of radius $b = (9\pi/2)^{1/3}w^{-1}$, where w is the WS radius of the solid. Further the $G = 0$ term in (24) is approximated by a k -independent constant in the BZ. The resulting model structure constant is approximately

$$S(\kappa^2, k) \simeq \frac{6}{w^2} \left[\frac{1}{\kappa^2 - k^2} + \frac{3}{b^2} g \left(\frac{\kappa^2}{b^2} \right) \right] \quad \text{for } k < b. \quad (25)$$

The k -independent function $3b^{-2}g(\kappa^2/b^2)$ can be determined in such a way that, as required, the integral of $S(\kappa^2, k)$ in the BZ vanishes. It is thus possible to define $g(\kappa^2/b^2)$ for complex κ^2 in such a manner that g is an analytical function in the circle $\kappa^2 < b^2$ with the circle $\kappa^2 = b^2$ being a branch cut, and g is another analytical function outside the branch cut. On the real axis, g is always decreasing from $-b^2$ to b^2 with $g(-1) = 1 + \frac{1}{4}\pi$, and $g(0)$ for $\kappa^2 = 0$ equals 1. It is negative from $\kappa^2 = 0.59b^2$ and tends logarithmically to $-\infty$ when $\kappa^2 \rightarrow b^2$. By choosing $\alpha(\kappa^2)$ so that $1/\alpha(\kappa^2)$ traces a little above $3g(\kappa^2/b^2)(1/b^2)$, i.e.

$$\alpha(\kappa^2) \equiv (6/w^2)[\delta(\kappa^2/b^2) + (3/b^2)g(\kappa^2/b^2)] \quad (26)$$

then the k zeros of

$$S(\kappa^2, k) - \alpha(\kappa^2)^{-1} = \frac{6}{w^2} \left[\frac{1}{\kappa^2 - k^2} - \delta \left(\frac{\kappa^2}{b^2} \right) \right] \quad (27)$$

move off to $k_0(\kappa^2) = \pm\kappa^2 - 1/[\delta(\kappa^2/b^2)]^{1/2}$. So for positive and sufficiently high δ , these zeros are imaginary so that the screened structure constant is localized in real space. If $\delta \equiv 1/(\kappa^2 + \lambda^2)$ with λ real, i.e.

$$\alpha(\kappa^2) \equiv \frac{6}{w^2} \left[\frac{1}{\kappa^2 + \lambda^2} + \left(\frac{3}{b} \right)^2 g \left(\frac{\kappa^2}{b^2} \right) \right] \quad (28)$$

then $k_0 = \pm i\lambda_0$ which is independent of κ^2 , and the screened structure matrix is

$$\mathbf{S}^\alpha(\kappa^2, k) = -\alpha(\kappa^2)^{-1} + \alpha(\kappa^2)^{-2} \frac{w^2}{6} (\kappa^2 + \lambda^2) \left(\frac{k^2 - \kappa^2}{k^2 + \lambda^2} \right) \quad (29)$$

having simple poles at $k_0 = \pm i\lambda$ and as a function $\alpha(\kappa^2)$ is analytical in $|\kappa^2| < b^2$. In real space it decays almost like $\exp(-\lambda|R - R'|)$. For $\lambda \rightarrow \infty$ the following simple expression for \mathbf{S}^α is obtained:

$$\alpha(\kappa^2) = g(\kappa^2/b^2)/0.325 \quad (30)$$

and

$$\frac{\mathbf{S}^\alpha(\kappa^2, k) + \alpha(\kappa^2)^{-1}}{(w^2/6)\alpha(\kappa^2)^{-2}} = k^2 - \kappa^2 \quad (31)$$

$$\mathbf{S}^\alpha(\kappa^2, k) + \alpha(\kappa^2)^{-1} = (k^2 - \kappa^2)(w^2/6)\alpha(\kappa^2)^{-2}. \quad (32)$$

A model of a substitutional binary alloy is constructed by us from this model by assuming random occupancy of the sites with the potential function having the form in (8) and the

screened structure constant having the form in (31). We have applied the formalism of Kudrnovsky and co-workers to the model. From (18) for spherical symmetry, we obtain, by converting the k -summation to a volume integral in k -space,

$$\begin{aligned} \phi^\beta(z) &= 4\pi \int_0^b \frac{k^2 dk}{P^\beta(E + i0) + \alpha(\kappa^2)^{-1} - (k^2 - \kappa^2)(w^2/6)\alpha(\kappa^2)^{-2}} = 4\pi \int_0^b \frac{k^2 dk}{A - Bk^2} \\ &= 4\pi \left[\frac{A/B}{(4AB)^{1/2}} \ln \left(\frac{(4AB)^{1/2} + 2Bb}{-2Bb + (4AB)^{1/2}} \right) - 4\pi \frac{b}{B} \right] \end{aligned} \quad (33)$$

where

$$A = [P^\alpha + \alpha^{-1} + \kappa^2 \alpha^{-2} (w^2/6)] \quad (34)$$

$$B = (w^2/6)\alpha(\kappa^2)^{-1}. \quad (35)$$

α and κ were suitably chosen for the calculation.

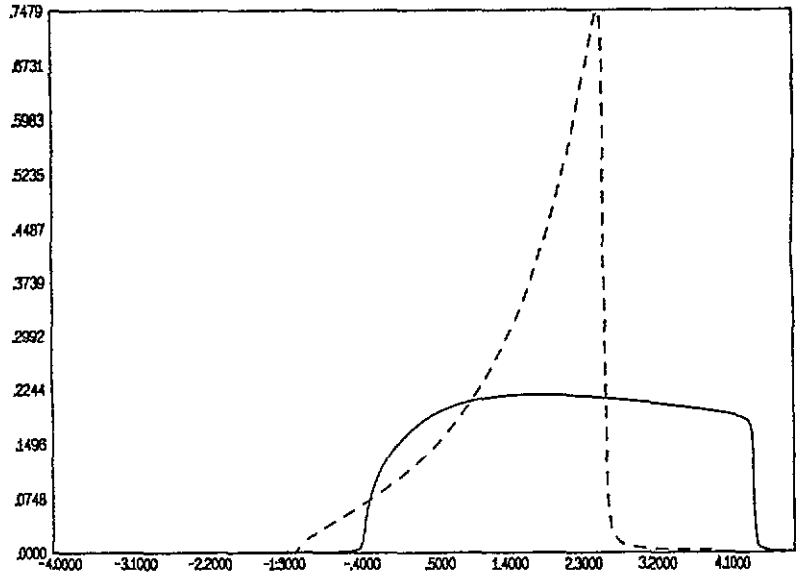


Figure 1. DOS: ---, $C = 1.05$, $\Delta = 0.5$, $\gamma = 0.24$; —, $C = 1.05$, $\Delta = 0.5$, $\gamma = 0.4$.

3. Results and discussion

As noted earlier, care was taken during calculations to have the poles in \hat{P}^α well outside the bands of all the constituents. The input parameters were C , Δ , γ and the concentrations of the binary substitutional alloys of type $A_x B_{1-x}$; the first three have a very marked influence on the shape of the DOS. We have presented three single-component calculations of the DOS to emphasize this point. Figure 1, broken curve, is a DOS calculated for $C = 1.05$, $\Delta = 0.5$ and $\gamma = 0.24$ which is found to rise to a sharp peak and resembles d-type states

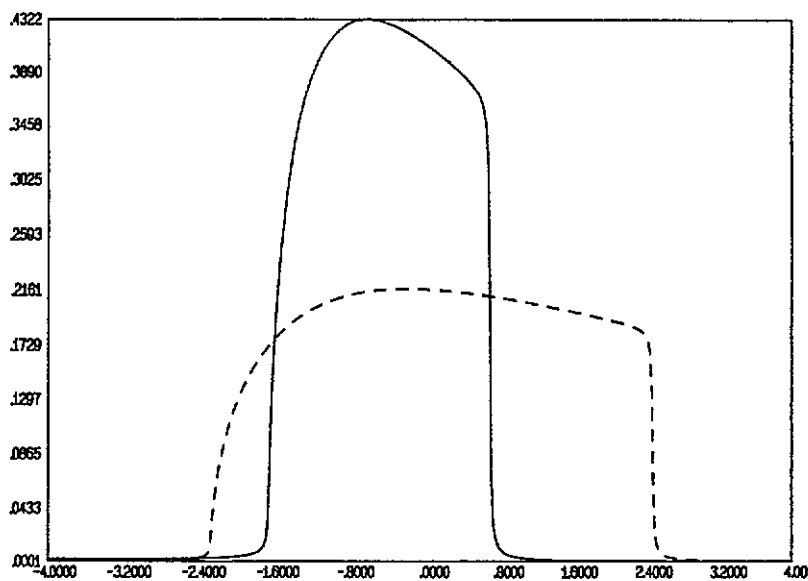


Figure 2. DOS: ---, $C_A = -1.0$, $\Delta_A = 0.25$, $\gamma_A = 0.4$; —, $C_B = -1.0$, $\Delta_B = 0.5$, $\gamma = 0.4$.

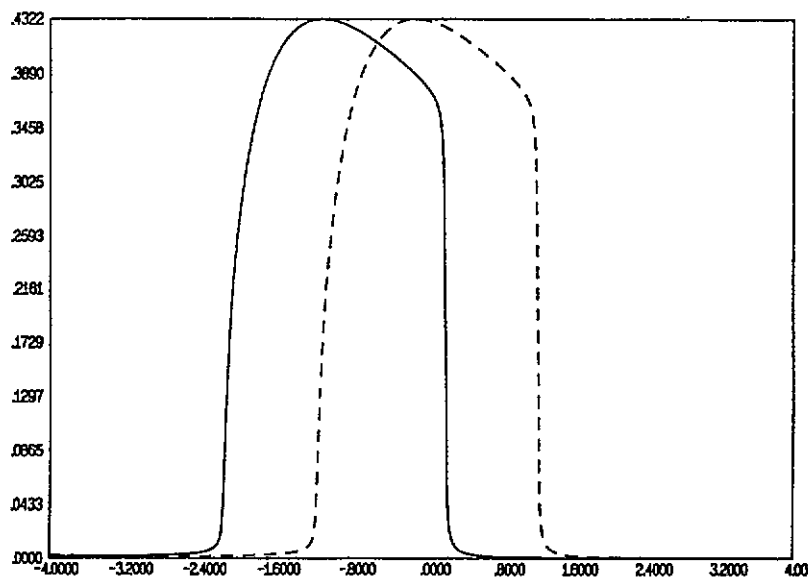


Figure 3. Shift of the band due to the change in C : ---, $C_A = -1.5$, $\Delta_A = 0.25$, $\gamma_A = 0.4$; —, $C_B = -0.5$, $\Delta_B = 0.25$, $\gamma_B = 0.4$.

in transition metals. The shape of this DOS is similar to the form obtained by Kirkpatrick *et al* (1970) in the so-called 'steep model' introduced by them to study the consequences of sharp structure and overall asymmetry in the d states of transition metals. The DOS shape also closely resembles that obtained by Butler (1976) on the basis of the KKR phase shift

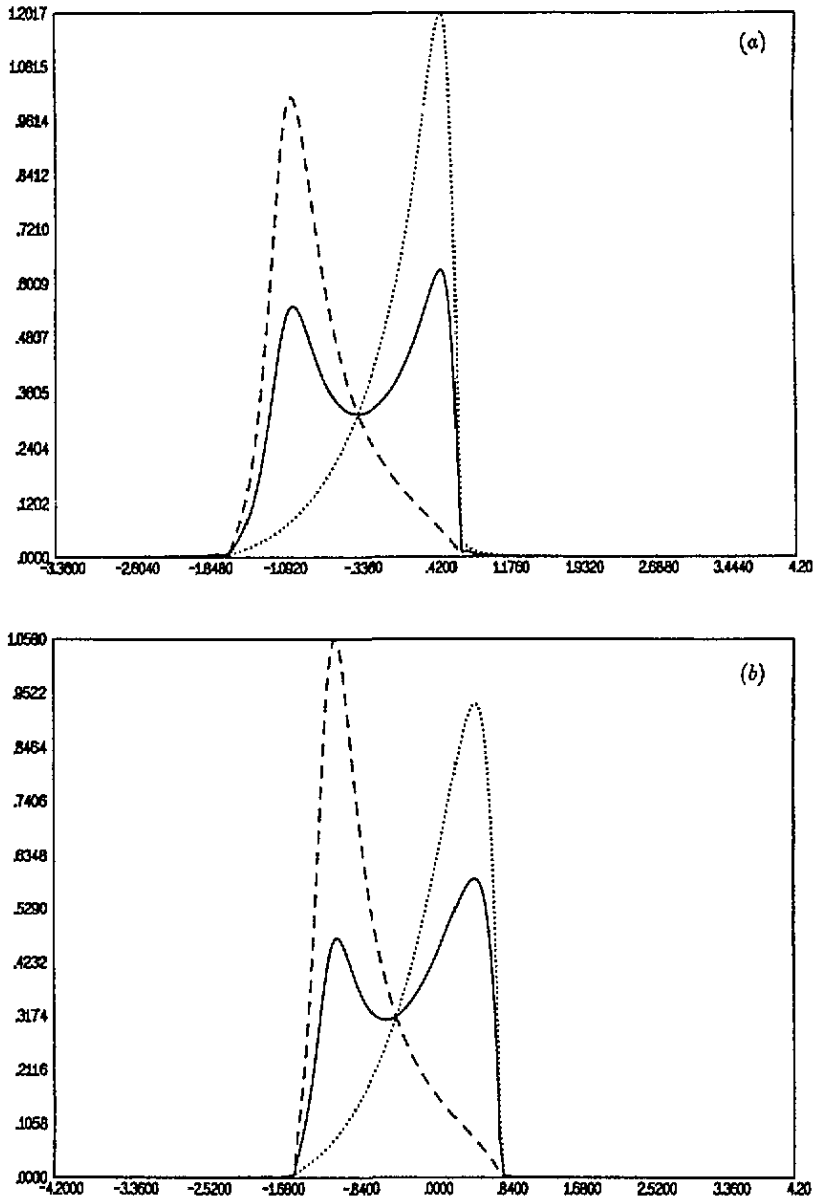


Figure 4. Purely diagonal disorder, the split-band case for (a) $x_A = 0.5 = x_B$, $C_A = -1.5$, $C_B = -0.5$, $\Delta = 0.25$ and $\gamma = 0.4$, (b) $x_A = 0.6$, $x_B = 0.4$, $C_A = -1.5$, $C_B = 0.5$, $\Delta = 0.25$ and $\gamma = 0.4$. (c) $x_A = 0.4$, $x_B = 0.6$, $C_A = -1.5$, $C_B = 0.5$, $\Delta = 0.25$ and $\gamma = 0.4$, and (d) $x_A = 0.7$, $x_B = 0.3$, $C_A = -1.5$, $C_B = -0.5$, $\Delta = 0.5$ and $\gamma = 0.4$: —, alloy DOS; ---, component A DOS; ·····, component B DOS.

analysis of d bands in transition metals. Figure 1, solid curve, is for a different γ -value (0.4) and is much wider than the broken curve.

By increasing Δ we can increase the width of a band significantly as demonstrated in figure 2, broken curve, which has $\Delta = 0.25$ and figure 2, solid curve, which has $\Delta = 0.5$: the latter looks like a free-electron s-type band. This DOS is similar to the semicircular

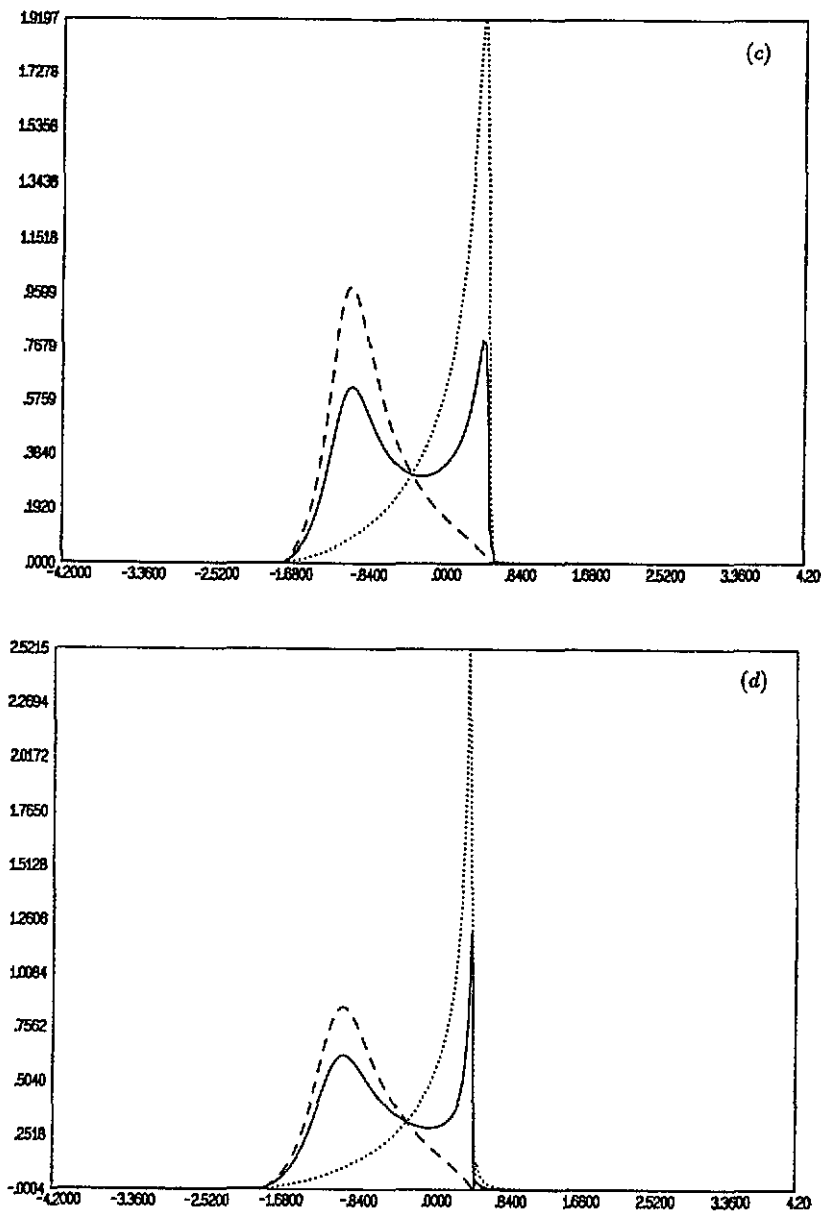


Figure 4. (Continued)

bands considered by Velicky (1969) to analyse the s-type bands in random metallic alloys.

Finally we see the effects of alterations in C , the band centre parameter, in figure 3 which show how a band becomes shifted from a different C .

For our random substitutional binary alloy model we have considered four types of disorder:

- (i) diagonal disorder only, i.e. random C ;
- (ii) off-diagonal disorder only, i.e. random Δ ;
- (iii) both diagonal and off-diagonal disorders, i.e. random C and Δ ;

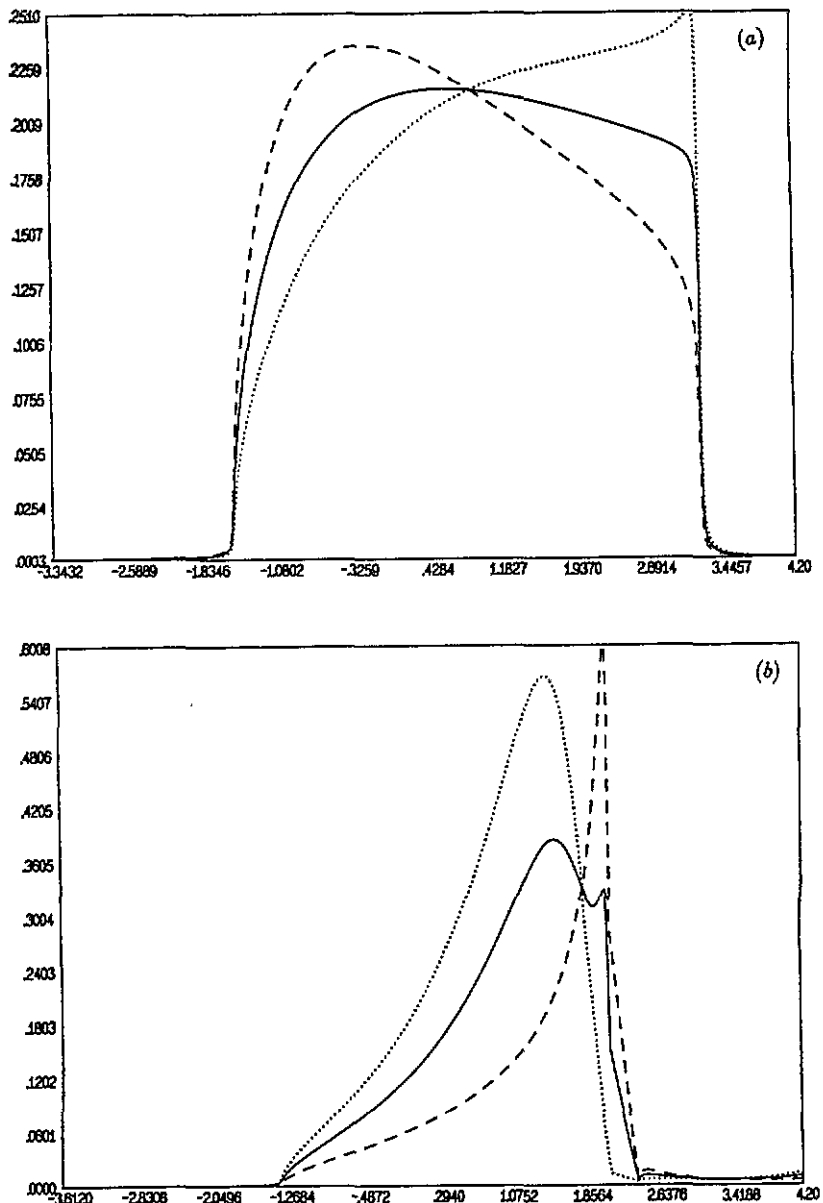


Figure 5. (a) Diagonal disorder with considerable overlap between the constituent Bands for $x_A = x_B = 0.5$, $C_A = -0.5$, $C_B = -0.05$, $\Delta_A = \Delta_B = 0.5$, $\gamma_A = \gamma_B \approx 0.4$; —, alloy DOS; ---, component A DOS; ·····, component B DOS. (b) Another case of purely diagonal disorder with good overlap for $x_A = x_B = 0.5$, $C_A = 1.25$, $C_B = 0.35$, $\Delta_A = \Delta_B = 0.5$, $\gamma_A = \gamma_B = 0.24$: —, alloy DOS; ---, component A DOS; ·····, component B DOS.

(iv) random band distortion parameter, i.e. random γ .

This is a novel feature obtainable in the TB LMTO ASA formalism. In actual calculations, we started for each energy value with the virtual-crystal approximation for P , i.e. $P_{VCA} = x_A P_A + x_B P_B$, and the coherent-potential function was obtained by successive iterations

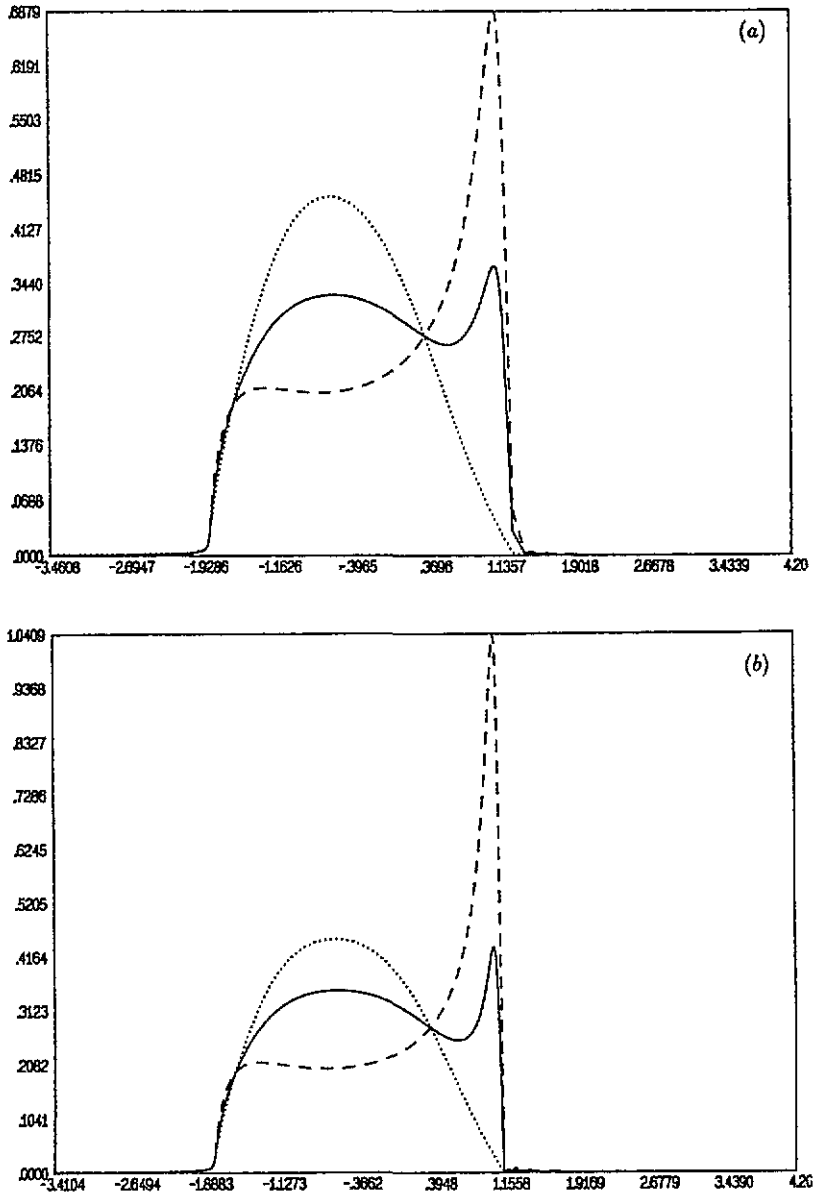


Figure 6. Purely off-diagonal disorder for (a) $x = 0.5$, $C_A = C_B = -1$, $\Delta_A = 0.5$, $\Delta_B = 0.25$, $\gamma_A = \gamma_B = 0.4$, (b) $x_A = 0.6$, $x_B = 0.4$, $C_A = C_B = -1$, $\Delta_A = 0.5$, $\Delta_B = 0.25$, $\gamma_A = \gamma_B = 0.1$, (c) $x_A = 0.3$, $x_B = 0.7$, $C_A = C_B = -1$, $\Delta_A = 0.5$, $\Delta_B = 0.25$, $\gamma_A = \gamma_B = 0.1$ and (d) $x_A = 0.7$, $x_B = 0.3$, $C_A = C_B = -1$, $\Delta_A = 0.5$, $\Delta_B = 0.25$, $\gamma_A = \gamma_B = 0.1$.

with equations (17), (18) and (33) and finally equations (21) and (22). A small positive imaginary part of about 0.01 was given and fast convergence was obtained. The convergence was found to be slower in the vicinity of poles in \hat{P} .

Case (i), i.e. for random C only, is presented in figures 4(a)–(c). The constituent bands are widely separated with small overlap and the resultant alloy DOS using the CPA

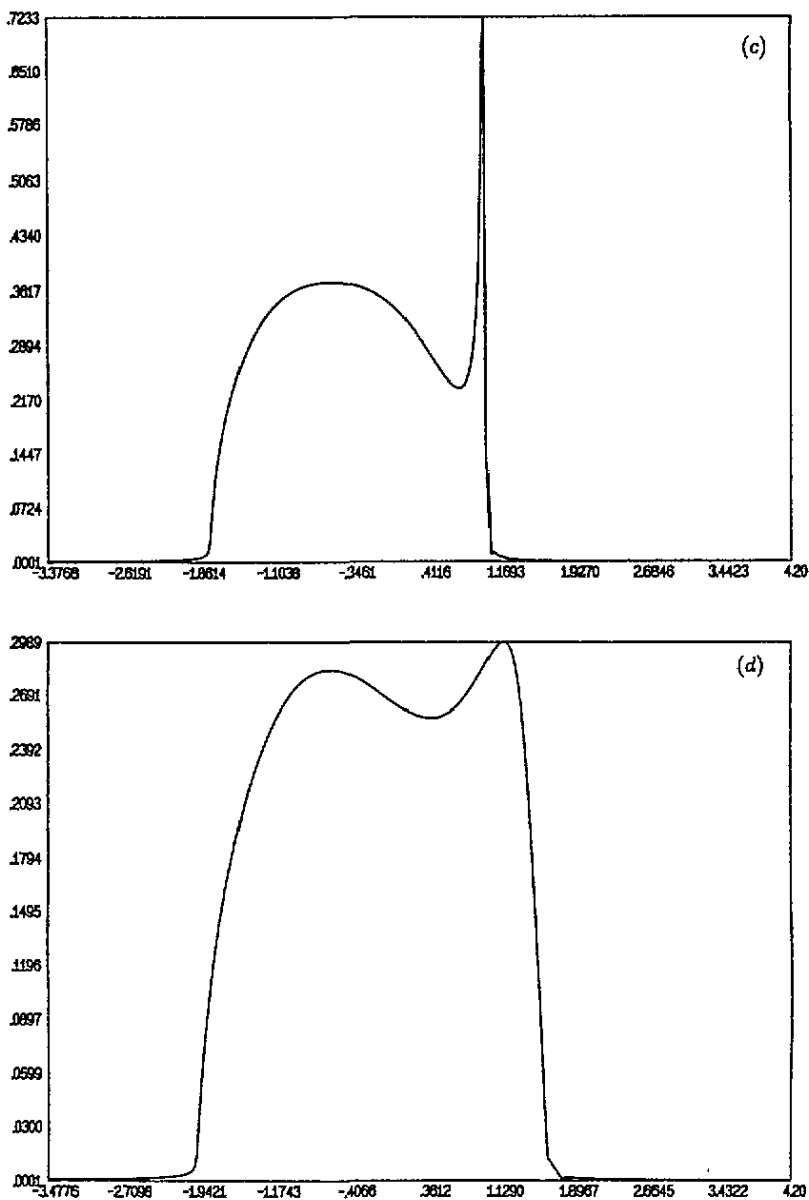


Figure 6. (Continued)

is of split-band type. Note that in figure 4(a) for $x_A = 0.5$ and $x_B = 0.5$ the alloy has almost symmetrically placed component DOSs, and the alloy DOS itself looks somewhat like a Lorentzian. However, the symmetry has largely disappeared in figure 4(b) for $x_A = 0.4$ and $x_B = 0.6$, or in figure 4(c) for $x_A = 0.6$ and $x_B = 0.4$. In figure 4(d) corresponding to $x_A = 0.7$ and $x_B = 0.3$ the alloy DOS drastically changes shape and adopts the shape of the A-type component DOS with the emergence of a large impurity peak owing to the low concentration of B.

This of course highlights the high sensitivity of the calculation to the changes in

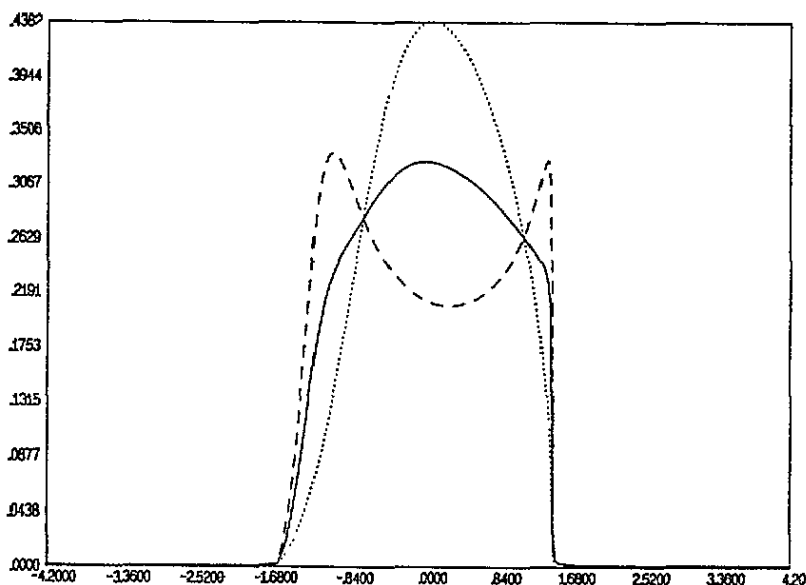


Figure 7. Both diagonal and off-diagonal disorder for $C_A = -1.5$, $C_B = -0.5$, $\Delta_A = 0.5$, $\Delta_B = 0.25$, $\gamma_A = \gamma_B = 0.4$, $x_A = x_B = 0.5$.

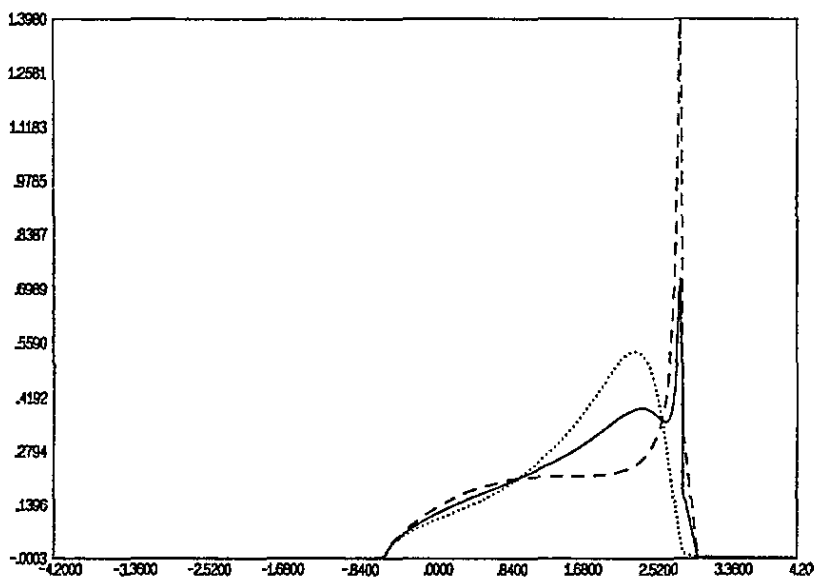


Figure 8. Disorder in γ for $C_A = C_B = 1.05$, $\gamma_A = 0.4$, $\gamma_B = 0.24$, $\Delta = 0.5$, $x_A = x_B = 0.5$.

concentration. In figure 5 the constituent bands have significant overlaps and as a result the alloy DOS exhibits much less splitting than in the previous case. For purely off-diagonal disorder in random Δ the results are even more interesting. In figure 2 we have shown the constituent DOSs of A and B. They have the same C , i.e. band centre, and thus strong overlap, but the width of one is twice that of the other. The alloy DOS in figure 6(a) has

$x_A = x_B = 0.5$ and it has a splitting in the vicinity of the crossing of the two component DOSs. Neither of the component DOSs resembles the DOSs for pure A and B. We also note that the effective band width is in between the band widths of the constituents. The same features are more or less repeated in the alloy DOS for $x_A = 0.4$ and $x_B = 0.6$ in figure 6(b). For $x_A = 0.3$ and $x_B = 0.7$, figure 6(c) shows a sharp impurity peak in the vicinity of the band edge of B but, for $x_A = 0.7$ and $x_B = 0.3$ in figure 6(d), the shape is entirely changed, again highlighting the sensitivity of the calculations to the change in concentrations. It should be pointed out that in figure 6(c) and 6(d) we have not drawn any component DOSs because they would not show any marked change from those shown in figures 6(a) and 6(b). The alloy DOS, however, show a significant change with variation in concentration from the two earlier cases.

Figure 7 presents case (iii), i.e. both diagonal and off-diagonal disorder, where we see that off-diagonal disorder prevents the band splitting due to random C , by giving a broadened DOS although the component DOSs are markedly different from the alloy DOS. In figure 8 we present an interesting DOS arising out of random γ . A drastic change in the shape of the alloy DOS from the component DOSs (figure 1) is obtained.

4. Conclusion

We thus see that the application of the TB LMTO CPA formalism by Kudrnovsky and co-workers to this simple model reproduces many features observed in realistic calculations. We have made an attempt to cluster generalize the single-site formalism of Kudrnovsky and co-workers with augmented space formalism (Datta *et al* 1993). Quite independently, Razez and Prasad (1993) have also developed a similar formalism. It will be of interest to apply this formalism to intuitive models such as this single-band model.

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