

Electronic densities of states of semi-infinite disordered chains: Comparisons of exact and analytic calculations

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Results of exact and analytic calculations of the electronic densities of states (DOS's) associated with semi-infinite substitutionally disordered chains are presented using the exact position-space renormalization-group (PSRG) method, the augmented-space (AS) formalism, and the embedded-cluster method (ECM). In addition to total DOS's, the PSRG method allows the calculation of exact partial DOS's associated with local atomic configurations in a disordered material. Comparisons with the exact results indicate that as in the case of infinite materials the ECM provides a reliable method for the calculation of single-particle properties, such as the DOS, of semi-infinite systems. Furthermore, the ECM is found to be much more accurate than the AS formalism, especially in the case of concentrated substitutionally disordered alloys.

I. INTRODUCTION

The theoretical understanding of the properties of cleaved, ordered or substitutionally disordered, materials is of great scientific and technological importance. Consequently, a large number¹⁻¹¹ of approaches have been developed (of which we cite only a small representative sample) for the study of surface properties within various and diverse physical models and formalisms for ordered¹⁻⁶ as well as disordered⁷⁻¹¹ materials. Most of these approaches are concerned primarily with obtaining analytic expressions for the single-particle surface Green function from which all single-particle properties, in particular the density of states (DOS), can be obtained. In this paper we examine the applicability to disordered surfaces of various techniques which have been used previously to calculate the DOS's of bulk substitutionally disordered systems.

The development of analytic theories in general, and in connection with the study of surfaces in particular, can be aided and guided by direct comparison with experimental results, e.g., photoemission studies, where such results are available. It is in this regard that computer simulations on simple, one-dimensional disordered materials have played a significant role in sorting out various formal methods on the basis of analytic behavior and the accuracy of calculated quantities such as the DOS. Corresponding comparisons for the case of semi-infinite solids have not been reported thus far, creating an uncertainty as to the reliability of various models for the study of surfaces of disordered materials. In this paper we present the first exact computer-simulated DOS's for semi-infinite substitutionally disordered linear chains, and compare them with the corresponding results obtained within two different analytic methods which have been used¹²⁻¹⁷ in the study of the bulk properties of substitutionally disordered alloys. We hope that our exact numerical results will provide a convenient testing arena for judging the validity and reliability of other formal methods for the study of surfaces.

A commonly used technique for obtaining the exact spectral distribution of disordered systems describable by a tight-binding (TB) Hamiltonian is that based on the negative-eigenvalue counting theorem as developed by Dean.¹⁸ This technique, although convenient for applications to many bulk systems, especially one-dimensional systems, is inapplicable to materials characterized by the presence of surfaces. On the other hand, a position-space renormalization-group (PSRG) approach (also called the decimation method), which has been used^{19,20} in connection with one-dimensional mass-disordered alloys, can be modified in a straightforward way and applied to the calculation of the exact DOS's of semi-infinite substitutionally disordered chains. For semi-infinite linear chains this technique yields accurate spectral distributions with only a moderate computational effort.

The analytically calculated DOS which we are comparing with the exact results were obtained within the generalization to the treatment of surfaces of two real-space methods originally developed for the study of bulk substitutionally disordered systems: One generalization is based on the augmented-space (AS) formalism,¹²⁻¹⁵ and the other on the embedded-cluster method^{16,17} (ECM). A brief review of some relevant computational aspects of both of these methods is given in the body of the paper.

The results presented in this paper correspond to a semi-infinite, single-band binary-alloy chain, $A_C B_{1-C}$, described by the usual TB model Hamiltonian,

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i \neq j} W_{ij} c_i^\dagger c_j . \quad (1.1)$$

Here, ϵ_i can take the values ϵ_A or ϵ_B with corresponding probability C and $1-C$, depending on whether site i is occupied by an atom of type A or B , respectively. The hopping terms W_{ij} are restricted to nearest neighbors and are taken as independent of the configuration (occupation) of sites i and j . Although the Hamiltonian of Eq. (1.1) is far from being physically realistic, it can serve as a proper testing case for differentiating between different methods for the treatment of disordered surfaces. We seek expres-

sions for the Green functions G_{00} and G_{jj} for the surface atom (0) and for the j th atom away from the surface, respectively, associated with the substitutionally disordered Hamiltonian of Eq. (1.1). The corresponding densities of states are obtained by means of the familiar expression

$$n_j(E) = -\frac{1}{\pi} \text{Im} G_{jj}(E). \quad (1.2)$$

The term "surface" in our work is to be understood in the conventional terms, namely, as the atoms on the planes to the left (or the right) of a cleavage plane cutting through an infinite material. We assume further that the potentials and concentrations of atoms on the surface are identical to those of the bulk. This is certainly an approximation, but it is sufficiently broad to serve our purposes and can be removed in more realistic calculations without excessive effort. We are interested in obtaining the DOS's as a function of the distance from the surface averaged over an "infinite" number of disordered chains.

The remainder of the paper is arranged as follows. In Sec. II we present a brief formal discussion of the exact (numerical) and the analytic methods used in our calculations. The results of these calculations are given in Sec. III. Section IV contains a general discussion and some conclusions which can be drawn from this work.

II. METHODS AND FORMALISMS

A. The position-space renormalization-group method

The position-space renormalization-group (PSRG) method for calculating the DOS's of a disordered (or ordered) system consists of an iterative procedure for obtaining the local Green function of a given Hamiltonian. It is a particularly simple approach for the study of TB systems with nearest-neighbor hopping in one dimension. In the first paper of this approach, Goncalves da Silva and Koiller¹⁹ (GK) used this method to calculate the spectral distribution of mass-disordered infinite chains by asserting that the rescaling process commutes with the configuration average. Different generalizations of the GK scheme have been developed to investigate the problems associated with disordered systems. In our approach, we carried the rescaling process to convergence for each individual configuration and then performed the configurational averages. The exact limit is in principle reached when the number of configurations goes to infinity. It turns out that the application of this method to infinite or semi-infinite chains is computationally very easy, allowing the use of a large number (10^6 – 10^7) of configurations. The method allows us to pursue the iterative process until a specific local Green function has become stable or, in the language of renormalization-group theory, a fixed point has been reached. The local density of states is then obtained as the imaginary part of the local Green function (in all our calculations the energy is assigned a positive infinitesimal imaginary part, $E \rightarrow E + i\eta$). Formally, this method can be applied to systems with extended hopping in any dimension, but the difficulty of its numerical implementation increases drastically with dimensionality.

The essence of the PSRG method can be understood along the following lines.

For a one-dimensional TB Hamiltonian, with only nearest-neighbor hopping, Eq. (1.1) takes the form

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_i (V_{i-1} c_i^\dagger c_{i-1} + V_{i+1} c_i^\dagger c_{i+1}), \quad (2.1)$$

where ϵ_i and V_i are the site energy and hopping integral, respectively. The equation for the Green-function operator,

$$(E - H)G = 1, \quad (2.2)$$

involving a given site, say the zeroth site, can be written in the form

$$(E - \epsilon_n)G_{n0} = \delta_{n0} + V_{n-1}G_{n-1,0} + V_{n+1}G_{n+1,0}, \quad n = -\infty, \dots, \infty. \quad (2.3)$$

An iterative procedure can be used to solve for G_{00} by renumbering the sites and eliminating the equations containing odd sites at each iteration step. After each step the resulting simultaneous equations have a structure similar to that of Eq. (2.3) but with renormalized values of ϵ_n and V_n . The new equations can be interpreted as corresponding to a one-dimensional system with a lattice constant which is an integral multiple of that of the original lattice. After each iteration, we arrive at an equation of the form of Eq. (2.3) the renormalized coefficients of which are given by the recursion relations,

$$\epsilon_n^{\text{ren}} = \epsilon_{2n} + \frac{V_{2n-1}^2}{E - \epsilon_{2n-1}} + \frac{V_{2n}^2}{E - \epsilon_{2n+1}} \quad (2.4)$$

and

$$V_n^{\text{ren}} = \frac{V_{2n} V_{2n+1}}{E - \epsilon_{2n+1}}, \quad (2.5)$$

where the site indices on the left-hand side refer to the new lattice. Upon repeating the decimation process, the values ϵ_n and V_n reach their limiting values, i.e., $\epsilon_n \rightarrow \epsilon_n^{\text{fixed}}$ and $V_n \rightarrow 0$. The above procedure is repeated for a large number of configurations, and an average is performed in order to obtain final results. This process is applicable to infinite one-dimensional materials, as well as to surfaces, and is ideally suited for probing local physical quantities.

The PSRG method is as efficient as the negative-eigenvalue theorem¹⁴ for the calculation of bulk properties. However, it is also applicable to cases not amenable to treatment by that theorem. For example, the PSRG method can be used to obtain partial DOS's associated with local configurations of atoms in bulk materials or on the surface of pure materials or alloys. The results of such calculations are presented in Sec. III.

B. The augmented-space formalism

The augmented-space (AS) Green function

$$\hat{G}(E) = (\hat{E}\hat{I} - \hat{H})^{-1} \quad (2.6)$$

is described in terms of a nonrandom Hamiltonian \hat{H} acting on the "augmented space" which is obtained as the direct product of the Hilbert space spanned by H , the given TB Hamiltonian of Eq. (1.1), with the "disorder space" comprising all possible configurations of the alloy.^{12,15} Through a substitution principles,¹⁵ each matrix element H_{ij} can be replaced by an operator \hat{H}_{ij} acting in the augmented space.

The matrix elements of the averaged Green function are now obtained by means of a scalar product in the augmented space,

$$\bar{G}_{ij}(E) = \langle \psi_i \otimes \gamma_0 | \hat{G}(E) | \psi_j \otimes \gamma_0 \rangle, \quad (2.7)$$

where the ψ_i are the states entering the definition $\langle \psi_i | H | \psi_j \rangle = H_{ij}$, and

$$\gamma_0 = v_0^1 \otimes v_0^2 \otimes \cdots \otimes v_0^N$$

is composed as the direct product of the two-dimensional basis vectors, $v_0^i = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$.

Calculations within the augmented-space method can be carried out by a variety of techniques appropriate for treating an ordered Hamiltonian. The most commonly used are the graphical procedure¹⁵ and the recursion method of Haydock *et al.*¹⁴ For our purposes, the graphical approach appears to be too cumbersome and not well suited to computer applications. We therefore applied the recursion method which basically consists in the transformation of an arbitrary tight-binding Hamiltonian H to a tridiagonal form. This is accomplished through the construction of an orthonormal basis set $|m\rangle$ such that

$$H|m\rangle = a_m|m\rangle + b_{m+1}|m+1\rangle + b_m|m-1\rangle, \quad (2.8)$$

where

$$a_m = \langle m | H | m \rangle, \quad (2.9a)$$

$$b_{m+1}^2 = \langle m | H^2 | m \rangle - a_m^2 - b_m^2, \quad \text{for } m > 0, \quad (2.9b)$$

and

$$a_0 = \langle 0 | H | 0 \rangle,$$

$$b_0^2 = \text{normalization of DOS}, \quad (2.9c)$$

$$b_1^2 = \langle 0 | H^2 | 0 \rangle - a_0^2, \quad \text{for } m = 0.$$

The coefficients a_m and b_m are the diagonal and off-diagonal elements of the tridiagonal matrix which appear in the continued fraction expansion of the density of states,

$$\begin{aligned} n(E) &= -\frac{1}{\pi} \text{Im} \bar{G}_{00}(E) \\ &= -\frac{1}{\pi} \text{Im} \frac{b_0^2}{E - a_0 - \frac{b_1^2}{E - a_1 - \frac{b_2^2}{E - a_2 - \cdots}}} \end{aligned} \quad (2.10)$$

Although we used Eq. (2.10) in our calculations, we did not directly apply the method of Haydock *et al.* for the calculation of the coefficients a_m and b_m , because of the large storage space this would require even for our very

simple linear chain example. Due to the peculiar construction of the augmented-space Hamiltonian, the vectors $|m\rangle$ have $(m+1) \times 2^{m+1}$ components, and for reasonably accurate results the maximum value of m should be of order 10. Instead, we calculated the moments of the DOS,

$$\mu_n = \langle \psi_0 \otimes \gamma_0 | \hat{H}^n | \psi_0 \otimes \gamma_0 \rangle, \quad (2.11)$$

by considering all closed paths of order n , $\hat{H}_{0i_1} \hat{H}_{i_1 i_2} \cdots \hat{H}_{i_n 0}$.

Now, the coefficients a_m, b_m can be calculated²¹ by means of well-known expressions involving appropriately defined determinants of the moments μ_n . In order to avoid the numerical problems of this procedure as much as possible, we calculated the coefficients in a different way by a linear expansion of the states $|m\rangle$ in terms of powers of H acting on $|0\rangle$.

In order to yield continuous densities of states the continued-fraction expansion, Eq. (2.10) has to be terminated in some appropriate manner. This was done by application of the self-consistent procedure of Beer and Pettifor²² which only needs the calculated pairs $[a_m, b_m]$ to estimate the asymptotic values a_∞, b_∞ . It should be noted that the simple square-root terminator of Ref. 21 is appropriate for our case because the augmented-space DOS's have no gaps.

C. The embedded-cluster method

In the ECM (Refs. 16, 17, 23) one calculates exactly the Green function for a cluster of atoms embedded in an effective medium which is determined in some optimal way. In substitutionally disordered alloys numerical investigations have indicated that the best embedding medium, in the majority of cases and especially for random alloys, is that determined within the coherent-potential approximation²⁴⁻²⁷ (CPA). Then the single-band TB Green function for a cluster C of atoms embedded in the medium is written in the form

$$G_{CC} = (z - H_C - \Delta_C)^{-1}, \quad (2.12)$$

where all quantities are $n \times n$ matrices for n -site clusters. Here, H_C is the intracluster part of the disordered Hamiltonian, and z is proportional to the $n \times n$ unit matrix. The cluster-renormalized interactor Δ_C describes the interaction of the cluster with the surrounding medium and in the absence of off-diagonal disorder is independent of the particular atomic configuration represented by H_C . Thus, Δ_C can be found easily by noting that \bar{G}_{CC} , the cluster-diagonal Green function for the effective medium can be evaluated in two different forms,

$$[\bar{G}_{CC}]_{ij} = [(z - \bar{H}_C - \Delta_C)^{-1}]_{ij} \quad (2.13)$$

and also

$$[\bar{G}_{CC}]_{ij} = \bar{G}_{ij} = \frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} \bar{G}(\mathbf{k}) e^{i\mathbf{K} \cdot \mathbf{R}_{ij}} d^3k, \quad (2.14)$$

where \bar{H}_C is the intracluster Hamiltonian for the effective medium, $\bar{G}(\mathbf{k})$ is the effective-medium Green function in the \mathbf{k} representation, \mathbf{R}_{ij} is the vector from site i to site j

and Ω_{BZ} is the volume of the Brillouin zone (BZ) of the reciprocal lattice. From Eqs. (2.17) and (2.18) we obtain

$$\Delta_C = z - \bar{H}_C - (\bar{G}_{CC})^{-1} \quad (2.15)$$

so that

$$G_{CC} = [\bar{H}_C - H_C + (\bar{G}_{CC})^{-1}]^{-1}. \quad (2.16)$$

The ECM can be used to calculate surface-cluster Green functions within a TB formalism in a straightforward way. For the case of one-dimensional systems one chooses a cluster large enough such that the surface atom has no direct interaction with the effective medium. Then for an $(n+1)$ -site cluster the renormalized interactor Δ_C for the surface cluster is equal to the corresponding quantity for a $(2n+1)$ -site cluster embedded in the bulk material. This is due to the fact that the "left" and "right" sides of the cluster interact only with that part of the medium with which they are in immediate contact. Similar considerations apply to higher-dimensional systems but with a certain increase in formal and computational labor, as will be discussed in a forthcoming publication. In any case, once G_{CC} has been determined, the corresponding local DOS's associated with any site in the cluster and for any cluster configuration is obtained in the usual way,

$$n_i(E) = -\frac{1}{\pi} \text{Im}[G_{CC}(E)]_{ii}. \quad (2.17)$$

Averaged results can be obtained by performing an ensemble average over all cluster configurations.

III. NUMERICAL RESULTS

It should be noted that E , the energy, in all the figures is given in arbitrary units. The DOS, $n(E)$, is always normalized to 1. Figure 1 shows the local DOS corresponding to sites at and below the surface and also for the bulk for a *pure* linear chain with parameters $\epsilon_i=0$, $W=1$. The transition from the surface DOS (leftmost panel) to the bulk DOS (rightmost panel) is indicated by the DOS at

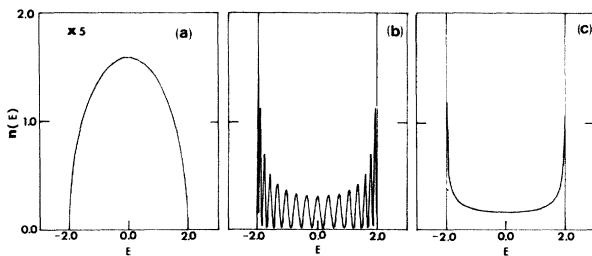


FIG. 1. Local DOS of a pure chain ($\epsilon=0$, $W=1.0$), (a) at the surface, (b) at the 16th site below the surface, and (c) for the bulk. All the energies are in arbitrary units.

the 16th site below the surface, $n_{16}(E)$ (middle panel). The origin of the "oscillation" in $n_{16}(E)$ can be understood upon examining the continued-fraction (CF) expansion of the Green function, Eq. (2.10).

Note that for the pure semi-infinite chain with nearest-neighbor hopping the CF method is exact and so is the ECM. In this case all three methods are computationally very similar and give identical results. Figure 2 depicts results analogous to those of Fig. 1, but for an *ordered binary* semi-infinite chain. Here, atoms of types A and B ($\epsilon_A=2.0$ and $\epsilon_B=-2.0$) alternate along the chain, thus producing a superstructure of diatomic unit cells. Again the middle panel, corresponding to the 4th atom below the surface, indicates the transition from the surface to the bulk DOS's.

The remaining figures depict DOS's for *binary randomly disordered* semi-infinite chains $A_C B_{1-C}$. Figures 3(a)–3(c) show the DOS of the surface site obtained by the AS method for 5, 8, and 10 pairs of coefficients a_m, b_m [cf. Eq. (2.10)], respectively, compared with an exact histogram of the DOS calculated in the PSRG approach for a 50 at. % alloy. The PSRG method converges quite rapidly and allows the inclusion of a large number ($\sim 10^7$) configurations in the evaluation of the ensemble average of the Green function. As is seen in these figures the AS approach yields a very smooth and rather poor representation of the richly structured surface DOS, as is also found in applications of this method to bulk systems. The structure of the surface DOS is produced primarily by local fluctuations in the environment of a site which cannot be taken properly into account by the AS method because of the averaged nature of the Hamiltonian \hat{H} . These results should be contrasted with those obtained in the ECM using 1, 5, and 13 sites, and continuing the chain with an effective potential obtained in the coherent-potential approximation for the infinite system [Figs. 4(a), 4(b), and 4(c)]. As is seen in Fig. 4 the DOS's corresponding to a 13-site cluster are practically indistinguishable from their exact PSRG counterparts in that they resolve all peaks and correctly reproduce all gaps and the weights of the various peaks. The results shown in Figs. 3 and 4 should also be compared with those of recent calculations²⁸ which apply a simplified traveling-cluster approximation. The surface DOS presented in

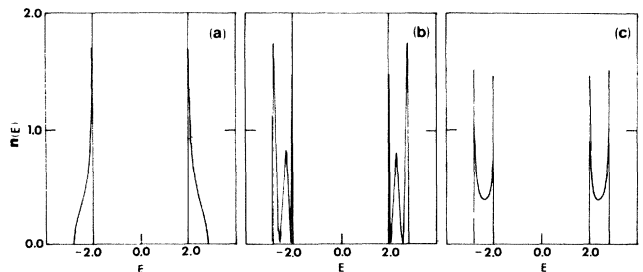


FIG. 2. Local DOS for an ordered binary chain of atoms ($\epsilon_A = -\epsilon_B = 2.0$ and $W=1.0$) (a) at the surface, (b) at the 4th site below the surface, and (c) for the bulk (right panel).

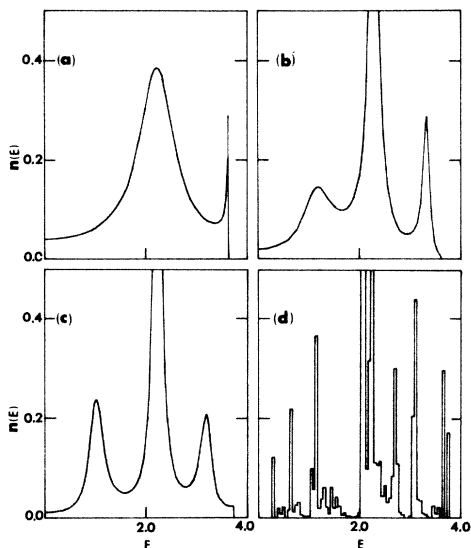


FIG. 3. Local DOS for a disordered binary chain (parameters of Fig. 2 and $C=0.5$) at the surface site as obtained by the AS approach with 5, 8, and 10 pairs of continued-fraction coefficients [(a), (b), and (c), respectively] compared to (d) the result of the PSRG calculation.

Ref. 28 seems to lack the detailed structure of the exact curves while being obtained on the basis of a conceptually more complicated method.

Figures 5 and 6 show results analogous to those of Figs. 3 and 4 but for alloys with $C=0.25$ and $C=0.05$, respectively. Since the DOS's are no longer symmetric in energy about $E=0.0$, the DOS is shown for the whole width of the band. The AS surface DOS (left panels) correspond-

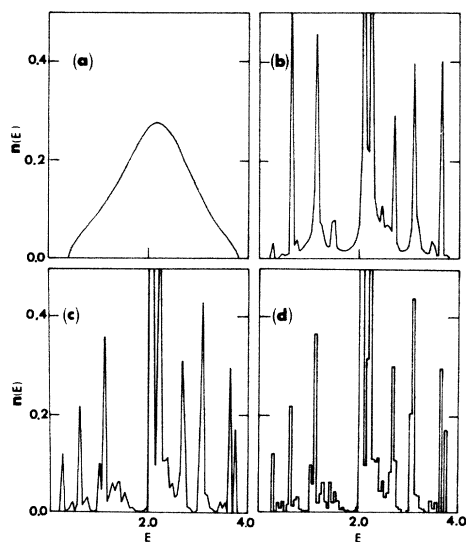


FIG. 4. Local DOS for the surface site analogous to Fig. 3 as obtained by the ECM using clusters of 1, 5, and 13 atoms [(a), (b), and (c), respectively] compared to (d) the result of the PSRG calculation.

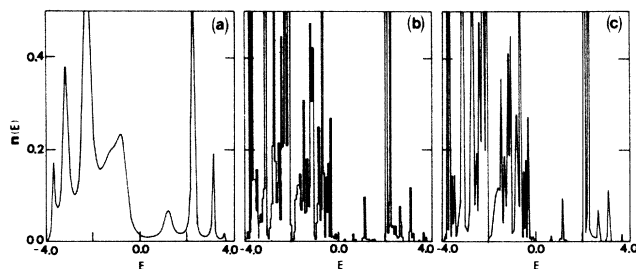


FIG. 5. Local DOS for the surface site of the disordered semi-infinite chain $A_C B_{1-C}$ with $C=0.25$ and the parameters $\varepsilon_A = -\varepsilon_B = 2.0$, $W=1.0$. (a) The AS calculated DOS with 10 pairs of continued-fraction coefficients; (b) exact (PSRG) DOS; (c) ECM results for a 13-atom cluster.

ing to ten pairs of CF coefficients and the analogous ECM results for 13-site clusters (right panels) are compared to the exact total DOS (center panels). For $C=0.05$ it is seen in Fig. 6 that the AS method reproduces accurately the position of the impurity peak, although it smooths out much of the structure in the host DOS which by contrast is faithfully reproduced by the ECM. The accuracy of the AS method in the dilute limit increases because in this limit the AS Hamiltonian approaches the Hamiltonian of a pure system, and for a semi-infinite chain with nearest-neighbor hopping the recursion method becomes exact. Note, incidentally, that a straightforward application of the CF expansion is not applicable to our study of a semi-infinite chain with diagonal disorder and constant nearest-neighbor hopping since the coefficients a_m in such an expansion are exactly the random ε_m and do not converge as $m \rightarrow \infty$.

As was done for pure semi-infinite chains, we also studied the rate of approach to the DOS's of infinite (bulk) disordered chains as a function of the distance from the surface. Using the ECM, we found that the local DOS's at the 13th site below the surface are almost indistinguishable from the bulk DOS's. This is in contrast to the rather large distances needed for corresponding similarity in the case of pure chains and attests to the fact that the DOS's in substitutionally disordered materials are primarily (but not totally) influenced by short-range local en-

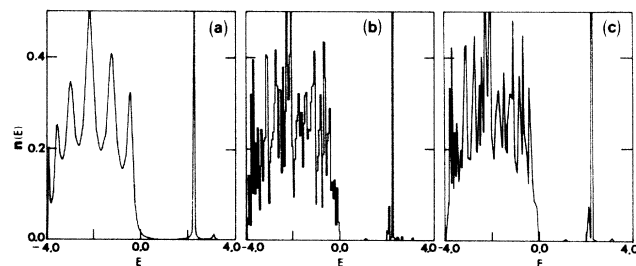


FIG. 6. Local DOS for the surface site analogous to Fig. 5 but with $C=0.05$.

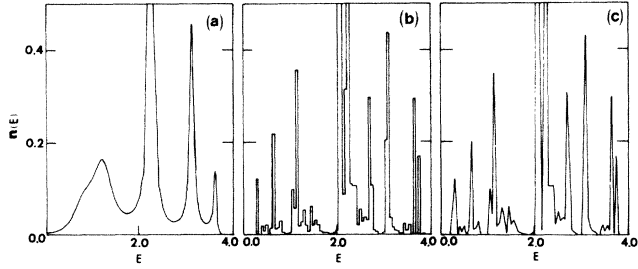


FIG. 7. Local DOS for an A atom on top of the disordered chain with $C=0.5$. Order of (a), (b), and (c) is as in Fig. 5.

vironment fluctuations. Alternatively, this is due to the rapid decrease of the electronic mean free path with increasing disorder.

Figures 7, 8, and 9 show, respectively, partial (species-resolved) surface DOS's for an A atom, a pair of A atoms, and an A atom followed by a B atom, for the case of the binary chain with $C=0.5$. The exact results shown in the center panel are to our knowledge the first exact partial DOS to be reported for substitutionally disordered materials. The ability to yield such decompositions is a great advantage held by the PSRG method over the negative-eigenvalue technique, worth the somewhat longer computing time. Once again, the ECM yields quite accurate results in contrast to the nearly featureless DOS's obtained in the AS method.

IV. CONCLUSIONS

We have compared exact surface DOS's for TB semi-infinite chains obtained by means of rigorous configurational averages with corresponding DOS's obtained by means of two analytic theories, the AS formalism and the ECM. All three methods, PSRG, AS, and ECM, yield identical results in the case of a semi-infinite *ordered* chain. For *disordered* materials, on the other hand, the

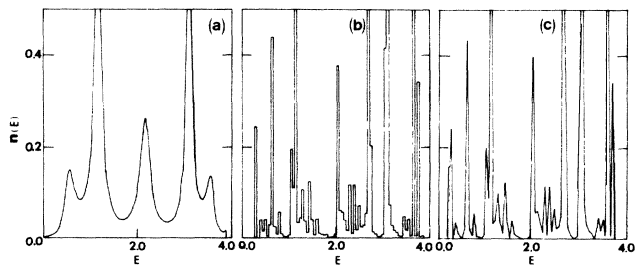


FIG. 8. Local DOS for an A atom followed by an A atom on the surface of a disordered ($C=0.5$) chain. Order of (a), (b), and (c) is as in Fig. 5.

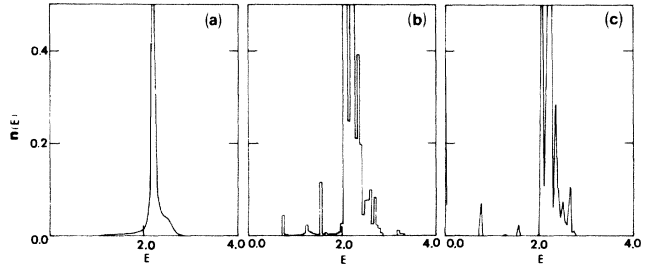


FIG. 9. Local DOS for an A atom followed by a B atom on the surface of a disordered ($C=0.5$) chain. Order of (a), (b), and (c) is as in Fig. 5.

two analytic methods, AS and ECM, were shown to yield vastly different results with the ECM providing a much more accurate, nearly exact, representation of the exact DOS's than the AS formalism.

Any analytic method applied to the study of surfaces must rely heavily on a real-space approach. This is especially true in the case of unidirectional semi-infinite systems, such as disordered linear chains. Both the AS method and the ECM are based on a real-space treatment of disorder, and both have been applied to disordered materials of infinite extent (no surfaces). A simple comparison shows that the ECM is much better suited for the treatment of local environment effects. Such treatment seems to be beyond the computational capabilities of any of the AS methods, which are based on an averaged Hamiltonian rather than treating exactly the Hamiltonian, or a part of the Hamiltonian, of a disordered material as is done within the ECM.

The ECM has been used²⁹ recently in an attempt to mimic the bandstructure of the surface of realistic three-dimensional ternary alloys by means of a one-dimensional model. The reliability of such procedures can be greatly enhanced on the basis of comparisons with exact results such as those presented in this paper. Our results allow us to identify the ECM as a viable technique for calculating local DOS's on the surface of real substitutionally disordered alloys as it has proved to be for such alloys in the bulk. These comparisons suggest rather strongly that for surface as well as for bulk disordered materials the correct treatment of local environment statistical fluctuations is a necessary prerequisite to obtaining accurate local DOS's. In our calculations using the ECM, we assumed that sufficiently far away from the surface the material can be described by means of an effective potential obtained in the CPA for the corresponding bulk alloy (infinite chain). That this assumption is indeed reasonable is substantiated by realistic slab calculation for pure materials.³⁰ In these calculations, it is found that the charge density and hence the potentials at the center layer of a 7- or even 5-layer film is quite similar to that of the corresponding bulk material. The convergence with respect to distance from the surface of a disordered alloy is expected to be even faster due to impurity scattering, as is indeed verified by our one-dimensional calculations.

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