

Electronic Spatial Structures of Eigenstates in Amorphous Alloys

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Abstract

A simple method is proposed for calculating the spatial extensions of wavefunctions in a tight-binding system. By means of the cluster Green functions, site-coefficients (amplitudes of the Wannier functions) of central sites in various type clusters within the system are derived, and the structures of the wavefunctions are discussed. As an example, the theoretical results for a ternary alloy are obtained and compared with the results from exact calculation of the 300-site model.

§ 1 Introduction

Recently, the problem of localization in random systems has been studied in various ways. As one of the ways the numerical study has been presented by J.T. Edwards and D.J. Thouless (1972)¹⁾, and extensively by S. Yoshino and M. Okazaki (1977)²⁾, by the use of eigenvectors of a secular matrix in two dimensional square lattices. The criterion of the localization by this numerical method is not simple due to miscellaneous natures of the eigenstates, so that it is needed to discuss the electronic spacial structures of all eigenstates.

In this paper, we derive the site-coefficients of locations and discuss the electronic structures in amorphous alloys by utilizing the results of our previous work (S. Obata and S. Shinohara 1980)³⁾. The constants, the symbols, the equations and calculations of the density of states are also used in the same way both theoretically and numerically as the our previous work. The tight-binding Hamiltonian is defined

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$$H = \sum_i |i\rangle e_i \langle i| + \sum_{l \neq m} \sum_l |l\rangle V_{lm} \langle m|, \quad (1)$$

where $|i\rangle$ are the Wannier functions at sites i . The eigenfunction (eigenvector) in the N -site system

$$|\varphi\rangle = \sum_i^N a_i(E_\varphi) |i\rangle \quad (2)$$

is obtained in the relation $H|\varphi\rangle = E_\varphi |\varphi\rangle$, where E_φ is an eigenvalue. $a_i(E_\varphi)$ are the site-coefficients at sites i , which show the electronic spatial structures of the eigenstates (figure 1), and these are

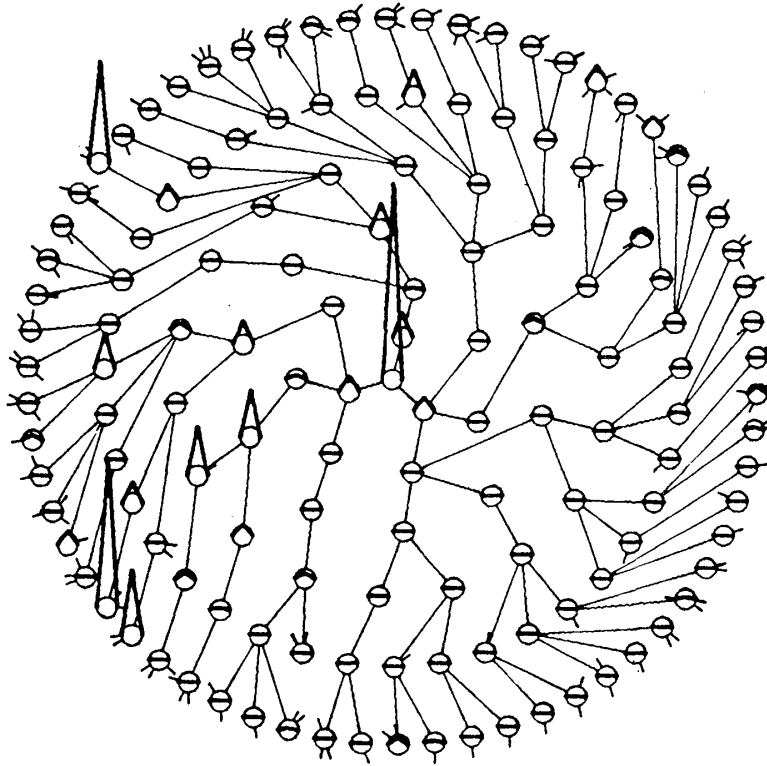


Figure 1. The numerical results of the electronic spatial structure of a eigenstate ($E_\varphi=3.0278$) with the quantity $\alpha=0.043$ in the ternary alloy. The height of the circular cones represent the probability $|a_i|^2$. The peak of the probability at the central site becomes $|a_0|^2=0.121$.

set to be normalized. As one measure of localization the quantity

$$\alpha = \sum_{i=1}^N |a_i(E_\varphi)|^4 \quad (3)$$

has been used. This parameter α indicates the inclination of the probability $|a_i(E_\varphi)|^2$ to concentrate upon several sites as shown in figure 1, and depends on the eigenvalue in the density of states as shown in figure 2.

§ 2 Formulation

The site-coefficients are able to be derived from the cluster Green functions formulated in the our previous work or earlier works^{4)~10)}.

The Green operator is defined as $G=(E-H)^{-1}$. The site diagonal Green functions expanded by the eigenfunctions

$$\sum_{\varphi} \langle i | \varphi \rangle \langle \varphi | G | \varphi \rangle \langle \varphi | i \rangle \text{ become}$$

$$G_{ii}(E) = \frac{1}{E - \sum_i} = \sum_{\varphi} \frac{|a_i(E_{\varphi})|^2}{E - E_{\varphi}} \quad (4)$$

If N is large and last equation of (4) is continuous, $G_{ii}(E)$ are integrated as

$$G_{ii}(E) = NP \int \rho(E_{\varphi}) \frac{|a_i(E_{\varphi})|^2}{E - E_{\varphi}} dE_{\varphi} + i\pi N\rho(E) |a_i(E)|^2, \quad (5)$$

where the first term of equation (7) is a principal value of the integral. The density of states $\rho(E)$ is obtained from the averaged Green function as

$$\text{Im } \bar{G}(E)/\pi = \sum_i^N \text{Im } G_{ii}(E)/N\pi = \rho(E) \sum_i^N |a_i(E)|^2 = \rho(E) \quad (6)$$

Where $\text{Im } G_{ii}(E)/\pi$ mean the local density of states^{11)~13)}. Recently B.Y. Tong et al¹⁴⁾ discussed the localization of the states by the local density of states which was treated within discrete energy spectrums. In this place our formulations are treated in the continuous energy spectrum, so that the calculation of the states are generally simplified. From equations (4) and (5), a relation

$$|a_i(E)|^2 = \frac{\text{Im } G_{ii}(E)}{\sum_l \text{Im } G_{ll}(E)} \quad (7)$$

is obtained.

Here we think clusters bonding up to L th nearest neighbors about every sites within the system and the cluster Green functions corresponding to these clusters. The number of L is several. Denoting p as types of atoms occupying sites i , x_p as the concentration and $F(p,u)$ as the probability of u th cluster pattern centered by a p atom, the averaged Green function is expanded by the cluster Green functions $G_{p,u}(E)$. Equation (6) is rewritten

$$\text{Im } \sum_p^n x_p \bar{G}_p(E)/\pi = \text{Im } \sum_p^n \sum_u x_p F(p,u) G_{p,u}(E)/\pi = \rho(E), \quad (8)$$

where

$$G_{p,u}(E) = \frac{1}{E - \bar{\Sigma}_{p,u}(E)} \approx \frac{\sum_{i \in \text{cluster}}^{N_{p,u}} G_{ii}(E)}{N_{p,u}} \quad (9)$$

For u th cluster type in the system, $N_{p,u}$ is the number of the clusters and $\bar{\Sigma}_{p,u}$ is the selfenergy of the clusters. Rewriting equation (6), the relationship between the cluster Green functions and the site-coefficients of the clusters become

$$\text{Im } G_{p,u}(E) / \pi = \rho(E) |a_{p,u}(E)|^2, \quad (10)$$

where $a_{p,u} = \sqrt{N} a_{p,u}$ indicate the site-coefficients compensated by the system size N .

Now, the quantity α is estimated from the site-coefficients of the central sites in the every clusters,

$$\begin{aligned} \hat{\alpha}(E) &= \sum_p \sum_u^n |a_{p,u}(E)|^4 x_p^F(p,u) \\ &= \sum_p \sum_u^n [\text{Im } G_{p,u}(E)]^2 x_p^F(p,u) / \pi^2 \rho^2(E). \end{aligned} \quad (11)$$

Obviously, the density of states $\rho(E)$ is calculated from equation (8).

§ 3 Example for a ternary alloy

Equation (11) should be applied to the precise cluster Green functions, but the Green functions of the clusters bonding up to second nearest neighbors are not clear enough to determine the quantity α . Here, especially on localized states, it is needed to modify the equation (11) to find better estimation of α . For the example of the ternary alloy in the our previous work, most of the states seem to be localized as in figure 2-(f), the coefficients of the sites (the central sites of the clusters distributed in a same pattern within the system) have not same magnitude of values but tend to localize to one site. If an amount of the site-coefficients concentrates upon several sites in eigenstates, the equation (11) is modified to

$$\alpha(E) = \sum_p \sum_u^n [\text{Im } G_{p,u}(E) x_p^F(p,u) / \pi \rho(E)]^2. \quad (12)$$

Equation (12) is applied to the second-order equations (2.18b) and (2.19) of the ternary alloy in the our previous work and the results are presented in figure 2-(e), which shows a good agreement with the numerical results from 300-site model as shown in figure 2-(f).

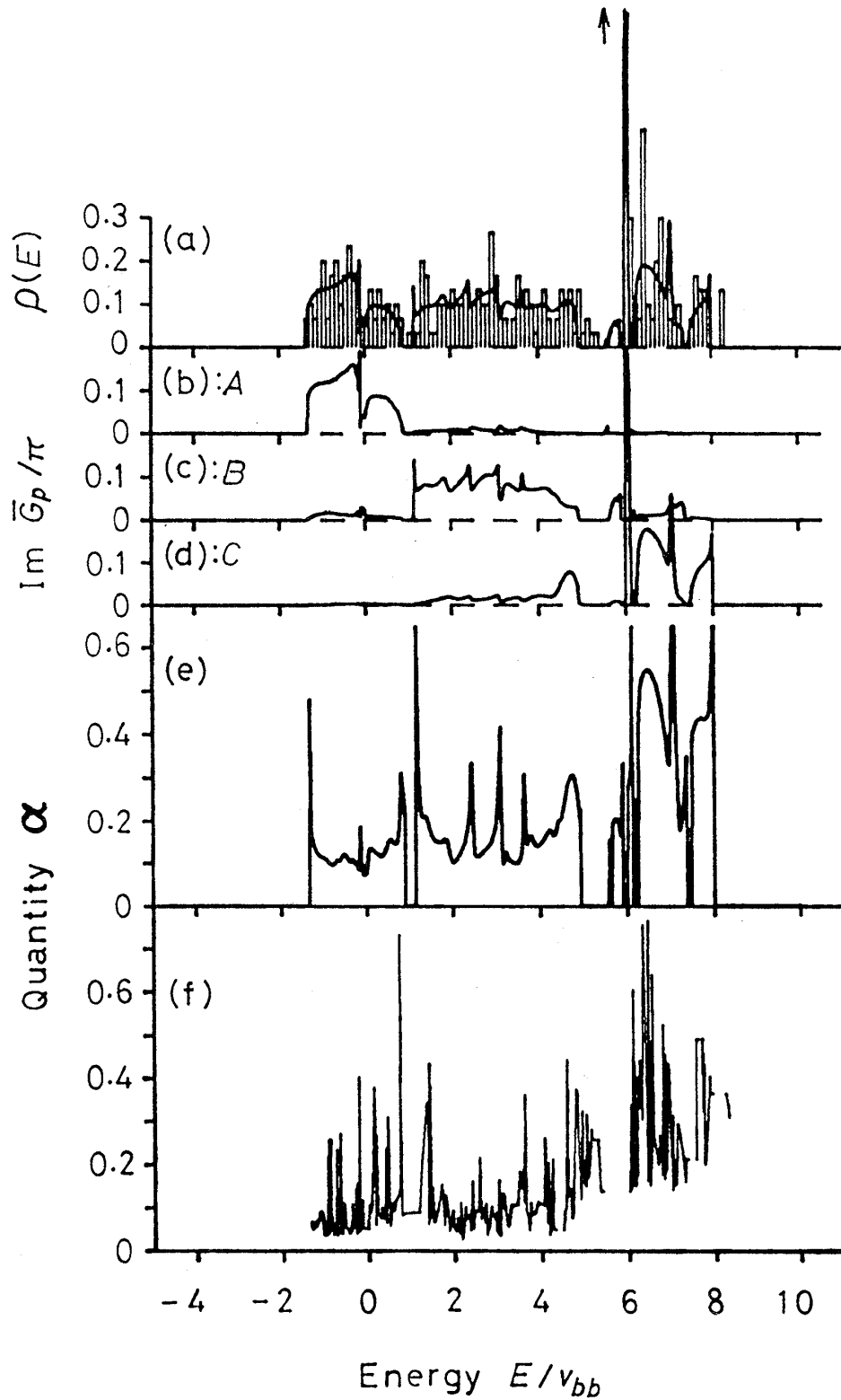


Figure 2. The density of states $\rho(E)$ and the quantity α . (a) the solid lines indicate the theoretical results and the histogram $\Delta E=0.1$ shows the numerical results, which have been calculated in our previous work. (b), (c) and (d) solid lines indicate $\text{Im } \bar{G}_p/\pi$ of A, B and C atoms respectively. The quantity α ; (e) are calculated from the equation (12) and (f) present the numerical results from the 300-site model.

In figure 1, the height of the circular cones represents the probability $|a_i|^2$. The cluster (about one half of the system) is constructed from the sites (small circles) bonding to 6th nearest neighbors around the peak site ($|a_0|^2 = 0.121$). The full lines linking the small circles represent the bonds corresponding to V_{lm} . In order to represent the Bethe lattice which is considered as a ideal system to calculate the density of states, several parts of the bonds are shown with short cutting lines on the small circles. These short lines facing each other represent the bonds making the loops, and these short lines going out of the cluster represent the bonds linking to the next nearest neighbors. The coordination number K_p are known by the number of these lines. In figure 2, the density of states $\rho(E)$ are shown in (a), which have been presented in the our previous work, the solid line is the result from the second-order equations and the histogram is the result from the numerical calculation. The peak at $E=6.01$ in the theoretical line is over 1.4. (b), (c) and (d) indicate the averaged local density of states $\text{Im}\bar{G}_a/\pi$, $\text{Im}\bar{G}_b/\pi$ and $\text{Im}\bar{G}_c/\pi$ respectively. Dividing these quantities by $\rho(E)$, we obtain the total site-coefficients about a, b, c atoms separately. The quantity α becomes the order of $N^{-1}=1/300$ in the extended states. The most parts of the eigenstates in (f) are seemed to be localized judging from the most of the quantity α of being over 0.043, which represents the value of the practical structure of figure 1 in weak localized states. As an comment, it is presented that the quantity α has a sharp peak at a center of the energy states in a feebl disordered system.

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