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Calculation of electronic states of a disordered binary alloy

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Abstract

We present an extension of the Beeby and Hayes method for the calculation of electronic states of a binary disordered alloy in the form A_xB_{1-x} on a square lattice. The calculation demonstrates the application of the disordered system approach to the substitutionally disordered square lattice. The densities of states of the binary alloy are calculated for different cases in the tight-binding limit.

1. Introduction

Electronic states of substitutional random alloys have become an active research topic over the past few decades, and they are still a challenging problem to study using alternative methods based on different approaches. The structure of these systems possessing the lack of translational symmetry is the main difficulty and obstacle for developing a general and quantitative method. Therefore, various methods, for example, coherent potential approximation (CPA) [1–11], recursion [12–14] and the augmented-space recursion method [15], have been proposed and used for investigating the electronic properties of these systems. Among these, the Beeby and Hayes method [16] is one which has been applied to both structural disordered solids and substitutional disordered alloys in the tight-binding approximation for many years. But the method has not fully been explored because it has been applied to a limited number of problems.

In this work, an application of the Beeby and Hayes method is performed on a two-dimensional artificial binary alloy model. The goal is to demonstrate the application of the disordered system approach to substitutionally disordered alloys. This argument will be described on a 50–50 AB binary alloy distributed with a certain order on a square lattice before it is applied to a real system, and for which some numerical examples for the density of states (DOS) are carried out. We should emphasize that this paper will look only at the case where the bandwidth is much greater than the spread of binding energies. Before the calculation, however, the resulting dynamic matrix associated with evaluating the DOS is reduced to a simple computational form, which was thought of as a future study in one of our previous papers [17]. Moreover, we consider a different case for the two-dimensional (2D) system by taking two kinds of the hopping integral, h_w (weak) and h_s (strong), corresponding to long and

short bonds, which is of interest for the application of the approach to 2D quasicrystals like a Fibonacci lattice [18].

The remainder of the paper is divided into four sections. In section 2 the formal relations of the method and the way that it is treated for a binary alloy are briefly presented. In section 3 the model system and the structural parameters are described, and the application of the method leading to the dynamic matrix is illustrated. In section 4 some numerical calculations are carried out. The paper ends with a short discussion in the last section.

2. The Beeby and Hayes method and binary alloy model

The technique used to evaluate the electronic states of disordered systems is based on multiple-scattering theory and the calculated function is the total scattering function, the T -matrix, discussed in previous studies in [16, 17, 19] and given by

$$\mathbf{T} = \sum_i \mathbf{t}_i + \sum_{j(\neq i)} \mathbf{t}_i \mathbf{G}_0^{ij} \mathbf{t}_j + \sum_{\substack{j(\neq i), \\ k(\neq j)}} \mathbf{t}_i \mathbf{G}_0^{ij} \mathbf{t}_j \mathbf{G}_0^{jk} \mathbf{t}_k + \dots + . \quad (1)$$

Here \mathbf{t}_i is the single-site matrix describing electron scattering from atom i and \mathbf{G}_0 is the free electron propagator between two atoms. The elements of each \mathbf{t} and \mathbf{G}_0 are matrices labelled by angular momentum indices and both are functions of momentum (\mathbf{k}) and of energy (E). Each factor G_0 in the expansion for s-wave scattering contributes a factor

$$G_0 = -2\pi K_0(\mu R) \exp(i\mathbf{k}\mathbf{R}_{ij}) \quad (2)$$

where $\mu = (-E)^{1/2}$ is real for $E < 0$, \mathbf{R} is the distance between two atoms and K_0 is a modified Bessel function associated with the hopping term. Once the T -matrix is defined in terms of the structural parameters of the system the DOS can be evaluated from the imaginary part, which at negative energy arises only where the scattering series diverges. Hence, the well-known physical quantity of interest related to the imaginary part is the spectral function, $\rho(\mathbf{k}, E)$, given by

$$\rho(\mathbf{k}, E) = -\frac{1}{\Omega} \frac{1}{(E - k^2)^2} \text{Im}\langle T(\mathbf{k}) \rangle \quad (3)$$

where, as seen, the main task is to determine the imaginary part of the T -function, which is

$$\begin{aligned} \text{Im}\langle T(\mathbf{k}) \rangle = & 2\pi \left\langle \left\{ \sum_i t_i(k, k) + \frac{1}{2\pi} \sum_{i \neq j} t_i(k, \sqrt{E}) G_{ij}(\sqrt{E}, k) t_j(\sqrt{E}, k) + \frac{1}{(2\pi)^2} \right. \right. \\ & \times \left. \left. \sum_{\substack{i \neq j \\ l(\neq j)}} t_i(k, \sqrt{E}) G_{ij}(\sqrt{E}, k) t_j(\sqrt{E}, \sqrt{E}) G_{il}(\sqrt{E}, k) t_l(\sqrt{E}, k) + \dots \right\} \right\rangle. \end{aligned} \quad (4)$$

Here the subscripts refer to the atom type and for simplicity the scattering is assumed to be only s-wave scattering so that t -matrices can be replaced by energy-dependent scalar functions. The initial approximations made to the potential are that it is in the muffin-tin form of non-overlapping spheres.

We can now use the properties of t -matrices derived in detail in [19], i.e. $t_i(k, \sqrt{E}) = \frac{s_i(k)}{s_i(\sqrt{E})} t_i(\sqrt{E}, \sqrt{E}) = t_i(\sqrt{E}, k)$ and $\text{Im} t_i(k, k) = \frac{s_i^2(k)}{s_i(\sqrt{E})} \text{Re} t_i(\sqrt{E}, \sqrt{E})$. The series in equation (4) can then be written

$$\begin{aligned} \text{Im}\langle T(\mathbf{k}) \rangle = & \left\langle 2\pi \left\{ \sum_i \frac{s_i^2(k)}{s_i(\sqrt{E})} \text{Re } t_i(\sqrt{E}, \sqrt{E}) + \text{Im} \sum_{ij} \frac{s_i(k)}{s_i(\sqrt{E})} t_{ij}(\sqrt{E}, \sqrt{E}) \right. \right. \\ & \left. \left. \times \left[1 - \frac{1}{2\pi} \mathbf{G}t(\sqrt{E}, \sqrt{E}) \right]^{-1} \frac{1}{2\pi} \mathbf{G}_{ij} t_j(\sqrt{E}, \sqrt{E}) \frac{s_i(k)}{s_i(\sqrt{E})} \right\} \right\rangle \end{aligned} \quad (5)$$

which can be reduced to the form

$$\text{Im}\langle T(\mathbf{k}) \rangle = 2\pi \left\langle \sum_i \frac{s_i(k)}{s_i(\sqrt{E})} \text{Im } T_i(\mathbf{k}) \right\rangle \quad (6)$$

where

$$T_i(\mathbf{k}) = t_i(\sqrt{E}, \sqrt{E}) \frac{s_i(k)}{s_i(\sqrt{E})} + t_i(\sqrt{E}, \sqrt{E}) \sum_{j(\neq i)} \frac{G_{ij}(\sqrt{E}, k)}{2\pi} T_j(\mathbf{k}). \quad (7)$$

Hence we shall seek a solution of the equation

$$\sum_j \left[t_i^{-1}(\sqrt{E}, \sqrt{E}) \delta_{ij} - \sum_{j(\neq i)} \frac{G_{ij}(\sqrt{E}, k)}{2\pi} P_{ij} \right] \cdot T_j = \frac{s_i(k)}{s_i(\sqrt{E})}. \quad (8)$$

Now if a binary alloy with concentrations c_A and c_B of A and B, respectively, is considered, the function $T_i(\mathbf{k})$ in equation (7) can be supposed to depend for each pattern only on the distribution in terms of the near-neighbourhood atoms. The sum in (6) is then $2\pi \sum_A \frac{s_i(k)}{s_i(\sqrt{E})} c_A \text{Im } T_A$. Here c_A is the total concentration of neighbourhood A and its central atom is of type i . Here the sum over neighbours is made of a sum over all bonds from a particular atom and over all possible patterns which can occur at the end of those bonds. The sum over all the pattern probabilities at the end of a particular bond must be unity, and the sum over bonds then gives simply the number of bonds. P_{AB} is the probability of neighbourhood B neighbouring A. Hence the number of AB pairs is given by $c_A P_{AB} = c_B P_{BA}$. From expression (8) it is better to solve for $\sqrt{c_A} T_A$ which satisfies

$$\sum_B \left[t_i^{-1} \delta_{AB} - \frac{G^{AB}}{2\pi} P_{AB} \sqrt{c_A/c_B} \right] \sqrt{c_B} T_B = \sqrt{c_A} \frac{s_i(k)}{s_i(\sqrt{E})} \quad (9)$$

in which $(\sqrt{c_A/c_B}) P_{AB} = (\sqrt{c_B/c_A}) P_{BA}$ is symmetrical and the atom at the centre of the pattern A is of type i . Moreover, in defining the T -function for the patterns each T_A will be taken to be a function of the axis directions and $\exp(i\mathbf{k} \cdot \mathbf{R})$ expansion in (2) gives an exponential factor such as $\exp[i\nu(\theta_R - \theta_k)]$, as will be illustrated on the model system below.

3. The model system and the application of method

In disordered systems it has been very common to study the effects of some physical parameters (e.g. a defect or disorder, SRO, etc) on a model system which may give very illustrative physical results for a theoretical technique before it is applied to a real material. It should however be emphasized that such model systems might correspond poorly at best to realistic materials which might have been studied intensively by various approaches for different purposes [15, 21–25]. Therefore, it is still of great interest for the simplicity of comparison and exact results for alternative theoretical studies.

In this sense we first consider a binary alloy described in tight-binding form, and atoms of two different kinds, say A and B, distributed over the sites of a 2D square perfect lattice with concentration c and $1 - c$, respectively. If each atom in the alloy has n neighbours with these occupation probabilities, then the various probabilities for the total distribution can be derived

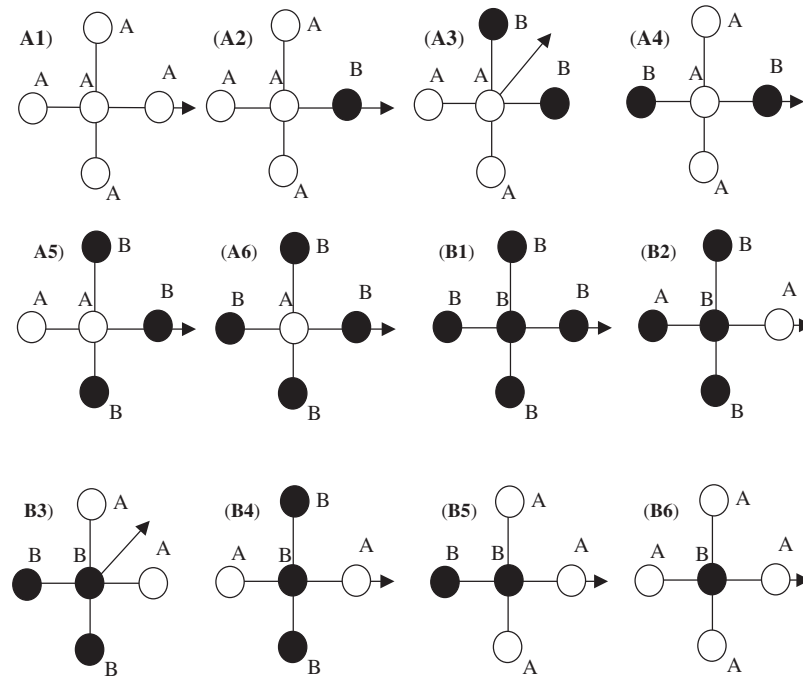


Figure 1. The diagram of possible distribution of A_cB_{1-c} binary alloy on square lattice.

from the expansion of $(c + (1 - c))^n$. Considering this distribution a 2D random system with concentrations of A and B of c and $(1 - c)$, respectively, may have 12 possible distribution patterns assigned as A1–A6 and B1–B6 as given in figure 1. The structural parameters associated with each pattern of the system, such as the total frequency of each pattern and the probability distribution of neighbourhoods, can be determined using the expansion procedure. The probabilities of the patterns in figure 1 are $P_{A1} = c^5$, $P_{A2} = 4c^4(1 - c)$, $P_{A3} = 4c^3(1 - c)^2$, $P_{A4} = 2c^3(1 - c)^2$, $P_{A5} = 4c^2(1 - c)^3$, $P_{A6} = c(1 - c)^4$, $P_{B1} = (1 - c)^5$, $P_{B1} = 4c(1 - c)^4$, $P_{B1} = 4c^2(1 - c)^3$, $P_{B1} = 2c^2(1 - c)^3$, $P_{B1} = 4c^3(1 - c)^2$ and $P_{B1} = c^4(1 - c)$, respectively. As can be seen, the sum equals unity. In addition, it is straightforward to calculate the available number of bonds, which is associated with the weighting along the bonds. Hence, consider movement along AA bonds, $N_{AA} = 4P_{A1} + 3P_{A2} + 2P_{A3} + 2P_{A4} + P_{A5} = 4c^2$ and similarly along BB bonds, $N_{BB} = 4(1 - c)^2$ and AB or BA bonds, $N_{AB} = N_{BA} = 4c(1 - c)$. We must note that there may be various possible distributions of such systems, but we have considered only the distribution illustrated in figure 1.

The next argument is to define the T -functions corresponding to the structural environment of each pattern and leading to the dynamic matrix. To do this, a coordinate axis is defined for each of the twelve individual patterns in figure 1 while every neighbouring pattern has a fixed orientation relative to the axis defined. The axis is shown by θ_b fitted on a symmetric bond as seen in the figure, and 12 different T -functions, each of which represents a pattern in the figure in terms of the structural parameters of the neighbouring atoms. To avoid confusion the T -function for each pattern will be denoted \mathbf{F} with a environment of the pattern label (for more detail see [17]). Then, if we write down \mathbf{F} only for the pattern A1 in an open form as a function of the rotation of its axis relative to the absolute axis, it can be defined as

$$F^{A1}(\theta_b) = \mathbf{1} + t_0[G(\theta_b)P_{AA}F^A(\theta_b) + G(\theta_b + \pi/2)P_{AA}F^A(\theta_b - \pi/2) + G(\theta_b - \pi)P_{AA}F^A(\theta_b - \pi) + G(\theta_b - 3\pi/2)P_{AA}F^A(\theta_b - 3\pi/2)]. \quad (10)$$

Here the propagator \mathbf{G} given in equation (2) is defined only in terms of angular functions in the last equation, while \sqrt{E} and \mathbf{k} in this function are suppressed for convenience, and $P_{\alpha\beta}$ is the probability of finding a neighbouring β of pattern α . The probability of each pattern can be calculated from the distribution of figure 1. If we consider the diagrams A and B joining along a particular bond, the propagator \mathbf{G} has the form $\sum_v K_0(\mu R)(-i)^v J_v(kR)e^{-iv\theta_R}\delta_{v,m-m'}$. Here θ_R is the direction of the vector between the two atoms. The \mathbf{F}^α for the other patterns can be written in the same way as equation (10). The general form for the scattering function describing each pattern environment can then be written as

$$\mathbf{F}^\alpha(\theta) = \mathbf{1} + \sum_\beta t_0 P_{\alpha\beta} \mathbf{G}^{\alpha\beta} \mathbf{F}^\beta(\theta \pm \gamma) \quad (11)$$

where α and β denote the patterns and γ the allowed orientations to the symmetric axis. If both sides of this equation are Fourier transformed to polar angles, this gives

$$\mathbf{F}_m^\alpha = \mathbf{1}\delta_{m,0} + \sum_\beta t_0 P_{\alpha\beta} K_0(\mu R) \sum_{m'} (-i)^m (-i)^{m-m'} J_v(kR) \Gamma^{\alpha\beta}(m, \theta) \mathbf{F}_{m'}^\beta. \quad (12)$$

Here \mathbf{F}^α and \mathbf{F}^β are vectors depending on the integers m and m' , $0, \pm 1, \pm 2, \dots$, and Γ is the structural function involving the terms related to the rotational angles. Thus the coefficient of \mathbf{F} satisfies a matrix equation which can be written in compact form as

$$\mathbf{F} = \mathbf{e} + t_0 \mathbf{M} \mathbf{F} \quad (13)$$

where \mathbf{M} is the structural matrix of the system, and is due to the 12 different patterns, \mathbf{F} is a block vector with blocks labelled by pattern type and elements of the blocks labelled by m . \mathbf{e} is a block vector consisting of the identity matrix if $m = 0$, and zero elsewhere. In the present case the matrix \mathbf{M} is a complex and non-symmetric block matrix, but it can be transformed to a real symmetric matrix as was done and discussed in detail in previous studies [17, 19, 20]. As a result, following the same way of symmetrization, equation (13) takes the form

$$t_0^{-1} \Lambda = t_0^{-1} \mathbf{e}' + \mathbf{M}' \Lambda \quad (14)$$

where \mathbf{e}' is $\sqrt{p_{\alpha i}} \cdot \mathbf{e}_{\alpha i}^m \delta_{m,0}$, $\Lambda_m^{\alpha i} = i^m \sqrt{p_{\alpha i}} \cdot \mathbf{F}_m^{\alpha i}$ and $p_{\alpha i}$ is the concentration of each pattern. The matrix \mathbf{M}' then becomes a symmetric block matrix. We note here that though the symmetric matrix makes the solution one degree easier we found that the convergence of the DOS takes a very long computer time. To avoid this cumbersome solution, we introduce an alternative simple solution by writing the matrix in an open form below. Due to the rotational symmetry the bond factors are unchanged as θ_i is rotated through 2π , which is equivalent to shifting the integers, m and m' , by $\gamma = 2\pi/(\text{interbond angle} = \pi/4)$. We may form block matrices of side γ times the number of patterns in which all the blocks on a particular diagonal are identical. If the elements of a blocked eigenvector are Λ_i with eigenvalue λ_i , shifting the eigenvector by a block also give an eigenvalue. This yields the equation

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \mathbf{M}_3^T & \mathbf{M}_2^T & \mathbf{M}_1 & \mathbf{M}_2 & \mathbf{M}_3 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \mathbf{M}_3^T & \mathbf{M}_2^T & \mathbf{M}_1 & \mathbf{M}_2 & \mathbf{M}_3 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \mathbf{M}_3^T & \mathbf{M}_2^T & \mathbf{M}_1 & \mathbf{M}_2 & \mathbf{M}_3 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \Lambda_{-1} \\ \Lambda_0 \\ \Lambda_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} = \lambda \begin{bmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \Lambda_{-1} \\ \Lambda_0 \\ \Lambda_1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{bmatrix} \quad (15)$$

where $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3 \dots$ are 48×48 block matrices given in explicit form as

$$\mathbf{M}_1 = \begin{bmatrix} J_0 \mathbf{m}_{00} & J_1 \mathbf{m}_{01} & J_2 \mathbf{m}_{02} & J_3 \mathbf{m}_{03} \\ J_1 \mathbf{m}_{01}^T & J_0 \mathbf{m}_{11} & J_1 \mathbf{m}_{01} & J_2 \mathbf{m}_{02} \\ J_2 \mathbf{m}_{02}^T & J_1 \mathbf{m}_{01}^T & J_0 \mathbf{m}_{22} & J_1 \mathbf{m}_{01} \\ J_3 \mathbf{m}_{03}^T & J_2 \mathbf{m}_{02}^T & J_1 \mathbf{m}_{01}^T & J_0 \mathbf{m}_{33} \end{bmatrix} \quad (16a)$$

$$\mathbf{M}_2 = \begin{bmatrix} J_4 \mathbf{m}_{00} & J_5 \mathbf{m}_{01} & J_6 \mathbf{m}_{02} & J_7 \mathbf{m}_{03} \\ J_5 \mathbf{m}_{01}^T & J_4 \mathbf{m}_{11} & J_5 \mathbf{m}_{01} & J_6 \mathbf{m}_{02} \\ J_6 \mathbf{m}_{02}^T & J_5 \mathbf{m}_{01}^T & J_4 \mathbf{m}_{22} & J_5 \mathbf{m}_{01} \\ J_7 \mathbf{m}_{03}^T & J_6 \mathbf{m}_{02}^T & J_5 \mathbf{m}_{01}^T & J_4 \mathbf{m}_{33} \end{bmatrix} \quad (16b)$$

and so on.

Note that each \mathbf{m} is a 12×12 block of the matrix \mathbf{M}_i . Here, since the system is four-fold each \mathbf{m}_{ij} repeats itself on each \mathbf{M}_i . As can be appreciated, it is very hard to truncate the matrix for solving the finite problem exactly. But in the infinite problem the situation is better. For a given eigenvalue λ , the eigenvectors Λ_i satisfy the same equation except that they differ by a phase factor. In this case, each row of the eigenvector equation can be written

$$\mathbf{M}_1 \Lambda_0 + (\mathbf{M}_2 e^{i\alpha} + \mathbf{M}_2^T e^{-i\alpha}) \Lambda_0 + (\mathbf{M}_3 e^{i2\alpha} + \mathbf{M}_3^T e^{-i2\alpha}) \Lambda_0 + (\mathbf{M}_N e^{i(N-1)\alpha} + \mathbf{M}_N^T e^{-i(N-1)\alpha}) \Lambda_0 = \lambda \Lambda_0 \quad (17)$$

which is a 48×48 Hermitian matrix equation. The normalization can be done as $\Lambda_0^*(\alpha = 2\pi j/N) \Lambda_0(\alpha = 2\pi j/N) = 1/N$, ($j = 0, 1, N - 1$). Thus equation (17) can be reduced to the form

$$[\mathbf{M}_1 + (\mathbf{M}_2 e^{i\alpha} + \mathbf{M}_2^T e^{-i\alpha}) + \dots] \Lambda_0 = \lambda \Lambda_0 \quad (18)$$

which has N sets of 48 eigenvectors and eigenvalues. The imaginary part is written as

$$\text{Im } \Lambda_0 = -\frac{\pi}{N} t_0^{-1} \sum_i \left| \sum_j \sqrt{p_{\alpha\beta}} \Lambda_{ij} \cdot \mathbf{e} \right|^2 \delta(t_0^{-1} - \lambda_i) \quad (19)$$

and the spectral function related to the DOS is

$$\rho(\mathbf{k}, E) = \frac{1}{\Omega_0} \frac{1}{[E - k^2]^2} \sum \left[\frac{s_0(k)}{s_0(i\mu)} \right]^2 \cdot \text{Im } \Lambda_0. \quad (20)$$

4. Results

In this section, as a first calculation we shall calculate the DOS for the system having the patterns as in figure 1 and distributed on a square lattice, on which the system is a 50–50 AB binary alloy and the structural parameters have already been calculated in section 3. For this system if we consider one energy scale and only s-states, we then expect that the system behaves like the well-known perfect square lattice in two dimensions. The second part of the calculation is focused on the case of variable overlap integrals. We shall consider the binary system as a 2D system having two different hopping integrals between site atoms on each pattern and neighbouring atoms, for which the DOS will be calculated for the 50–50 binary alloy. In one sense this is a kind of investigation of the structural effect for disordered alloys. Note here that the system need no longer be a square lattice for this calculation.

Let us then represent by h_{ij} the magnitude of the hopping integral between the central atom on the patterns and neighbouring atoms along the bond, which is given by $h_{ij} = WK_0(\mu R_i)$ [17], where R_i is the length of the bond and W is a parameter related to the

band width. Following [16], t_0^{-1} in equation (14) is energy dependent and given to within a constant approximately by $(E - E_b)/W$ in the tight-binding approximation, which can be combined with the appropriate factors in equation (2) to form what is effectively an overlap integral. Here E_b is the bound-state energy of a single muffin-tin potential. We must note that since the magnitude of the overlap integrals between neighbouring atoms is related to the hopping term h_{ij} , the second part of the calculation is focused on this term.

We note that the analytic form of the hopping term was approximated by the standard representation of the hopping integrals in the tight-binding calculations such that the values of the overlap integrals were first fixed and then substituted in the matrix equation in (18) as done exactly in [17]. Then the spectral density function in (20) was evaluated using the eigenvalues and eigenvectors of the matrix. The potential used in this calculation has been taken in the form $v(\mathbf{r}) = \lambda\delta(\mathbf{r} - \alpha)$, for which values of $s_0(k)$ and $s_0(i\mu)$ were derived in [20]. However, it should be emphasized that the results do not depend on the potential in the extreme tight-binding limit because the total number of states in the band equals one per atom. We shall take appropriate values for atomic parameters such as the strength of the potential, as was done in the previous calculations [17, 19]. For example, $r = 0.5$ (au) and the bond length between two atomic potential centres $R = 2.0$ (au), for which the ground state energy $E_0 = -30$ (au). Thus the density of states, $N(E)$, has been calculated from

$$N(E) = \frac{\Omega_0}{4\pi^2} \int_{\mathbf{k}} \rho(\mathbf{k}, E) d\mathbf{k}. \quad (21)$$

Let us now calculate the first case, i.e. the system in figure 1, for which the structural parameters have been given in section 3 and the concentrations of A and B atoms, c_A and c_B , are taken equal. In order to approximate the system to a perfect square lattice, we take $E_A = E_B = E_0$ ($\Delta E \ll h$) so that one single common band is expected. Using these conditions, evaluating the eigenvalues and the eigenvectors from equation (18), the DOS was calculated through equations (19)–(21) and the result is given in figure 2(a). As expected, the DOS is symmetric about the band centre $E_0 = 0.0$, and has a Van Hove singularity peak resembling approximately the DOS of the perfect square lattice, but the singularity is not as sharp and smooth as expected for the perfect case or as calculated by Chakrabarti and Mookerjee in [15]. This is due to the nature of the theoretical treatment based on the structural disordered systems. In the next calculation of the same system the concentrations of the composition in the system were taken as $c_A = 0.49$ and $c_B = 0.51$, and $c_A = 0.51$ and $c_B = 0.49$, respectively, but leaving the other parameters the same. The results are presented in figures 2(b) and (c). As can be seen, the symmetry is broken down, and on panel (b) the weight has slightly shifted to the top of the band due to c_B , while on panel (c) it has shifted to the bottom of the band due to c_A . From these results it can be emphasized that the singularity was not removed since the approach to substitutionally disordered alloys treated our system as a partially disordered alloy rather than a randomly disordered alloy, so that the variation of the DOS was due to the concentration values. However, at this point if it is possible to compare our treatment with the study done by Chakrabarti and Mookerjee using the augmented-space recursion method (ASR) [15], in which the singularities appearing for the ordered square lattice were removed as the disorder was defined in terms of two different concentrations values ($A = 49.5, B = 50.5$ and $A = 50.5, B = 49.5$) for a perfectly disordered lattice distributed randomly, but the two results were exactly the same for two concentration values. In contrast, we have shown in panels (b) and (c) that the symmetry disappeared as the concentrations were different. This demonstrates the sensitivity of the approach to the compositional effects of the system. Obviously, although both the binding energies and the hopping integrals are the same, the difference between (b) and (c) shows that the electron cares about the site label and concentrations, which demonstrates how accurate the method is.

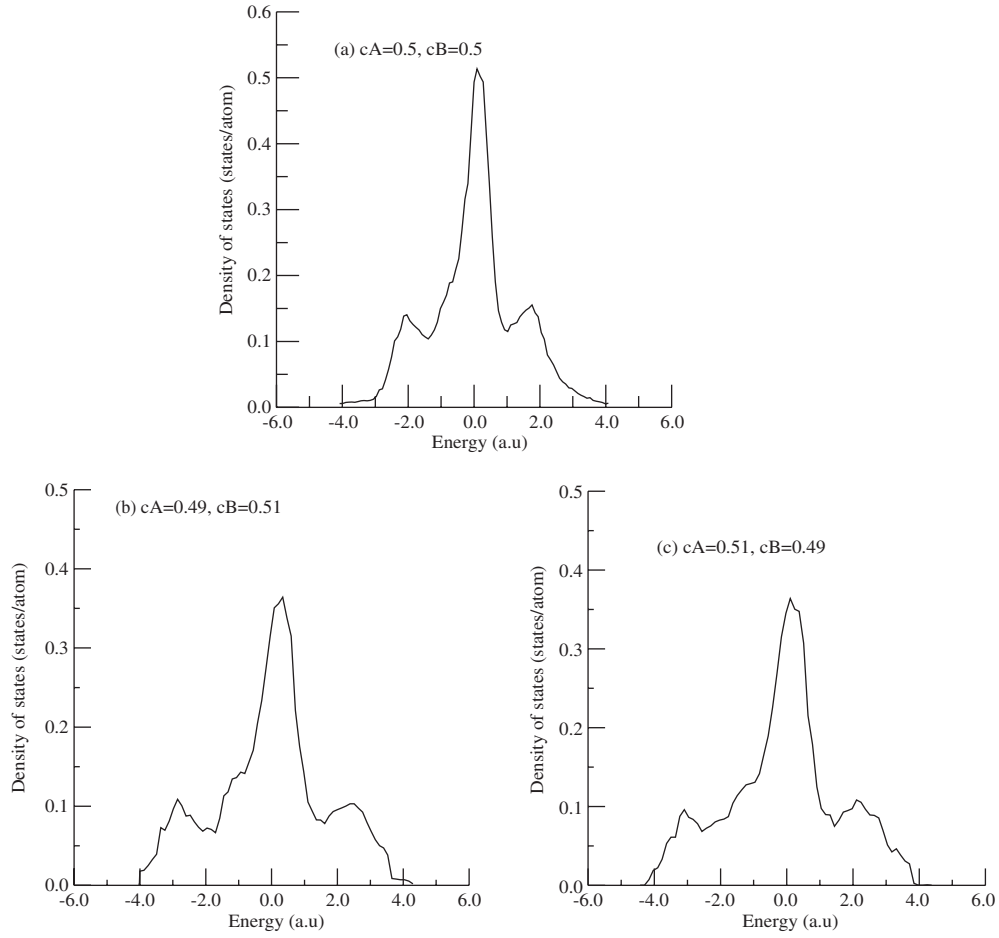


Figure 2. The density of states (states/atom) for a partially disordered binary alloy with concentration: (a) $c_A = c_B = 0.5$, (b) $c_A = 0.49$, $c_B = 0.51$, (c) $c_A = 0.51$, $c_B = 0.49$.

In the second part of the calculation, we assume that the system is no longer a perfect square lattice, but a two-dimensional lattice having two different bonds of the binary alloy. In other words we shall seek the DOS of the system for the case of variable integral overlaps. This case may resemble Fibonacci lattices in two dimensions [18]. Then we consider two kinds of hopping integral (or transfer matrix), h_w (weak) and h_s (strong), corresponding to long and short bonds. First, the long bonds are taken between atoms A, and short bonds between atoms B, and then we have assumed the inverse case, i.e. short bonds between atoms A and long bonds between atoms B. In the first case, the hopping integrals are chosen as $h_{BB} (=h_s) = \Delta E/0.326$, $h_{AA} (h_w) = \Delta E$ and $h_{AB} = \Delta E/0.564$, where ΔE is the unit of energy and it defines the overlap integral, fixing the energy scale. In the second case we have taken $h_{AA} (=h_s) = \Delta E$ and $h_{BB} (=h_w) = \Delta E/3.13$, and the hopping terms between atoms A and B, $h_{AB} = \Delta E/1.77$ which are averaged over h_s and h_w . The numerical results are presented in terms of this unit. Thus, using these values the calculations were carried out for the 50–50 binary system and the results have been presented in figures 3(a) and (b). As seen in figure 3(a), one single band appeared as expected and the Van Hove singularities at $E_0 = 0.0$ have also vanished. The

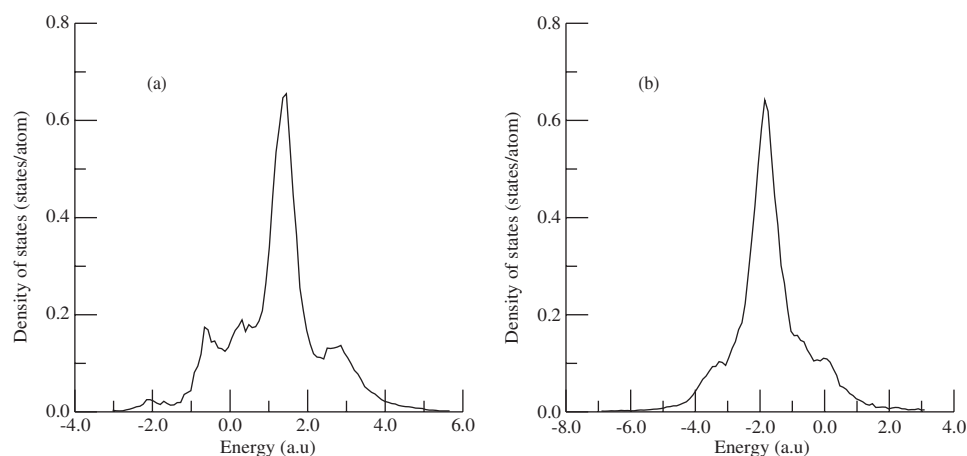


Figure 3. The density of states (states/atom) for a partially disordered binary alloy with $c_A = c_B = 0.5$, and different hopping terms: (a) $h_{AA} = \Delta E$, $h_{BB} = \Delta E/0.326$ and $h_{AB} = \Delta E/0.564$; (b) $h_{AA} = \Delta E$, $h_{BB} = \Delta E/3.13$ and $h_{AB} = \Delta E/1.77$.

structure shifted to the top of the band appearing at energy 2.0 (au) is due to the weight of short bonds (strong interaction) coming from atoms B. On the other hand, in the case of (b) the structure was shifted to the bottom of band with a single band at energy 2.0 (au) due to atoms A giving strong interactions. Hence, these calculations demonstrated that the approach can be used to calculate the DOS for systems having different hopping integrals and concentrations if the bandwidth is much greater than the spread of binding energies. In one sense such systems are also some kind of disordered system having different bond distances between atoms and consisting of sublattices like the Fibonacci lattice in two dimensions [19, 26].

5. Discussion

With this paper we have demonstrated the application of a structurally disordered system approach to substitutionally disordered alloys on a 2D 50–50 binary alloy. For these purposes, some numerical calculations were performed on a 2D binary alloy for different concentration values and the case $|Ea - Eb| \ll$ different hopping terms. The approach used in this calculation does not involve a single-site approximation or the solution of any self-consistent equation if we compare with the CPA. At this point, however, one comment might be regarding the results of Chakrabarti and Mookerjee in [15] if we make a comparison with the Beeby and Hayes method. The two figures presented for different concentration of compositions (A = 49.5 and B = 50.5, and A = 50.5 and B = 49.5) of complete disorder in [15] are symmetric and show exactly the same structure, whereas we might expect that the symmetric case could slightly be broken in completely disordered binary alloys depending on the composition ratio, but this may not be true for structurally disordered systems.

In conclusion, the results showed sufficient confidence to look at the case where the bandwidth is greater than the spread of binding energies for 2D binary disordered alloys. We hope in a future publication to be able to demonstrate the application of the method to variable binding energies. In addition, we have achieved a position of being able to apply this formalism to systems such as Fibonacci lattices in two dimensions, which will also be the subject of a future study.

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