PHYSICAL REVIEW B VOLUME 29, NUMBER 2 15 JANUARY 1984

Tight-binding view of alloy scattering in III-V ternary semiconducting alloys

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(Received 6 September 1983)

The contribution of alloy scattering to the electronic scattering rate at the Brillouin-zone center in 18 III-V ternary semiconducting alloys is calculated in the Born approximation using the semiempirical tight-binding parameters of Vogl, Hjalmarson, and Dow. Three types of disorder for a ternary alloy of the type $A_xB_{1-x}C$ are included in these calculations. These are (1) ordinary diagonal disorder or disorder in the diagonal tight-binding energies associated with the constituents A and B, (2) off-diagonal disorder or disorder in the tight-binding transfer energies between the constituents A and C and the constituents B and C, and (3) redistribution disorder which takes into account the fact that the diagonal tight-binding energy of constituent C is different in substance AC than in substance BC. The latter two types of disorder are taken into account for the first time by our calculations, and we show that all three types of disorder can make roughly equal and sometimes competing contributions to the alloy scattering rate. Scattering rates appropriate for both conduction-band and valence-band scattering are presented and chemical trends in these rates for the alloys considered are predicted.

I. INTRODUCTION

The increasing technological importance of the III-V ternary semiconducting alloys has generated considerable basic experimental and theoretical research on their electronic properties. An important parameter of these materials for most device applications is the carrier mobility. Of particular interest for this parameter is its variation with alloy composition and from alloy to alloy.

Among other scattering mechanisms, the alloy or disorder scattering contribution to the mobility can be significant. Furthermore, this mechanism contributes to the scattering of electrons throughout the Brillouin zone. Most previous treatments of alloy scattering have been based on an effective impurity potential that is localized to within an atomic cell. Although square wells[1] or screened effective charges[2] have sometimes been used to describe this potential, the alloy scattering relaxation rate in the Born approximation depends only on its volume integral. The relaxation rate can thus be characterized by a single parameter, which is often chosen to be an energy denoted as ΔE. Once this relaxation rate is calculated, it can be used to calculate drift mobilities[3] or high-field mobilities.[4] Various guesses for the energy parameter ΔE exist[1,5] but, in fact, it cannot be related to any other theoretical parameters or to any experimental results except the mobility. Furthermore, although it is usually not explicitly stated, the implication in this type of treatment is that the scattering potential and thus ΔE are the same for both the conduction and the valence bands.

Recently, coherent-potential approximation (CPA) calculations of band structures of III-V ternary alloys have been published.[6] These calculations include disorder only in the diagonal bonding and antibonding energies and not in all of the various energies that go into the alloy Hamiltonian in the tight-binding picture. However, these calculations do illustrate the fact that the effects of the alloy disorder on the conduction and valence bands are different.

In this paper we investigate alloy or disorder scattering in both the conduction and valence bands of the III-V ternary alloys. Our approach is based on an effective tight-binding Hamiltonian that can be related to many other properties of the alloy considered. We thus believe that our treatment is considerably more fundamental than those based on an effective potential. Our theory is limited to the Born approximation for states near the Γ point and the effects of spin-orbit coupling are neglected. The actual calculation uses parameters from the semiempirical tight-binding model of Vogl, Hjalmarson, and Dow[7] (VHD), although it could also be adapted to other tight-binding-like models. There are no adjustable parameters in the theory other than the ones used in this band-structure model.

Since the VHD model includes ten bands,[7] a treatment of the disorder problem in general would involve 10×10 matrix equations. However, for states near the Γ point ($\vec{k}=\vec{0}$), the disorder part of the calculation for either the conduction or valence band can be described by 2×2 matrix equations. Thus in that region of the Brillouin zone, each band can be described by an anion energy E_a, a cation energy E_c, and a transfer matrix element or overlap energy V. In a ternary semiconducting alloy at the Γ point, one therefore expects disorder in V (usually denoted as off-diagonal disorder) and in one of the two diagonal energies (usually denoted as diagonal disorder). For example, in a ternary alloy with cation disorder ($A_xB_{1-x}C$) one expects disorder in V and E_c but not in E_a. However, by examining Table I of VHD one can see that E_a is also disordered. That is, the diagonal entries for the anion C are different in compound AC than in compound BC. This implies a third type of disorder. That is, the anion energies for C must be partially determined by the number of A and B neighbors. This disorder is physically due to charge redistribution within an atomic cell and between atomic cells and will thus be denoted henceforth as redistribution disorder. To our knowledge, redistribution disorder has never been discussed in the literature before. Furthermore, other than a recent CPA calculation of the alloy scattering contribution to the mobility done by us and discussed elsewhere,[8] off-diagonal disorder has never been explicitly included in any theory of alloy scattering. In Sec. II we calculate the alloy scattering contribution to the scattering rate taking into account all three types of disorder.

The starting point for our theory is the virtual-crystal approximation, which treats the alloy as a perfect crystal with average energies for each atom and between each pair of atoms. We then treat the fluctuations about the virtual crystal in the Born approximation or weak scattering limit. Further, we consider the constituents of the alloy to be distributed at random and treat the overlap energy V between a given pair of atoms as a constant depending only on the two atoms and independent of the composition of the rest of the alloy. This last assumption obtains from recent observations[9] that AC and BC nearest-neighbor distances are virtually independent of alloy composition in $A_xB_{1-x}C$.

The VHD semiempirical tight-binding model has been successfully used to predict a large number of properties of semiconductors and semiconducting alloys.[10–24] However, the tight-binding energy parameters in the model are reliable only to about 0.1 eV,[10–24] and our calculations depend heavily on differences between energies. Thus the detailed numbers resulting from our theory should not be taken too seriously. Nevertheless, we feel that these numbers should give a reasonable estimate of the strength of alloy scattering and particularly of the relative contributions of diagonal, off-diagonal, and redistribution disorder, and the importance of the interference effects between them. They should also illustrate the difference between scattering in the conduction and valence bands. Finally, in keeping with the spirit of the numerous previous calculations using the VHD parameters,[10–24] we feel that our calculations should predict the correct chemical trends or relative orderings of the scattering rates in the alloys considered here.

The calculational details of the paper are contained in Sec. II, which may be omitted by the reader without loss of continuity. The results and their implications are presented and discussed in Secs. III and IV.

II. CALCULATION

In this section we derive expressions for the alloy or disorder scattering contribution to the relaxation rate for III-V ternary alloys. This is easiest to do by first calculating the single-particle relaxation rate and then constructing the transport rate from it. Our calculation is based on the tight-binding VHD model and it is easiest to approach within a Green's-function formalism. The electronic Green's function for the alloy is defined as[25]

$$\tilde{G}_{\alpha\beta}(E)=\langle \psi_\alpha | (E-H)^{-1} | \psi_\beta \rangle \,, \tag{1}$$

where E is the energy variable, H is the Hamiltonian for the alloy, Greek indices denote both a spatial atomic site and a band or atomic level, and ψ_α is the appropriate wave function. The equation of motion for $\tilde{G}_{\alpha\beta}(E)$ is easily found to be

$$(E-E_\alpha)\tilde{G}_{\alpha\beta}(E)-\sum_\gamma T_{\alpha\gamma} W_{\alpha\gamma} \tilde{G}_{\gamma\beta}(E)=\delta_{\alpha\beta} \,, \tag{2a}$$

where we have defined

$$E_\alpha=\langle \psi_\alpha | H | \psi_\alpha \rangle \tag{2b}$$

and

$$T_{\alpha\beta}=\langle \psi_\alpha | H | \psi_\beta \rangle \,, \quad \alpha\neq\beta \,. \tag{2c}$$

We assume only nearest-neighbor interactions throughout this calculation. Thus we have introduced the quantity $W_{\alpha\gamma}$ in Eq. (2), which equals one if α and γ are nearest-neighbor sites and zero otherwise. Since, as is stated above, we are considering fluctuations about the virtual-crystal approximation, we make the following definitions:

$$\delta E_\alpha=E_\alpha-\langle E_\alpha \rangle \tag{3a}$$

and

$$\delta T_{\alpha\beta}=T_{\alpha\beta}-\langle T_{\alpha\beta} \rangle \,, \tag{3b}$$

where the angular brackets refer to the alloy configuration average. Thus $\langle E_\alpha \rangle$ and $\langle T_{\alpha\beta} \rangle$ are the virtual-crystal-averaged diagonal and off-diagonal energies, and δE_α and $\delta T_{\alpha\beta}$ refer to the fluctuations about these quantities.

The inverse of the Green's function $\tilde{G}_0$ for the alloy in the virtual-crystal approximation is defined as

$$(\tilde{G}_0^{-1})_{\alpha\beta}=(E-\langle E_\alpha \rangle)\delta_{\alpha\beta}-\langle T_{\alpha\beta} \rangle W_{\alpha\beta} \,. \tag{4}$$

By combining Eqs. (2)–(4) and expressing the result in matrix form, it can easily be shown that the true alloy Green's function $\tilde{G}$ and the virtual-crystal Green's function $\tilde{G}_0$ are related by the Dyson equation

$$\underline{\tilde{G}}=\underline{\tilde{G}}_0+\underline{\tilde{G}}_0\underline{\Omega}\,\underline{\tilde{G}} \,, \tag{5}$$

where we have defined

$$\Omega_{\alpha\beta}=\delta E_\alpha\, \delta_{\alpha\beta}+\delta T_{\alpha\beta}\, W_{\alpha\beta} \,.$$

By construction, the configuration average of Ω is zero. It is straightforward to iterate Eq. (5) to second order in Ω, solve for $\underline{\tilde{G}}^{-1}$, and then average over configurations. This is equivalent to the usual Born approximation and yields the results

$$\begin{gathered}(\underline{G}^{-1})_{\alpha\beta}=(\underline{G}_0^{-1})_{\alpha\beta}-\sigma_{\alpha\beta} \,, \\ \sigma_{\alpha\beta}=\sum_{\gamma,\delta}\langle \Omega_{\alpha\gamma}(\underline{G}_0)_{\gamma\delta}\Omega_{\delta\beta} \rangle \,, \\ \underline{G}=\langle \underline{\tilde{G}} \rangle \,, \quad \underline{\tilde{G}}_0=\langle \underline{\tilde{G}}_0 \rangle=\underline{\tilde{G}}_0 \,,\end{gathered} \tag{6}$$

where the angular brackets again denote a configuration average. This equation can be Fourier-transformed and we will let $G(q,E)$ denote the Fourier transform of $G_{\alpha\beta}(E)$.

In the VHD scheme, each Greek index refers to a space point and to one of ten bands[7] so that Eqs. (6) are in general 10×10 matrix equations. However, at the Γ point ($k=0$), the 10×10 Hamiltonian matrix of VHD reduces to five uncoupled 2×2 matrices. Thus Eqs. (6) similarly reduce to five uncoupled 2×2 matrix equations and the conduction and valence bands are described separately by such equations. For finite k these matrices are, of course, connected to other elements of the 10×10 matrix. However, for small k and in the weak scattering limit it can easily be shown that the disorder in these connecting matrix elements is of the order of $(\delta E)^2 k^2$, where δE is a typical fluctuation about the virtual-crystal average. We thus neglect these terms here since we are only interested in developing a lowest-order theory where only terms of order $(\delta E)^2$ and k^2 are kept. The virtual-crystal parts of these connecting matrix elements are, however, kept as the effective-mass part of the energy. Thus in our calculations we use Eqs. (6), with only two bands, but include the k^2-dependent effective-mass energy in the virtual-crystal Green's function G_0.

In the rest of this section we consider only alloys of the form $A_xB_{1-x}C$ with cation disorder. In the 2×2 matrix equations obtained from Eqs. (6) in the weak scattering limit, we let the indices 1 and 2 refer to the cation and anion, respectively. Results for alloys with anion disorder may be similarly obtained. When the atomic site part of α is 1, then we denote E_α as e_a, if an A atom occupies that site, and as e_b if a B atom is situated there. Similarly, we denote the quantity $T_{\alpha\beta}$ as t_a, if it connects neighboring A and C atoms, and as t_b if it connects neighboring B and C atoms. Finally, if α is 2, we denote E_α as $\frac{1}{4}\bar{e}_a$ times the number of neighboring A sites plus $\frac{1}{4}\bar{e}_b$ times the number of neighboring B sites. In this notation, the virtual-crystal diagonal and off-diagonal energies are

$$\langle E_1\rangle = xe_a+(1-x)e_b\ , \quad \langle E_2\rangle = x\bar{e}_a+(1-x)\bar{e}_b\ , \tag{7}$$

and

$$\langle T_{12}\rangle = xt_a+(1-x)t_b\ .$$

In the evaluation of $\sigma_{\alpha\beta}$ in Eq. (6), it is necessary to evaluate expressions of the form

$$\langle \delta E_\alpha\, \delta E_\beta\rangle = \langle (E_\alpha-\langle E_\alpha\rangle)(E_\beta-\langle E_\beta\rangle)\rangle\ ,$$

$$\langle \delta T_{\alpha\beta}\, \delta T_{\gamma\delta}\rangle = \langle (T_{\alpha\beta}-\langle T_{\alpha\beta}\rangle)(T_{\gamma\delta}-\langle T_{\gamma\delta}\rangle)\rangle\ , \tag{8}$$

and

$$\langle \delta E_\alpha\, \delta T_{\beta\gamma}\rangle = \langle (E_\alpha-\langle E_\alpha\rangle)(T_{\beta\gamma}-\langle T_{\beta\gamma}\rangle)\rangle\ .$$

In evaluating these expressions one makes use of Eqs. (7) and the formal expression

$$E_\alpha = \sum_\beta W_{\alpha\beta} h_\beta\ , \tag{9}$$

where α is on sublattice 2 and where h_β is $\frac{1}{4}\bar{e}_a$ ($\frac{1}{4}\bar{e}_b$) if β is an A (B) site. Equations (8) can be easily evaluated in the notation just discussed. They have the explicit forms

$$\langle \delta E_\alpha\, \delta E_\beta\rangle = x(1-x)[\delta_{\alpha\beta}\delta_{\alpha 1}(e_a-e_b)^2+\delta_{\alpha 2} f_{\alpha\beta}(\bar{e}_a-\bar{e}_b)^2 + \tfrac{1}{4}(e_a-e_b)(\bar{e}_a-\bar{e}_b)W_{\alpha\beta}]\ , \tag{10a}$$

$$\langle \delta T_{\alpha\beta}\delta T_{\gamma\delta}\rangle = x(1-x)(t_a-t_b)^2[\delta_{\alpha\gamma}\delta_{\alpha 1}+\delta_{\alpha\delta}\delta_{\alpha 1} + \delta_{\beta\gamma}\delta_{\beta 1}+\delta_{\beta\delta}\delta_{\beta 1}]\ , \tag{10b}$$

$$\langle \delta E_\alpha \delta T_{\beta\gamma}\rangle = x(1-x)(t_a-t_b)[(e_a-e_b)\delta_{\alpha 1}(\delta_{\alpha\beta}+\delta_{\alpha\gamma}) + (\bar{e}_a-\bar{e}_b)\delta_{\alpha 2}\tfrac{1}{4}(W_{\alpha\beta}+W_{\alpha\gamma})]\ , \tag{10c}$$

where

$$f_{\alpha\beta} = \sum_\gamma W_{\alpha\gamma}W_{\gamma\beta}/16\ , \tag{10d}$$

and we have used the shorthand notation $\delta_{\alpha 1}$ ($\delta_{\alpha 2}$) to denote that α refers to a cation (anion) site.

By using Eqs. (10) one can easily evaluate the components of $\sigma_{\alpha\beta}$ in the small-k limit. They have the form

$$\begin{aligned} \sigma_{11} &= x(1-x)[(\Delta e_c)^2 g_{11}+(\Delta v)^2 g_{22}+2(\Delta e_c\Delta v)g_{12}]\ ,\\ \sigma_{22} &= x(1-x)[(\Delta e_a)^2 g_{22}+(\Delta v)^2 g_{11}+2(\Delta e_a\Delta v)g_{12}]\ ,\\ \sigma_{12} = \sigma_{21} &= x(1-x)[(\Delta e_c\Delta e_a)g_{12}+(\Delta v)^2 g_{12} + (\Delta e_c\Delta v)g_{11}+(\Delta e_a\Delta v)g_{22}]\ , \end{aligned} \tag{11}$$

where

$$\Delta e_c = e_a-e_b\ , \quad \Delta e_a = \bar{e}_a-\bar{e}_b\ , \quad \Delta v = (t_a-t_b)/4\ . \tag{12}$$

In Eq. (11) we have defined

$$g_{\alpha\beta}(E) = \frac{1}{n}\int \frac{d^3q}{(2\pi)^3}[G_0(q,E)]_{\alpha\beta}\ , \tag{13}$$

where n is the number of atoms per unit volume and E is understood to have an infinitesimally small positive imaginary part.

The single-particle relaxation rate can be extracted from the energy eigenvalues of Eqs. (6). From these equations one can easily obtain the roots of the characteristic equation,

$$E_\pm = \tfrac{1}{2}\{E_c+E_a+\sigma_{11}+\sigma_{22}\pm[(E_c+\sigma_{11}-E_a-\sigma_{22})^2 + 4(V+\sigma_{12})]^{1/2}\}\ , \tag{14}$$

where $\langle E_1\rangle$, $\langle E_2\rangle$, and $\langle T_{12}\rangle$ have been replaced by E_c, E_a, and $V/4$, which denote the diagonal cation and anion energies and the transfer energy in the virtual-crystal approximation. The factor of 4, here and in Eq. (12), occurs because each atom has four nearest neighbors in a zinc-blende lattice. The upper and lower signs in Eq. (14) arise because of the mixing of two bands; the upper sign denotes the conduction band and the lower sign denotes the valence band.

The single-particle relaxation rate ν_1 is given by the imaginary part of $E_{\pm}/\hbar$. By evaluating Eq. (13), combining Eqs. (11)–(14), and expanding Eq. (14) to second order in the fluctuations, we obtain, for this quantity,

$$\nu_1 = [x(1-x)(m^*)^{3/2}E^{1/2}/2^{1/2}n\pi\hbar^4](\Delta E)^2 , \tag{15a}$$

where

$$\Delta E = [(E_c - E_a \pm E_s)\Delta e_c - (E_c - E_a \mp E_s)\Delta e_a + 4V\Delta v]/2E_s . \tag{15b}$$

Here we have defined

$$E_s = [(E_c - E_a)^2 + 4V^2]^{1/2} . \tag{15c}$$

In Eqs. (15), m^* is the electronic effective mass and E_c, E_a, and V are the virtual-crystal cation, anion, and overlap energies, respectively. The quantities Δe_c, Δe_a, and Δv are the differences between the cation, anion, and overlap energies for the compounds that make up the alloy. Finally, since the scattering is isotropic, the transport relaxation rate ν is just twice ν_1. The relaxation rate for the case of alloys with anion disorder (AB_xC_{1-x}) is obtained in a similar fashion and results in an energy parameter ΔE also given formally by Eq. (15).

III. RESULTS

In the last section an expression for the single-particle relaxation rate or inverse relaxation time due to alloy scattering was derived. The transport relaxation rate which results from the single-particle rate is

$$\nu = [x(1-x)2^{1/2}(m^*)^{3/2}E^{1/2}/n\pi\hbar^4](\Delta E)^2 , \tag{16}$$

where ΔE is defined in Eqs. (15b) and (15c). As is pointed out in Sec. II, the equations for cation and anion disordered alloys are identical. The formalism used in that section was based on the semiempirical tight-binding model of VHD. For this model, the upper signs in Eq. (15) are appropriate for the conduction band and the lower signs are appropriate for the valence band. Equation (16) is the scattering rate for a ternary alloy of two pure substances where x is the fraction of substance 1 and $1-x$ is the fraction of substance 2. For the conduction band, the relationship of the alloy parameters to those of VHD for III-V materials is

$$\begin{aligned} E_c &= xE_1(s,c) + (1-x)E_2(s,c) , \\ E_a &= xE_1(s,a) + (1-x)E_2(s,a) , \\ V &= xV_1(s,s) + (1-x)V_2(s,s) , \\ \Delta e_c &= E_1(s,c) - E_2(s,c) , \\ \Delta e_a &= E_1(s,a) - E_2(s,a) , \\ \Delta v &= V_1(s,s) - V_2(s,s) , \end{aligned} \tag{17}$$

where the E's and V's on the right-hand sides of the equations are tabulated in Table I of VHD. For the valence band, Eqs. (17) are appropriate if $E(s,c)$, $E(s,a)$, and $V(s,s)$ are replaced by $E(p,c)$, $E(p,a)$, and $V(x,x)$, respectively. Equation (16) is very similar to expressions derived by Brooks[5] and by Harrison and Hauser.[1,26] We believe that our Eq. (16) is somewhat more natural than the corresponding expressions derived by these workers, because with one-band diagonal disorder, ΔE would be the difference in the diagonal energies.

Before presenting numerical results, we shall discuss a number of points that are not particularly dependent on the VHD model. First we note that the equations for the relaxation rate for the conduction and valence bands, although formally identical, are unrelated from a numerical point of view because they depend on different input energies. This should not be too surprising because the wave functions and energies of the states in the two bands are very different. However, in an effective-mass picture where the scattering is due to an effective localized impurity potential, one would conclude that the energy parameter ΔE should be the same for the conduction and valence bands. The resolution of this paradox is simply that free-electron-like effective-mass theory is valid only over regions of a crystal containing many atomic cells. Therefore, it will work for the long-ranged Coulomb potential, but not for potentials whose length scale is of order atomic dimensions. Note also that while Eq. (16) contains the expected $x(1-x)$ dependence, an additional composition dependence is included in $(\Delta E)^2$. This point has been discussed recently[2] in the literature, and we only note here that this additional composition dependence vanishes only if two of the three disorder parameters Δe_c, Δe_a, and Δv vanish and that (see Table I), with the notable exception of the alloy $InAs_xSb_{1-x}$ the composition dependence of ΔE is very weak. It should also be pointed out that the effective mass m^* is also composition dependent.

The three terms in Eq. (15b) for ΔE are proportional to Δe_c, Δe_a, and Δv, corresponding to disorder in the cation, anion, and overlap energies. For a ternary alloy with cation disorder, $A_xB_{1-x}C$, these terms would thus correspond to diagonal, redistribution, and off-diagonal disorder, respectively. On the other hand, for a ternary alloy with anion disorder, AB_xC_{1-x}, these terms would correspond to redistribution, diagonal, and off-diagonal disorder, respectively. As can be seen from Eqs. (5) and (16), these three types of disorder do not contribute additatively to the relaxation rate. Instead, there exist interference terms between them that are a quantum-mechanical effect.

By using Table I and VHD with Eqs. (15) one can easily

TABLE I. List of ΔE for the conduction band at $x=0$ and 1 for 18 III-V ternary alloys. The last column denotes the largest contribution to ΔE where *d*, *o*, and *r* stand for diagonal, off-diagonal, and redistribution disorder, respectively. All energies are in eV.

Alloy	ΔE $(x=0)$	ΔE $(x=1)$	Largest term
$Ga_xIn_{1-x}Sb$	0.59	0.50	*o*
$Al_xI_{n1-x}Sb$	1.66	1.65	*d*
$Al_xGa_{1-x}Sb$	1.12	1.09	*d*
$Ga_xIn_{1-x}As$	1.18	1.06	*o*
$Al_xIn_{1-x}As$	2.64	2.57	*d*
$Al_xGa_{1-x}As$	1.44	1.49	*d*
$Ga_xIn_{1-x}P$	1.60	1.30	*o*
$Al_xIn_{1-x}P$	2.28	2.08	*o*
$Al_xGa_{1-x}P$	0.73	0.71	*d*
$InAs_xSb_{1-x}$	0.27	0.12	*r*
InP_xSb_{1-x}	1.29	1.06	*r*
InP_xAs_{1-x}	0.98	0.98	*r*
$GaAs_xSb_{1-x}$	0.84	0.70	*r*
GaP_xSb_{1-x}	2.14	2.06	*o*
GaP_xAs_{1-x}	1.34	1.32	*o*
$AlAs_xSb_{1-x}$	1.18	1.12	*o*
AlP_xSb_{1-x}	1.73	1.70	*o*
AlP_xAs_{1-x}	0.56	0.56	*o*

compute the energy parameters ΔE for a wide variety of substances. This parameter for the conduction band at $x=0$ and 1 is tabulated for 18 alloys in Table I of the present paper. The values of ΔE at intermediate values of x are reasonably well fit by a constant term and a term linear in x. In addition, Table I relates which of the three terms in Eq. (15b) is largest in magnitude, although rarely can one of the terms be said to dominate the other two. It should be noted from the table that, for the conduction band, typical values of the paramter ΔE are in the range $\simeq 0.5-2$ eV for all compositions and for all alloys considered here. Furthermore, we find that ΔE is positive in all such cases. A similar calculation for scattering in the valence band of these alloys yields results which are very different from those of the conduction band. In particular, we find that in this case, the values of ΔE at the end points $x=0$ and 1 are typically of the order of only a few milli-electron-volts and thus almost 3 orders of magnitude smaller than the corresponding quantities for the conduction band. We further find that the sign of ΔE changes between the end points and thus, at x near 0.5 $(0.4 \leq x \leq 0.6)$ this parameter and the relaxation rate vanishes for all 18 alloys considered here. The individual contributions from the three terms in Eq. (15b) are of the order of 100 meV in this case, and the resulting very small values of ΔE are due to an almost complete cancellation between the terms. As discussed in Sec. I, the values of the input energy parameters from VHD are uncertain to within about 0.1 eV. The vanishing of ΔE for the valence band near $x=0.5$ may thus be an artifact of the fitting procedure used by VHD. We feel, however, that our calculations are a step towards predicting the chemical trends or relative ordering of both the conduction- and valence-band scattering rates in the alloys considered. This view is consistent with that of previous calculations using the VHD parameters.[10-24]

We have also computed all of the energy parameters ΔE for the alloys in Table I using the universal model discussed by VHD. Within this model, the above-discussed cancellation for the valence band does not occur. Furthermore, with these universal model parameters we find ΔE's for the valence and conduction band differing by only about an order of magnitude, with typical values of the order of 0.1 eV for the valence band and of the order of 1 eV for the conduction band. The results for the conduction band in this case are not particularly well correlated with the results of Table I in their prediction of the relative ordering of the ΔE's for the alloys considered. Even within the universal model, however, different types of scattering dominate in different materials and the interference terms are often important.

We have also attempted to estimate the energy parameters ΔE from the band theory numbers computed by Chen and Sher[6] in their tight-binding model. Strictly speaking, their tight-binding parameters are not compatible with our formalism because of overlap and second- and third-neighbor effects which are included in them, but excluded in our theory. It is clear from our estimates, however, that redistribution and off-diagonal disorder effects and interference between the three types of disorder are still important with their numbers.

IV. SUMMARY AND CONCLUSIONS

In summary, using a nearest-neighbor Born-approximation formalism which takes into account the fluctuations of the alloy tight-binding energy parameters about the virtual-crystal approximation, we have derived a formula, Eq. (16), for the contribution of alloy scattering to the scattering rate in ternary semiconducting alloys. In our formalism, we have included the effects of diagonal, off-diagonal, and redistribution disorder in these parameters. We believe that we are the first to discuss redistribution disorder and the first to include off-diagonal and redistribution disorder in an alloy scattering formalism. The scattering rate we derive is expressible in terms of an energy ΔE, Eq. (15b), which we have numerically evaluated for both conduction-band and valence-band scattering in 18 III-V ternary semiconducting alloys using the semiempirical tight-binding parameters derived for the alloy constituent semiconductors by VHD.[7]

The explicit results of our calculations show the following: (1) for the parameters of VHD and for all 18 alloys, the energy parameter ΔE, and thus the scattering rate, is much greater for conduction-band than for valence-band scattering, (2) the composition dependence of this parameter is very weak, and (3) for compositions near $x=0.5$ this parameter vanishes for valence-band scattering. Since the VHD tight-binding energy parameters which we have input into our calculations have uncertainties of the order of 0.1 eV,[7] the absolute magnitudes of our numbers cannot be taken too seriously. However, even viewed on such a coarse scale, we believe that our predictions of the chemical trends or relative orderings in the alloy scattering rates should be valid for the alloys considered here.

The results of our calculations furthermore show that all three types of disorder—diagonal, off diagonal, and redistribution—can make important contributions to ΔE and thus to the scattering rate. Furthermore, there can be quantum-mechanical interference effects between these three types of disorder which can make the resulting scattering rate very small. We thus believe that any correct theory of alloy scattering in semiconducting alloys must necessarily include the effects of all three types of disorder.

ACKNOWLEDGMENTS

We are grateful for advice and many stimulating discussions with D. L. Rode, B. A. Shrauner, J. D. Dow, and O. F. Sankey. One of the authors (P.A.F.) thanks the U. S. Navy Office of Naval Research for their continuing support (Contract No. N0014-80C-0762). The other author (C.W.M.) thanks the National Science Foundation for partial support of this work through Grant. No. ECS-80-20322.

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