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Alloy broadening of impurity electronic spectra: One-dimensional-model calculations for a ternary alloy

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The embedded-cluster method is used to investigate the inhomogeneous alloy broadening of impurity spectral lines in substitutional crystalline ternary alloys, within a simple model. The model considered is that of a defect in a tight-binding, one-state-per-atom, one-dimensional ternary alloy $A_xB_{1-x}C$ with nearest-neighbor interactions. The dependences of the impurity energy levels and the alloy-broadened linewidths on the composition x, the alloy tight-binding parameters, and the impurity site are discussed and compared with previous results obtained for defects in binary alloys.

I. INTRODUCTION

Fluctuations of local potential energy in the neighborhood of a defect in a disordered alloy can both inhomogeneously broaden the defect spectral lines lying within a band gap and produce local environments which can immobilize and hold excitations for relatively long times as they move from one defect site to another. A few years ago, the importance of this alloy-broadening effect on luminescence spectra of impurities in semiconducting alloys was convincingly demonstrated by Wolford *et al.*[1] in their experiments on excitons bound to nitrogen in $\text{GaAs}_{1-x}\text{P}_x$. They determined that the alloy fluctuations which broaden the nitrogen impurity line can also greatly inhibit exciton transport to traps, thereby enhancing the luminescence yield for this material. Wolford *et al.*[1] measured the alloy-broadened width and shape of the nitrogen luminescence line as a function of the host-alloy composition x. Although a few semiempirical theories have been proposed to treat alloy-broadening effects on defect spectra in semiconducting alloys,[2–4] to our knowledge a satisfactory microscopic theory of the line shape observed by Wolford *et al.*[1] does not exist. In previous work,[5] the foundations for such a theory were developed. In that work, a quantitative theory of inhomogeneous alloy broadening of impurity electronic spectra was developed and applied to impurities in a one-dimensional binary alloy. The purpose of the present paper is to use that theory to investigate such alloy-broadening effects in a simple model of a substitutional crystalline ternary alloy, present some results based on this simple model, and contrast these results with the previous results for defects in binary alloys. In a later work,[6] we plan to present a detailed theory of the inhomogeneous alloy broadening of deep energy levels in real semiconducting alloys.

In this paper, we treat the effects of alloy disorder on impurity spectra in a one-dimensional, one-state-per-atom ternary alloy in the nearest-neighbor tight-binding approximation. This model contains much of the essential physics of the effects of alloy disorder on impurity spectra in ternary alloys without the mathematical and computational complexities inherent in a more realistic model. The treatment of such a simple model, while certainly not allowing us to make any quantitative statements about alloy broadening of impurity electronic spectra in real alloys, enables us to obtain a qualitative understanding of such effects in ternary alloys and to compare these effects with those found previously for defects in the binary-alloy system. The technique used here is based upon the embedded-cluster method, which was originally developed for alloy systems by Gonis and Garland[7] and by Myles and Dow[8] and which has been subsequently applied to a number of alloy problems by several workers.[5–11] Much of the formalism and many of the equations needed for carrying out the calculations described here may be found in Ref. 5, where a discussion of the embedded-cluster method applied to the treatment of alloy-broadening effects on impurity spectra is given, and in Ref. 11, where a detailed discussion of the present model of the alloy host is given.

II. MODEL AND METHOD

In this paper, we consider a ternary alloy $A_xB_{1-x}C$ which serves as the host for an isolated impurity, I. All of our calculations are done for a one-dimensional, one-state-per-atom, nearest-neighbor tight-binding-model alloy system with diagonal disorder only, although most of the formalism is, in principle, generalizable to more realistic models. The alloy-host one-electron Hamiltonian for this model is discussed in detail in Ref. 11. Here we will use, where possible, the notation of that reference. Inserted in this host at the origin on sublattice α ($\alpha=1$ or 2) is an impurity with on-site tight-binding matrix elements ϵ_I and a nearest-neighbor transfer-matrix element which is taken to be t, the same as for the rest of the crystal. The Hamiltonian for the alloy plus impurity system is thus

$$H=H_0+U\ , \tag{1a}$$

where H_0 is the host Hamiltonian shown in Eq. (1) of Ref. 11 and U has the form

$$U=|0,\alpha\rangle(\epsilon_I-\epsilon_{0\alpha})\langle 0,\alpha|\ . \tag{1b}$$

Here $|0,\alpha\rangle$ and ϵ_0 are the atomiclike orbital and corresponding on-site tight-binding matrix element of the alloy-host atom on the αth sublattice at the origin and $\alpha=1$ ($\alpha=2$) refers to the sublattice with A or $B(C)$ atoms. The quantity $\epsilon_{0\alpha}$ is equal to ϵ_C if $\alpha=2$. On the other hand, if $\alpha=1$, it is a random variable taking on the values ϵ_A and ϵ_B with probabilities x and $1-x$, respectively. Here ϵ_A, ϵ_B, and ϵ_C are the atomiclike energies characterizing atoms A, B, and C of the alloy.

In this paper, we seek the configuration-averaged local density of states at the impurity site for energies E in the band gap of the pure alloy. This quantity is defined by the equation

$$l_{0\alpha}(E)=\langle\langle\langle 0,\alpha|\delta(E-H)|0,\alpha\rangle\rangle\rangle , \tag{2}$$

where the double angular brackets denote an average over all alloy configurations. We compute this quantity using the embedded-cluster method as developed by Gonis and Garland[7] and Myles and Dow.[8] Subsequent workers have also found this method to be useful in a number of applications to problems in alloy physics.[5-11] The basic idea of this method is that the host alloy is treated by embedding a finite cluster containing N_C unit cells of alloy constituents in an effective medium, described here by the coherent-potential approximation (CPA).[12-14] The host-plus-defect problem is then solved by replacing one of the atoms in the central cell of the cluster by an impurity and by then applying Koster-Slater defect theory.[15] This impurity is responsible for the persistent defect level. Further, every distinct configuration of the N_C alloy constituent unit cells which surround the impurity leads to a defect level at a different energy.[16] The levels associated with these cluster configurations are the components of the inhomogeneously broadened impurity line shape.

A. CPA and embedded cluster theories for the alloy host

In the single-cell CPA, one approximates the disordered alloy by a self-consistently determined, translationally invariant effective medium. The CPA Green's function g_0, defined as the configuration average of the alloy Green's function G_0, is approximated as

$$g_0=\langle\langle G_0\rangle\rangle\simeq(E-\langle\langle H_0\rangle\rangle+i0)^{-1} , \tag{3}$$

where G_0 is defined in the usual manner, [12]$i0$ is a positive imaginary infinitesimal, and $\langle\langle H_0\rangle\rangle$ is the self-consistently determined configuration-averaged alloy Hamiltonian discussed in Ref. 11.

In order to account for the clustering effects of alloy constituents which are responsible for inhomogeneously broadening the defect spectral lines but which are not accounted for by the CPA, we treat the alloy host via the embedded-cluster method.[5-11] In order to implement this theory, an ensemble of clusters is embedded in the CPA medium. Each particular member of the ensemble contains N_C unit cells with the alloy constituents arranged in a specific configuration.[16] Following Ref. 5, here we include *all* possible configurations for a given cluster size, even those whose compositions differ from the average composition x.[17] It should also be noted that, in contrast to the cluster CPA theories,[12,18] in this theory the cluster is not included self-consistently in the medium. This approximation makes the method computationally tractable, even for large N_C, and furthermore, it has been shown to be accurate in application to a variety of alloy problems.[5-11]

In this approximation, the Green's function which describes the alloy-host has the form

$$G_0=(I-g_0V)^{-1}g_0 , \tag{4a}$$

where V is a scattering potential which is defined as

$$V=H_0-\langle\langle H_0\rangle\rangle , \tag{4b}$$

for sites inside the cluster and which is equal to zero outside the cluster. For large enough cluster size N_C and if all possible configurations of alloy constituents for a given N_C are considered, the number of local environments sample by an impurity placed near the center of the cluster will approach that seen by an impurity in a random alloy.

The embedded-cluster method calculations in Refs. 5 and 11 have shown that, for one-dimensional models, the properties of interest do not change appreciably if the cluster size is changed from $N_C=6$ to $N_C=8$. Thus, for the calculations discussed below, we have fixed the cluster size at $N_C=6$ unit cells. This enables us to obtain almost the same accuracy as one would obtain for $N_C=8$ but saves a considerable amount of computational effort.

B. Defect theory

An impurity whose defect potential is described by Eq. (1b) is placed in the alloy host at the origin on sublattice α. With the alloy-host modeled by the embedded-cluster method discussed above, this is accomplished for a given cluster configuration by replacing one of the atoms in the central cell of the embedded cluster by the impurity. Following essentially the same procedure as is commonly employed in the theory of deep levels in semiconductors,[19] the persistent defect level which is produced by this impurity for this configuration is then found by application of the defect theory due originally to Koster and Slater.[15] Every distinct cluster configuration for an N_C unit-cell cluster[16] which surrounds such an impurity will give rise to a defect energy level at a different energy. The levels which result from following this procedure for all possible cluster configurations are the components of the alloy-broadened local density of states at the impurity site, Eq. (2). In the following discussion, this local state density will be referred to as the impurity "line shape."

Within the embedded-cluster formalism, the impurity-produced bound-state energies for a particular (say the ith) cluster configuration, are solutions to the implicit Fredholm determinantal equation

$$\det[I-G_0(E_i)U]=0 , \tag{5a}$$

where G_0 is given by Eq. (4a), I is the unit matrix, and E_i is the bound-state energy desired. This is the standard result of Koster-Slater defect theory.[15] In the present case Eq. (5a) reduces to the scalar equation

$$\langle 0,\alpha|U|0,\alpha\rangle[\langle 0,\alpha|G_0(E_i)|0,\alpha\rangle]^{-1} . \tag{5b}$$

III. RESULTS

The use of the embedded-cluster and Koster-Slater formalisms discussed above results in an impurity line-shape spectrum $l_0(E)$ for energies in the bandgap of the host alloy which is a series of δ-function lines, one for each distinct configuration of the cluster.[16] For a given cluster size N_C and composition x, this function may thus be written as

$$l_0(E)=\sum_i P_i \delta(E-E_i)\ , \tag{6}$$

with the normalization condition $\sum_i P_i=1$. Here, P_i is the probability of occurence of the ith cluster configuraton, the sum goes over all possible cluster configurations[16] and E_i is the solution to Eq. (5b). Because we are interested only in persistent impurity spectra in the band gap, if a particular cluster configuration produces an energy E_i which is resonant with one of the host-alloy bands, that configuration is excluded from the sum.

Because of the form of Eq. (6), it is of interest to characterize the impurity line shape in terms of its configuration-averaged moments. Of particular interest in the present paper are the first moment or configuration-averaged energy, the square root of the second moment about the mean or linewidth, and the cube root of the third moment about the mean, or skewness. For these quantities we use the symbols

$$L_1=\langle\langle E\rangle\rangle\ , \tag{7a}$$

$$\Delta=[\langle\langle(E-L_1)^2\rangle\rangle]^{1/2}\ , \tag{7b}$$

and

$$\alpha=[\langle\langle(E-L_1)^3\rangle\rangle]^{1/3}\ . \tag{7c}$$

It is sometimes useful to artificially broaden the δ functions in Eq. (6) to enable one to "see" the line shape. This is also physically reasonable, since for a real impurity in a real alloy, effects other than the alloy-broadening mechanism under consideration here will also contribute to the width of the impurity line. In this paper, we thus artificially broaden the δ functions in Eq. (6) by convolving that equation with a Gaussian of width Γ, which we take to be an adjustable parameter. The line shape which we display in the discussion below thus has the form

$$l_0(E)=\frac{1}{2\pi\Gamma}\sum_i P_i e^{-(E-E_i)^2/2\Gamma^2}\ . \tag{8}$$

We now present some results for some specific alloy parameters.

A. Results for impurities in an amalgamated alloy, $\epsilon_C=-\epsilon_B=t$ and $\epsilon_A=0.0$.

This choice of alloy parameters corresponds to the case of a ternary alloy in the "amalgamation" limit,[12] where the band spectra of the unalloyed crystals AC and BC overlap and where the alloy band spectra for $A_xB_{1-x}C$ are characteristic of the alloy as a whole rather than of any component.[11] Most of the technologically important semiconducting alloys are expected to have amalgamated electronic spectra.[20,21] This choice of parameters also corresponds to the case of a ternary alloy $A_xB_{1-x}C$ with anion disorder. That is, the constituent atoms A and B are both more electronegative than atom C. An example of this type of alloy is $\mathrm{GaAs}_{1-x}\mathrm{P}_x$. For this (or any) set of parameters, there are two cases of interest. These correspond to the case where the impurity is on the ordered ($\alpha=2$) sublattice and to the case where the impurity is on the disordered ($\alpha=1$) sublattice. We now discuss results for these two cases in turn.

1. $\epsilon_I=-0.5t$ on the ordered ($\alpha=2$) sublattice

Since the nearest neighbors to the impurity are disordered in this case, we expect that the primary contribution to the alloy broadening will come from this nearest-neighbor disorder. Further, the atomiclike energy ϵ_I of the impurity has been chosen to be halfway between the atomiclike energies, ϵ_A and ϵ_B, of the alloy constituent atoms B and A, making the impurity I similar to atoms A and B and very dissimilar to atom C. Thus, this case corresponds to that of a very electronegative (anionlike) impurity occupying a cation site in a ternary alloy with anion disorder. An example of a similar case for a real system would be an As or P antisite defect in $\mathrm{GaAs}_{1-x}\mathrm{P}_x$.

In Fig. 1 we show the results of this case for the dependence of the configuration-averaged energy L_1 on the alloy composition x. The defect potential produces an impurity spectral line in the band gap of the alloy. The host energy bands are shaded and the band edges are the same as those predicted by the CPA. The conduction (valence) band is mostly C-atomlike (A- and B-atomlike) and is so labeled in the figure. The conduction-band edge is essentially independent of x on the scale of the figure. The first moment L_1 varies approximately linearly with x in the region $0.167<x<0.833$ which is the range $1/N_C<x<1-(1/N_C)$ for $N_C=6$. This is the region in which we expect our calculations to be most accurate, although we have also performed calculations for x outside of this range. By performing an exact calculation for an appropriate isolated impurity in a pure BC or AC lattice,

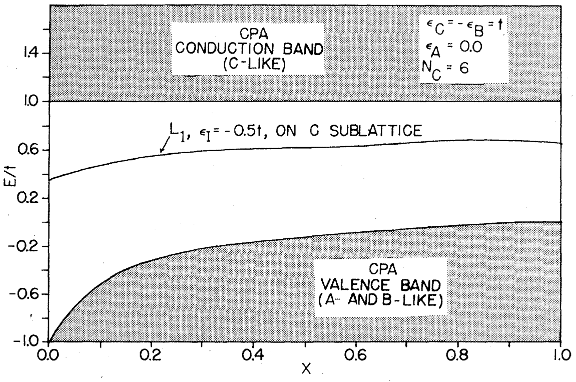

FIG. 1. The first moment L_1 of the alloy-broadened impurity line shape as a function of alloy composition x for $A_xB_{1-x}C$ in the case $\epsilon_C=-\epsilon_B=t$, $\epsilon_A=0$, $N_C=6$, and $\epsilon_I=-0.5t$ for the impurity on the ordered ($\alpha=2$) sublattice.

it is possible to extrapolate the present results to $x \rightarrow 1$ and $x \rightarrow 0$, respectively. We have done this for the case shown in Fig. 1 and in that figure the results of the embedded-cluster method have been joined smoothly to these isolated impurity results. At large ($x > 0.833$) and small ($x < 0.167$) compositions, it is clear from Fig. 1 that L_1 shows significant deviations from linear behavior. Finally, it is clear from the figure that the impurity line L_1 is not attached to either band edge as x is varied. This is characteristic of a deep level.[19]

In previous work on alloy broadening of impurity spectra in *binary* alloys,[5] it was possible to resolve the impurity line into three distinct components, corresponding to configurations in which the impurity atom I is surrounded by its three possible nearest-neighbor environments: two A atoms (AIA), two B atoms (BIB), and one A and one B atom (AIB or BIA). The present case presents a stark contrast to the binary-alloy case. We find that, while it is both formally and computationally possible to follow these component lines as a function of x, the spectra of the AIA, BIB, and AIB components are sufficiently overlapping that they have no distinct meaning. This is primarily due to the fact that the alloy under consideration here is amalgamated. (Reference 5 considers a binary alloy in the persistence limit.) Thus, the difference in the atomic potentials of the randomly placed A and B atoms which surround the impurity in the various cluster configurations are not great enough to cause a splitting. In addition, the presence of atom C on the ordered sublattice also affects the potential at the impurity site, tending to reduce the differences in the AIA, BIB, and AIB component lines.

In Fig. 2, we display the x dependences of the linewidth Δ and the skewness α for the same parameters as were used in Fig. 1. Since the impurity occupies a site on the ordered sublattice which is between two disordered sites, and since the atomiclike energy $\epsilon_I = -0.5t$, associated with the impurity, lies halfway between the corresponding quantities, $\epsilon_A = 0.0$ and $\epsilon_B = -t$, for the atoms on the disordered sublattice, this case should be analogous to the case of the "symmetric" impurity discussed in Ref. 5 for the binary-alloy impurity system. As can be clearly seen from Fig. 2, our results for this case predict a linewidth Δ and a skewness α which have marked asymmetries about $x = 0.5$, in sharp contrast with the symmetries about $x = 0.5$ which were found for these same quantities in Ref. 5. The reason for this asymmetry is due to the presence of C atoms on the ordered sublattice between each pair of disordered sites, which strongly affects the random potential seen by the impurity and causes the asymmetry. Thus, the differences between the binary- and ternary-alloy cases should not be too surprising because the analogy between the two cases is actually a poor one.

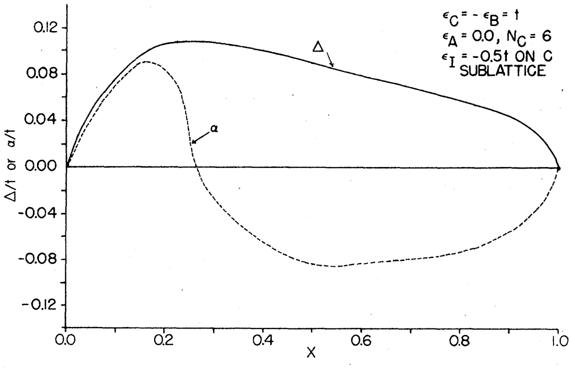

FIG. 2. The linewidth Δ (solid curve) and the skewness or asymmetry α (dashed curve) of the alloy-broadened line shape as functions of the alloy composition x for the same parameters as used in Fig. 1.

It is also worth noting that the linewidth and skewness displayed in Fig. 2 both show considerable deviations from the $[x(1-x)]^{1/2}$ and $[x(1-x)]^{1/3}$ dependences expected for Δ and α on the basis of a perturbation theory in powers of the minority concentration.[5] Such deviations are not too surprising since that perturbation theory is expected to be strictly valid only in the limits $x \rightarrow 0$ and 1. Because our embedded-cluster calculations are expected to be most accurate in the range $0.167 < x < 0.833$, however, in these extreme ($x \rightarrow 0, x \rightarrow 1$) composition limits our results have been smoothly joined to the perturbation-theory results.

We have also calculated, but not displayed, the fourth root of the fourth moment about the mean for this same case and find that it is of the same order of magnitude as and that it has a composition dependence which is similar to the linewidth Δ. Because the line shape in this case has significant third and higher moments, it is clear that it is probably not representable by a simple function. In fact, the usual moment expansions of impurity line shapes[22] would probably be, at best, slowly convergent in this case.

2. $\epsilon_I = 1.5t$ *on the disordered* ($\alpha = 1$) *sublattice*

Because the impurity is on the disordered sublattice in this case, the primary contribution to the alloy broadening will be expected to come from a second-neighbor effect. Furthermore, the impurity's atomiclike energy parameter ϵ_I has been chosen to be more electropositive than that of any of the alloy constituents. The impurity is most similar to atom C and very different than atoms A and B. Thus, this case corresponds to the case of a very electropositive (cationlike) impurity occupying an anion site in a ternary alloy with anion disorder. An example of a similar case for a real system would be a Ga antisite defect in $\mathrm{GaAs}_{1-x}\mathrm{P}_x$.

We have calculated the x dependences of the configuration-averaged energy L_1, the linewidth Δ, and the skewness α for these parameters. The results we have obtained for these quantities, while differing in quantitative detail from those obtained for the previously discussed case, are qualitatively very similar to the results presented in Figs. 1 and 2. In particular, the average energy L_1 is an essentially linear function of composition, except for large and small x, and the linewidth Δ and skewness α are very asymmetric functions of x which cannot be described by a simple perturbation theory in powers of x or $(1-x)$.[5] Of particular importance is the fact that Δ and α are both of the same order of magnitude for this case of an impurity on the disordered sublattice as they were for the previously discussed case of an impurity on the ordered sublattice, showing that a moment expansion theory of the line shape[22] would again be slowly convergent. The fact that Δ are α are of the same order of magnitude for the two cases is surprising, since one would expect that because the alloy broadening in the previous case was a first-neighbor effect and that in the present case it is a second-neighbor effect the broadening in the present case should be smaller. This result thus shows that the physics of alloy broadening of impurity electronic spectra is not intuitively obvious.

As our only illustration for this case, in Fig. 3 we display Gaussian-broadened impurity line shapes, computed by the use of Eq. (8), for alloy composition $x=0.5$, which is the case where the line shape contains the most structure. The vertical scale in this figure is arbitrary; the curves are normalized so that the highest-peak height is unity. The line shapes for three different choices of the Gaussian width Γ are shown. The narrowest peaks in Fig. 3 (solid curve) correspond to $\Gamma=(2.0\times10^{-3})t$, the next-narrowest peaks (dashed curve) to $\Gamma=(1.8\times10^{-2})t$, and the wide envelope (dot-dashed curve) correspond to $\Gamma=(1.6\times10^{-1})t$. It is clear from the figure that the predicted line shapes are very rich in structure that would be missed by most simple perturbation or moment-expansion approaches.

The finest resolution curve (solid curve) for the line shapes shows the existence of many impurity energy levels. Each level corresponds to the solution of Eq. (5) for a different configuration of alloy constituents within the cluster. Some of these levels are, of course, degenerate or nearly degenerate because of the physical equivalence or almost equivalence of particular configurations. The intermediate resolution curve (dashed curve) in Fig. 3 tends to smooth out all but the gross features of the energy-level structure, but still clearly reflects the fact that the spectrum is made up of multiple components. The curve in Fig. 3 with the largest broadening (dot-dashed curve) shows only an almost featureless Gaussianlike bump which forms an envelope over the curves for the smaller broadenings. In a real alloy, the actual alloy-broadened impurity line shape could range anywhere from that shown in Fig. 3 for the finest resolution to that shown for the broadest resolution, depending on the physical mechanism responsible for this level broadening.

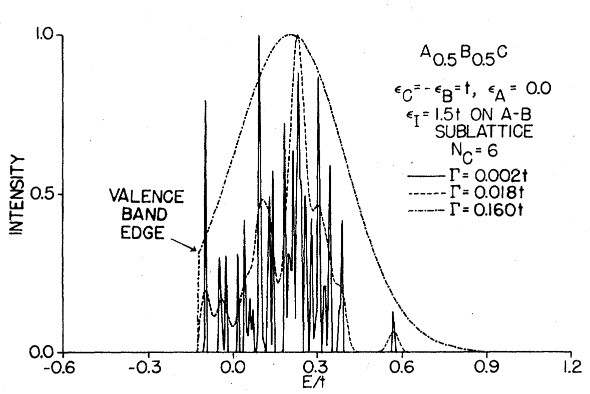

FIG. 3. Gaussian-broadened impurity line shape for the alloy $A_{0.5}B_{0.5}C$ in the case $\epsilon_C=-\epsilon_B=t$, $\epsilon_A=0$, $N_C=6$, and $\epsilon_I=1.5t$ for the impurity on the disordered ($\alpha=1$) sublattice. Three different Gaussian broadenings are displayed: $\Gamma=(2.0\times10^{-3})t$ (solid curve), $\Gamma=(1.8\times10^{-2})t$ (dashed curve), and $\Gamma=(1.6\times19^{-1})t$ (dot-dashed curve).

B. Results for impurities in a persistent alloy

We have also calculated results analogous to those discussed above for impurities in a ternary alloy in the "persistence" limit,[12] where the band spectra of AC and BC are nonoverlapping and where the alloy band spectra for $A_xB_{1-x}C$ thus display characteristics of both AC and BC. The results of these calculations show that the impurity line shapes and moments are all qualitatively similar and have similar magnitudes as the corresponding quantities presented and discussed above for impurities in a ternary alloy in the amalgamation limit. We find that this is true for an impurity on either the ordered or the disordered sublattice. Thus these results will not be shown here. Furthermore, we also find that none of the results obtained in this case are very similar to the analogous results for the case of an impurity in a persistent binary alloy.[5] In particular, even for the choice of parameters $\epsilon_C=-\epsilon_B=-2.0t$, $\epsilon_A=0.0$, and $\epsilon_I=-1.0t$, on the ordered sublattice, for which atoms A, B, C, and I are very different from one another, the alloy-broadened line shape does *not* split into three distinct groups, corresponding to the three possible nearest-neighbor environments of the impurity as it does in the analogous binary-alloy case.[5] Thus, the alloy-broadened line shapes of impurities in binary and ternary alloys are very different in this respect, even when the alloy and impurity parameters are chosen so that the two cases appear to be analogous. This is due to the presence of the ordered C sublattice in the present case.

IV. SUMMARY AND CONCLUSIONS

We have used the theory of inhomogeneous alloy broadening of impurity electronic spectra developed in Ref. 5, to investigate this effect for impurities in ternary alloys, within a simple one-dimensional model where the electrons are treated in the nearest-neighbor tight-binding approximation. By embedding an ensemble of clusters containing N_C unit cells in a CPA medium and then by replacing one of the central atoms of the cluster by an impurity and solving for the impurity levels using Koster-Slater defect theory, we have shown that one can calculate the alloy-broadened line shape of the impurity. We have furthermore presented results for impurities on both the ordered and the disordered sublattices. Although the model used here is a simple one, the method does produce accurate alloy broadened line shapes and shows promise for application to impurity spectra in real semiconducting alloy systems.

The results presented here enable us to make some general conclusions regarding the alloy broadening of impurity spectra in substitutionally disordered one-dimensional ternary alloys, which should also be qualitatively correct for impurity spectra in real ternary alloys. These are the following: (i) disorder in either the nearest-neighbor or the second-neighbor environments of an impurity greatly affects persistent impurity lines and can appreciably broaden them; (ii) this alloy-broadening effect is both qualitatively and quantitatively similar for the impurity on either the disordered or the ordered sublattice; (iii) disorder in the higher-neighbor environments of the impurity also contributes significantly to this effect and can often asymmetrically broaden the impurity lines; (iv) in contrast with the case for binary alloys the impurity spectra in ternary alloys are not in general split into distinct components corresponding to the near- or second-neighbor environments of the impurity, even when the alloy is in the persistence limit, and (v) the approach outlined here, while somewhat tedious, will usually produce an adequate alloy-broadened line shape.

V. ACKNOWLEDGMENTS

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[16] For a cluster containing N_C unit cells, with N_A of them containing AC cells and N_B of them containing BC cells ($N_A + N_B = N_C$) the total number of possible configurations is

$$\eta = \sum_{N_A=0}^{N_C} \frac{N_C}{N_A! N_B!}$$

However, not all cluster configurations are physically distinct. Furthermore, for the alloy $A_xB_{1-x}C$, for a given composition x, the probability of occurrence of a given configuration containing N_A unit cells of type AC and N_B unit cells of type BC ($N_C = N_A + N_B$) is

$$P = x^{N_A}(1-x)^{N_B} .$$

[17] This is in contrast to the work discussed in Refs. 8, 9, and 11, where the main thrust was to accurately mimic the alloy-host state density.

[18] There are a large number of cluster CPA theories, many of which suffer from nonanalyticity problems, in addition to their computational complexity. One which does not have this problem is R. Mills and P. Ratanavararaksa, Phys. Rev. B **18**, 5291 (1978); R. Mills, L. J. Gray, and T. Kaplan, *ibid.* **27**, 3252 (1983).

[19] See, for example, S. T. Pantelides, Rev. Mod. Phys. **50**, 797 (1978); M. Jaros, *Deep Levels in Semiconductors* (Adam Hilger, Briston, 1982); M. Jaros, Adv. Phys. **29**, 409 (1980); H. P. Hjalmarson, P. Vogl, D. J. Wolford, and J. D. Dow, Phys. Rev. Lett. **41**, 892 (1978); C. W. Myles and O. F. Sankey, Phys. Rev. B **29**, 6810 (1984), and references therein.

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