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David C. Look
Wright State University - Main Campus, david.look@wright.edu

D. K. Lorance

J. R. Sizelove

C. E. Stutz

K. R. Evans

See next page for additional authors

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Authors

David C. Look, D. K. Lorance, J. R. Sizelove, C. E. Stutz, K. R. Evans, and D. W. Whitson

Alloy scattering in p-type Al$_x$Ga$_{1-x}$As

D. C. Look
University Research Center, Wright State University, Dayton, Ohio 45435

D. K. Lorance,[a] J. R. Sizelove, C. E. Stutz, and K. R. Evans
Solid State Electronics Directorate, Wright Laboratory, WL/ELR, Wright-Patterson AFB, Ohio 45433

D. W. Whitson
Department of Physics, Indiana University of Pennsylvania, Indiana, Pennsylvania 15701

The hole mobility of Be-doped ($\sim 2 \times 10^{17}$ cm^{-3}) Al$_x$Ga$_{1-x}$As, for $x=0$–1, is analyzed both theoretically and experimentally. Alloy scattering is very important, and in fact reduces the hole mobility from 150 to less than 90 cm^2/V s at $x=0.5$. The main parameter in the alloy scattering formulation, the alloy potential E_{al}, is found to be about 0.5 eV for p-type Al$_x$Ga$_{1-x}$As.

I. INTRODUCTION

Hall-effect measurements constitute one of the most useful and effective ways to assess the quality of semiconductor materials, with the Hall mobility being a widely used figure of merit. Mobility data are especially useful when they can be compared with theory, allowing parameters such as impurity concentrations to be extracted. Such theory is well developed for simple systems that involve carriers in only a single, spherical band, such as for electrons in GaAs.[1] For holes in such semiconductors, on the other hand, the situation is usually much more complex because of degenerate valence bands.[2] A further complexity is added when alloys, such as Al$_x$Ga$_{1-x}$As, are considered because of electron or hole scattering from the alloy potential.[3-5] Alloy scattering is relatively weak for carriers with small effective masses, but can be strong for heavy carriers. Thus, it is very important to include alloy scattering when calculating hole mobilities in Al$_x$Ga$_{1-x}$As.[6-8] Such a calculation was carried out by Masu et al.[8] several years ago, and was compared with hole-mobility data in Be-doped Al$_x$Ga$_{1-x}$As. In this paper, we present a more accurate calculation, and also a more complete set of data, with x ranging from 0 to 1. Our fit of data and theory is excellent and an improved value of the alloy scattering potential is obtained.

II. SCATTERING RATES

The theory to be presented in this section has advantages over some of the previous works in that it explicitly takes into account band nonparabolicity, screening, and wave-function overlap, and also involves a numerical solution of the Boltzmann equation, rather than relying on the relaxation-time approximation or Matthiessen's rule. To derive most of the usual scattering rates, we basically follow the outline given in Nag's book.[1] From the scattering rates and Boltzmann's equation we can determine the light- and heavy-hole mobilities, and then weigh them in the proper manner to calculate the overall Hall coefficient.

The probability of an electron being scattered from wave vector k to k' is given by

$$S(\mathbf{k}) = \frac{V_c}{8\pi^3} \int \frac{2\pi}{\hbar} |M(\mathbf{k,k'})|^2 \delta(E_\mathbf{k} - E_{\mathbf{k'}}) d\mathbf{k'}, \qquad (1)$$

where V_c is the crystal volume and the material is assumed, for the moment, to be nondegenerate. The matrix element $M(\mathbf{k,k'})$ involves a perturbing potential ΔV and wave functions $U_\mathbf{k}$. For defect or impurity scattering, ΔV may be represented by a Fourier series

$$\Delta V = \sum_\mathbf{q} A(\mathbf{q}) \exp(i\mathbf{q}\cdot\mathbf{r}), \qquad (2)$$

whereas for lattice scattering

$$\Delta V = \sum_\mathbf{q} A(\mathbf{q}) [a_\mathbf{q} \exp(i\mathbf{q}\cdot\mathbf{r}) + a_\mathbf{q}^\dagger \exp(-i\mathbf{q}\cdot\mathbf{r})], \qquad (3)$$

where $\mathbf{q}$ is the lattice wave vector and $a_\mathbf{q}^\dagger$ and $a_\mathbf{q}$ are the usual creation and annihilation operators. The matrix element is then given by

$$M(\mathbf{k,k'})$$
$$= \int U_{\mathbf{k'}}^*(\mathbf{r}) e^{-i\mathbf{k'}\cdot\mathbf{r}} \Delta V U_\mathbf{k}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$$
$$= A(|\mathbf{k'}-\mathbf{k}|) I(\mathbf{k,k'}) \text{ for defect scattering}$$
$$= A(\mathbf{q})(n_\mathbf{q} + \tfrac{1}{2} \pm \tfrac{1}{2})^{1/2} I(\mathbf{k,k'}) \text{ for lattice scattering,} \qquad (4)$$

where $n_\mathbf{q}$ is the number of phonons of mode $\mathbf{q}$. The plus sign corresponds to the emission of a phonon, and the minus sign, absorption. Here $I(\mathbf{k,k'})$, the "overlap integral," is defined by

$$I(\mathbf{k,k'}) = \int U_{\mathbf{k'}}^*(\mathbf{r}) U_\mathbf{k}(\mathbf{r}) d\mathbf{r}, \qquad (5)$$

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[a] Present address: Corning, Inc., 310 N. College Rd., Wilmington, NC 28405.

where $U_k(r)$ is the cell-periodic part of the Bloch function. In the Kane k·p picture, the forms of $U_k(r)$ for the conduction band, light-hole band, or split-off band, are as follows:

$$U_{1k} = ia_k S\uparrow + (b_k/\sqrt{2})(X + iY)\downarrow + c_k Z\uparrow, \quad (6)$$

or

$$U_{2k} = ia_k S\downarrow + (b_k/\sqrt{2})(X - iY)\uparrow + c_k Z\downarrow, \quad (7)$$

and for the heavy-hole band,

$$U_{1k} = (1/\sqrt{2})(X + iY)\uparrow, \quad (8)$$

or

$$U_{2k} = (1/\sqrt{2})(X - iY)\downarrow. \quad (9)$$

An overlap function $G(k,k')$, which sums over the four possible combinations (1-1, 1-2, 2-1, 2-2) of the wave functions given in Eqs. (6)–(9) is defined as follows:

$$G(k,k') = \tfrac{1}{2} \sum_{i,j} |I_{ij}(k,k')|^2. \quad (10)$$

For electrons, whose wave functions are represented by Eqs. (6) or (7), a_k is near unity, and b_k and c_k near zero, except for nonparabolicity, which is small for nondegenerate GaAs. Thus, $G(k,k') \simeq 1$ for electrons, and this fact reduces the complexity of the scattering terms. For holes, the situation is not as simple, and the p-type basis set for the scattered wave vector $(X', Y', \text{and } Z')$ must be transformed into the basis set $(X, Y, \text{and } Z)$ of the initial wave vector, leading to complex functional dependences of the $|I_{ij}(k,k')|^2$ terms on k and Θ, the angle between k and k'. Fortunately, as shown by Wiley,[2] the overlap functions for GaAs are not strong functions of k, and can be well approximated by their values at $k=0$. In that case

$$G_{h\to h} = G_{l\to l} = (1 + 3\cos^2\Theta)/4, \quad (11)$$

$$G_{h\to l} = G_{l\to h} = 3(1 - \cos^2\Theta)/4, \quad (12)$$

and these are the values that we use.

Finally, we must take account of the fact that the free-carrier density can vary in the vicinity of potential discontinuities, and can act to screen the effects of the potential at large distances. This phenomenon can be roughly accounted for by modifying the Fourier coefficients as follows:

$$A(q) \to A(q)\frac{q^2}{q^2 + 1/\lambda^2}, \quad (13)$$

where the screening length λ is a function of the carrier concentration. For nondegenerate material

$$\frac{1}{\lambda^2} = \frac{e^2}{\epsilon kT}\{p + (p + N_D)[1 - (N_D + p)/N_A]\}, \quad (14)$$

where p is the total hole concentration. With these additions, we can now calculate the scattering rates for the important mechanisms.

A. Ionized-impurity scattering

The Coulombic scattering rate due to N_I ionized impurities of charge Ze is given by

$$S_{ii}(k) = \frac{N_I}{8\pi^3} \int \frac{2\pi}{\hbar} \frac{Z^2 e^4}{\epsilon^2}\left(\frac{1}{|k - k'|^2 + \lambda^{-2}}\right)^2$$
$$\times G(k,k')\delta(E_k - E_{k'})dk'. \quad (15)$$

By noting that

$$dk' = k'^2 \sin\Theta \, d\Theta \, d\phi \, dk' \quad (16)$$

and

$$\frac{\hbar^2 k^2}{2m^*} \simeq E(1 + \alpha E) \equiv \gamma(E), \quad (17)$$

where $\alpha \simeq 1/E_g$ for GaAs and similar compounds, Eq. (15) becomes

$$S_{ii}(k)$$

$$= \frac{Z^2 e^4 N_I m^*}{8\pi\epsilon^2\hbar^3} \frac{\gamma'(E_k)}{k^3} \int_{-1}^{1} \frac{G(y)}{(1 - y + k^{-2}\lambda^{-2}/2)^2} dy, \quad (18)$$

where $y \equiv \cos\Theta$ and $G(y) = G(\cos\Theta)$ is one of the overlap functions in Eqs. (11) and (12), depending on the initial and final hole bands. Also, m^* is the effective mass of the relevant band into which the holes are being scattered, and ϵ is the static dielectric constant. Note that if screening is neglected $(\lambda \to \infty)$, S_{ii} becomes infinite; thus, the inclusion of screening is absolutely necessary to properly deal with ionized-impurity scattering.

B. Piezoelectric scattering

The acoustic-mode lattice vibrations produce a potential due to the partial ionization of the atoms in crystals without inversion symmetry. By following an analysis similar to that outlined above, the piezoelectric-potential scattering rate is

$$S_{pz}(k) = \frac{e^2 h_{pz}^2 kT m^*}{2\pi\epsilon^2\hbar^3 \rho s^2} \frac{\gamma'(E_k)}{k}$$

$$\times \int_{-1}^{1} \frac{G(y)(1 - y)}{2(1 - y + k^{-2}\lambda^{-2}/2)^2} dy, \quad (19)$$

where ρ is the density, s the acoustic velocity, and h_{pz} the "piezoelectronic constant" which can be defined in terms of the elastic constants. As with the ionized-impurity case, free-carrier screening must be included to avoid an infinite $S_{pz}(k)$.

Equation (19) is often cast in different forms, which can be confusing. Sometimes the parameter e_{14} is used for h_{pz}. In other cases, the formulation is in terms of the piezoelectric stress tensor h_{ij} and the relationship here is $h_{14} = e_{14}/\epsilon = h_{pz}/\epsilon$. Finally, the piezoelectric coupling coefficient P is often used, where $P = h_{pz}/(\epsilon \rho s^2)^{1/2}$. The most commonly quoted[1] value of P is 0.052, which would give $|h_{pz}| = |e_{14}| = 0.211$ C/m^2. However, we have found that the value $|h_{pz}| = 0.136$ C/m^2 gives better temperature-dependent mobility fits to our data on high-purity samples. Adachi[9] quotes an $|e_{14}|$ value of 0.16 C/m^2 for GaAs, and 0.225 C/m^2 for AlAs. We will use our value of 0.136 C/m^2 for GaAs and linearly interpolate for Al$_x$Ga$_{1-x}$As to obtain 0.225 C/m^2 at the AlAs end point; i.e., $h_{pz} = 0.136 + 0.089x$.

C. Acoustic-mode deformation-potential scattering

The changes in lattice-atom positions due to acoustic-mode lattice vibrations produce a potential that scatters carriers. The scattering rate is

$$S_{ac}(\mathbf{k})$$

$$= \frac{E_1^2 kTm^*}{\pi \rho \hbar^3 s^2} \gamma'(E_k) k \int_{-1}^{1} \frac{G(y)(1-y)^2}{2(1 - y + k^{-2}\lambda^{-2}/2)^2} dy, \tag{20}$$

where E_1 is the deformation-potential constant, normally given in eV. The theoretical value for E_1 is about 5.6 eV, although our fitted value is higher, about 11.0 eV. For this scattering mechanism, screening is rather unimportant except at high carrier densities or low temperatures.

Masu et al.[8] fit their data with $E_1 = 7.0$ eV; however, their theory is much more approximate, and also, we believe the coefficient in front of their acoustic-scattering formula (Appendix, Ref. 8) is too small by a factor of 10. Adachi[7] quotes an "effective" acoustic-mode deformation potential as $E_{eff} = (6.7 - 1.2x)$ eV. One option would be to use this same relationship except scaled to 11.0 eV for GaAs: i.e., $E_1 = 11.0 - 1.8x$. However, we obtain a much better fit to the 296-K AlAs mobility ($x=1$) by letting $E_1 = 11.0 + 1.7x$. Note that this formula should not be employed for general use without a more critical evaluation.

D. Polar optical-mode scattering

The optical-mode lattice vibrations produce a polarization of the ionic charges on neighboring atoms, leading to dipole moments that can interact with the free holes. This is by far the most important scattering mechanism for electrons in GaAs at room temperature, and is also relatively strong for holes. The scattering rate is

$$S_{po}(\mathbf{k}) = \frac{e^2 m^* \omega_{po}}{4\pi \epsilon \hbar^2} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon} \right) \frac{1}{k^2} \left(\sum_{+,-} k_\pm \gamma'(E_k \pm \hbar\omega_{po})(n_{po} + \tfrac{1}{2} \pm \tfrac{1}{2}) \right.$$

$$\left. \times \int_{-1}^{1} \frac{G(y)[1 - 2(k_\pm/k)y + (k_\pm/k)^2]}{[1 - 2(k_\pm/k)y + (k_\pm/k)^2 + k^{-2}\lambda^{-2}]^2} dy \right), \tag{21}$$

where $n_{po} = 1/[\exp(\hbar\omega_{po}/kT) - 1]$ and ϵ_∞ is the high-frequency dielectric constant. Here, ω_{po}, the longitudinal optical phonon angular frequency, is assumed to be constant (weak dispersion). The equivalent temperature, $T_{po} = \hbar\omega_{po}/k$, is about 419 K in GaAs. The wave vectors $k_\pm$ correspond to energies $E \pm \hbar\omega_{po}$, respectively. In contrast with the acoustic-mode case, screening is important for polar optical-mode scattering. Note that for screening to be effective, we are implicitly assuming that the thermal hole velocity is larger than the velocity of the lattice waves, so that the holes can redistribute themselves in a short enough time.

A complication in Al$_x$Ga$_{1-x}$As is the presence of two types of optical phonon modes, one GaAs-like and the other, AlAs-like. As a simplification to the transport problem, we can define an "effective" phonon frequency, or temperature [Eqs. (16)–(17) in Adachi[9]]:

$$T_{po} = (1-x)T_{po}^{GaAs} + xT_{po}^{AlAs}$$

$$= 419 + 21.2x + 198x^2 - 59.2x^3.$$

This is equivalent to Adachi's Eq. (17) except that we have used 419 K for the first term, instead of 421 K.

E. Nonpolar optical-mode scattering

Besides the polarization mechanism, optical phonons may also produce a perturbing potential by deforming the lattice and locally changing the band gap. This mechanism is quite important for holes in GaAs near room temperature. The scattering rate is

$$S_{npo}(\mathbf{k}) = \frac{D_{npo}^2 m^*}{4\pi \rho \hbar^2 \omega_{npo}} \left(\sum_{+,-} k_\pm \gamma'(E_k \pm \hbar\omega_{npo})(n_{npo} + \tfrac{1}{2} \pm \tfrac{1}{2}) \int_{-1}^{1} \frac{G(y)[1 - 2(k_\pm/k)y + (k_\pm/k)^2]^2}{[1 - 2(k_\pm/k)y + (k_\pm/k)^2 + \lambda^{-2}k^{-2}]^2} dy \right), \tag{22}$$

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where D_{npo} is the appropriate deformation potential constant and $n_{npo} = 1/[\exp(\hbar\omega_{npo}/kT) - 1]$. Often D_{npo} is replaced by another term,

$$E_{npo} = (s/\omega_{npo})D_{npo} = (\hbar s/kT_{npo})D_{npo},$$

where E_{npo} has the units of energy. Theoretically, E_{npo} should be about double E_1 (see Sec. II C), and our data fitting is consistent with that relationship. As with acoustic-mode scattering, free-carrier screening is generally not an important factor except at high carrier densities or low temperatures.

Adachi,[9] following Wiley,[2] defines a phenomenological nonpolar optical deformation potential E_{npo} related to the optical deformation potential d_o. For d_o he gives an x variation of $d_o \simeq 41 + x$, and for E_{npo}, a constant value 5.9 eV. However, Brudevoll et al.[10] suggest that $E_{npo} \simeq 2E_1 \simeq 2(5.6) \simeq 11.2$ eV for GaAs. We find from temperature-dependent mobility fits of high-purity GaAs data that $E_1 \simeq 11.0$ eV and $E_{npo} \simeq 19.7$ eV. Thus, we will assume that $E_{npo} = 19.7$ eV for the whole range of x.

F. Alloy scattering

In a ternary alloy, consisting of binary components A(GaAs) and B(AlAs), the potential will change randomly if we assume that the two components are randomly distributed. Let the potential at an A site be V_A, and at a B site V_B; then the average potential will be $V = xV_A + (1 - x)V_B$ where x is the fraction of component A.[3] The potential discontinuity experienced by a hole at an A site is $V - V_A$, and at a B site, $V - V_B$. The scattering potential due to a particular A site at position $\mathbf{r}_A$ can be approximated by $\Delta V \simeq v_a(V - V_A)\delta(\mathbf{r} - \mathbf{r}_A)$, where v_a is the volume over which the scattering is effective. From a "hard-shell" point of view, v_a should simply be a cation volume, or $v_a \simeq 1/(N_a/2)$ where N_a is the atomic concentration (4.43×10^{22} cm^{-3} for GaAs). Then, from Eq. (2), the Fourier coefficient $A(\mathbf{q})$ can be written

$$A(\mathbf{q}) = \frac{1}{V_c} \int \Delta V e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r} = \frac{v_a}{V_c}(V - V_A)e^{-i\mathbf{q}\cdot\mathbf{r}_A}, \quad (23)$$

and from Eqs. (4)–(10), the squared matrix element for an A site is

$$|M_A(\mathbf{k},\mathbf{k}')|^2 = \frac{v_a^2}{V_c^2}(V - V_A)^2 G(\mathbf{k},\mathbf{k}'). \quad (24)$$

Noting that there are $(N_a V_c/2)x$ A sites and $(N_a V_c/2) \times (1 - x)$ B sites, the total matrix element should be

$$|M(\mathbf{k},\mathbf{k}')|^2 = \frac{v_a^2}{V_c^2}\frac{N_a V_c}{2}[x(V - V_A)^2$$

$$+ (1 - x)(V - V_B)^2]G(\mathbf{k},\mathbf{k}') \quad (25)$$

$$= \frac{v_a}{V_c}x(1 - x)(V_A - V_B)^2 G(\mathbf{k},\mathbf{k}'), \quad (26)$$

where we have made use of the fact that $v_a N_a/2 = 1$. From Eq. (1), the scattering rate can then be shown to be

$$S_{al}(\mathbf{k}) = \frac{v_a x(1 - x)(V_A - V_B)^2 m^*}{2\pi\hbar^3}\gamma'(E_k)k$$

$$\times \int_{-1}^{1} G(y)dy. \quad (27)$$

As a check, we see that for parabolic bands ($\gamma' = 1$; $k = \sqrt{2m^*E/\hbar^2}$), and s-like wave functions [$G(y) = 1$], we reproduce the standard formula for alloy scattering:

$$S_{al}(E) = \frac{2^{1/2}v_a x(1 - x)(V_A - V_B)^2 m^{*3/2}}{\pi\hbar^4}E^{1/2}. \quad (28)$$

(Note that the corresponding formula given in Nag's book is not quite correct because of his term N_0 instead of v_a.) The alloy mobility for parabolic bands and s-type wave functions is then

$$\mu_{al} = \frac{e\langle S_{al}^{-1}(E)\rangle}{m^*}$$

$$= \frac{e}{m^*}\frac{\int_0^\infty [E^{3/2}/S_{al}(E)]e^{-E/kT}dE}{\int_0^\infty E^{3/2}e^{-E/kT}dE}$$

$$= \frac{2^{3/2}\pi^{1/2}}{3}\frac{e\hbar^4}{v_a x(1 - x)(V_A - V_B)^2 m^{*5/2}(kT)^{1/2}}, \quad (29)$$

which is well known. However, for the p-type wave functions being considered here we will have to deal with the less restrictive formula, Eq. (27).

Note that we have not included the screening factor $[q^2/(q^2 + 1/\lambda^2)]$ in the alloy-scattering matrix elements. Indeed, this factor is non-negligible for the samples of this study which have $p \simeq 1 \times 10^{17}$ cm^{-3}, and thus $\lambda \simeq 135$ Å, at room temperature. However, the scattering centers in this case are only a few Å apart, on the average, so that the screened potentials overlap considerably. Another complication is the fact that the de Broglie wavelength (about 300 Å for carriers of energy 296 K) is much larger than the average distance between scattering centers. Thus, in reality, multiple scattering occurs. A more accurate treatment of alloy scattering should probably take account of the longer-range fluctuations in the average potential due to the inhomogeneous variations (clustering) of the cation concentrations. Interestingly enough, for electron scattering due to ionized impurities, Meyer and Bartoli[11] have shown that the relaxation time due to long-range fluctuations is roughly within a factor of 2 of that calculated by assuming that the ions scatter independently (the usual assumption). Therefore, we will proceed with our somewhat idealized alloy-scattering formalism (which is essentially equivalent to most of the other treatments in the literature) but will not attempt to ascribe too much meaning to the parameter $(V_A - V_B)^2$; i.e., we will view it simply as a fitting parameter.

III. TWO-BAND MODEL

The two hole bands are essentially treated as uncoupled except for allowing interband transitions in the deter-

mination of scattering rates. The Boltzmann equation is solved, by Rode's iterative technique, for each band separately. For interband scattering, the relevant mass in each scattering equation is taken to be that corresponding to the final band [the $d\mathbf{k}'$ in Eq. (1)]. This means, of course, that interband scattering will dominate for light holes, while intraband scattering will dominate for heavy holes. The overlap functions for intraband and interband scattering are given in Eqs. (11) and (12), respectively. The total hole concentration, $p = p_l + p_h$, is used for screening purposes.

The solutions to the Boltzmann equations for the two bands then give values of μ_l, μ_h, r_{sl}, and r_{sh}, where r_{sl} and r_{sh} are the values of the Hall r factors due to scattering alone. However, there are also contributions to the Hall r factors due to anisotropy; these have been found[2] to be $r_{Al} = 0.995$ and $r_{Ah} = 0.661$. The total r factors are $r_l = r_{sl} r_{Al}$ and $r_h = r_{sh} r_{Ah}$. Also, the hole concentrations in each band are approximately given by $p_h = p/[1 + (m_l/m_h)^{3/2}]$ and $p_l = p - p_h$. Then, the two-band conductivity σ, Hall coefficient R, and Hall r factor r, become[12]

$$\sigma = \sigma_l + \sigma_h = e(p_l \mu_l + p_h \mu_h), \tag{30}$$

$$R = \frac{\sigma_l^2 R_l + \sigma_h^2 R_h}{(\sigma_l + \sigma_h)^2} = \frac{r_l p_l \mu_l^2 + r_h p_h \mu_h^2}{e(p_l \mu_l + p_h \mu_h)^2}, \tag{31}$$

$$r = epR, \tag{32}$$

$$\mu_H = R\sigma. \tag{33}$$

IV. RESULTS

To begin with, we apply our model to undoped GaAs in order to obtain values of the acoustic deformation-potential constant E_1 [Eq. (20)], and the optical-phonon deformation potential E_{npo} [Eq. (20) and following]. Recently, Szafranek et al.[13] have carried out temperature-dependent Hall-effect measurements on a very pure p-type molecular-beam-epitaxial (MBE) GaAs layer, and found that $N_A = 6.5 \times 10^{13}$ cm^{-3} and $N_D = 2.5 \times 10^{12}$ cm^{-3}, uncorrected for Hall r factor. They also found that μ_H (77 K) $\simeq 10\,000$ cm^2/V s, which is close to or slightly higher than various values found by others for pure GaAs. The highest value for Hall mobility found at room temperature is usually about 450 cm^2/V s. Thus, to determine E_1 and E_{npo}, we have required the calculated Hall mobility μ_H [Eq. (33)] to be 450 cm^2/V s at 296 K, and 10 000 cm^2/V s at 77 K. The value of p at each temperature, needed for the screening parameter, was found from the usual statistical formula involving N_D and N_A; an acceptor activation energy of 0.025 eV (probably carbon) was assumed. Also, p is needed to determine the ionized impurity concentration N_I [Eq. (18)], since $N_I = 2N_D + p$ for a p-type sample. The results, which depend only weakly on p, N_D, and N_A, are shown in Fig. 1(a). The fitted parameters, $E_1 \simeq 11.0$ eV and $E_{npo} \simeq 19.7$ eV, are somewhat larger than those found by others.[2,8,10] For example, theoretical values are given as 5.6 eV for E_1, and about double that, or 11.2 eV for E_{npo}. Experimentally, Masu et al.[8] found that $E_1 \simeq 7$ eV and
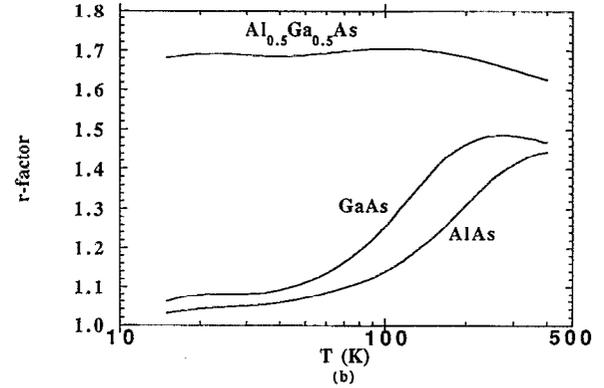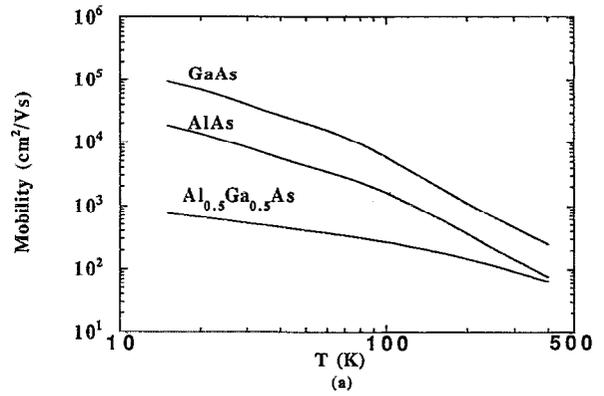

FIG. 1. (a) A comparison of the theoretical Hall mobilities for relatively pure p-type samples of GaAs, AlAs, and Al$_{0.5}$Ga$_{0.5}$As ($N_A = 6.5 \times 10^{13}$ cm^{-3}, $N_D = 2.5 \times 10^{12}$ cm^{-3}, and $E_A = 0.025$ eV, for each); (b) the Hall r factors for these same samples.

$E_{npo} \simeq 11.5$ eV. However, as mentioned earlier, we believe the prefactor in their formula for μ_{ac} (as evidently reproduced from Wiley[2]) may be a factor of 10 too small; this would give a larger fitted value of E_1. We believe our values for E_1 and E_{npo} may be somewhat more accurate than those measured by Masu et al. and others, because our theory is less approximate. However, it still must be remembered that E_1 and E_{npo} are simply fitting parameters in such analyses, and great care should be exercised in assigning theoretical significance to them. In any case, the alloy scattering parameter $|V_A - V_B| = E_{al}$ is not much affected by the choices of E_1 and E_{npo} since the mobility without alloy scattering is further fitted (by choice of N_I) to one of the samples at an end point (say $x=0$) anyway.

Also shown in Fig. 1(a) are the temperature dependencies of the theoretical hole mobilities for AlAs and Al$_{0.5}$Ga$_{0.5}$As, which are assumed for illustrative purposes to have the same values of N_A, N_D, and E_A as given for the GaAs case, while the other relevant parameters are taken from Table I. (It is known that E_A for carbon will vary somewhat with x but that effect has only a small impact on μ.) The effects of the alloy scattering are clearly seen here, and are especially strong at the lower temperatures. We have assumed $E_{al} = 0.53$ eV, as determined below. The Hall r factors are shown in Fig. 1(b), and it is apparent that the

TABLE I. Parameters used for the calculations in this paper

Symbol	GaAs	AlAs	$Al_xGa_{1-x}As$	Notes
ϵ(F/m)	$12.91\epsilon_0$[a]	$10.06\epsilon_0$[b]	$12.91 - 2.85x$	assume linear
ϵ_∞(F/m)	$10.91\epsilon_0$[a]	$8.16\epsilon_0$[b]	$10.91 - 2.75x$	assume linear
m_l/m_0	0.087[c]	0.150[b]	$0.087 + 0.063x$	assume linear
m_h/m_0	0.475[c]	0.760[b]	$0.475 + 0.285x$	assume linear
E_1 (eV)	11.0[d]	12.7[d]	$11.0 + 1.7x$	assume linear
E_{np0} (eV)	19.7[d]	...	19.7	assume equal, following Adachi[b]
ρ (kg/m^3)	5.31[a]	3.76[b]	$5.31 - 1.55x$	assume linear
s(m/s)	5.22[a]	...	$5.22 + 1.0x$	estimated from Fig. 7, Adachi[b]
$|h_{pz}|$ (C/m^2)	0.136[d]	0.225[b]	$0.136 + 0.089x$	assume linear
T_{p0} (K)	419[a]	...	$419 + 21.2x + 198x^2 - 59.2x^3$	approximately same as Eq. (17) of Adachi[b]

[a]Reference 1, and references therein.
[b]Reference 9, and references therein.
[c]H. C. Casey, Jr. and M. B. Panish, *Heterojunction Lasers* (Academic, New York, 1978), and references therein.
[d]Fitted from data in this laboratory (not to be accepted uncritically).

usual assumption of $r=1$ causes a significant error in the determination of p for these samples, except for the binary compounds below 100 K. Of course, the r factors will be different for doped materials, such as those presented below, but in that case they still range from about 1.3 to 1.5 as a function of x at room temperature. It is difficult to experimentally verify the μ vs T curves for AlAs and $Al_{0.5}Ga_{0.5}As$, because the background impurity levels are usually much higher than those assumed here. Since ionized impurities strongly affect μ at lower T, it is also more difficult to determine E_{al} from μ vs T data than from μ vs x data at room temperature.

The μ vs x results at 296 K are presented in Fig. 2. To increase statistical validity, three different $Al_xGa_{1-x}As$ sample groups (circles, squares, and triangles, respectively) grown at different times and in two different MBE systems (a Varian 360 and a Varian Gen II) were included in this study. In each case, the thickness was 2 μm, the substrate temperature 620 °C, and the doping level (Be),
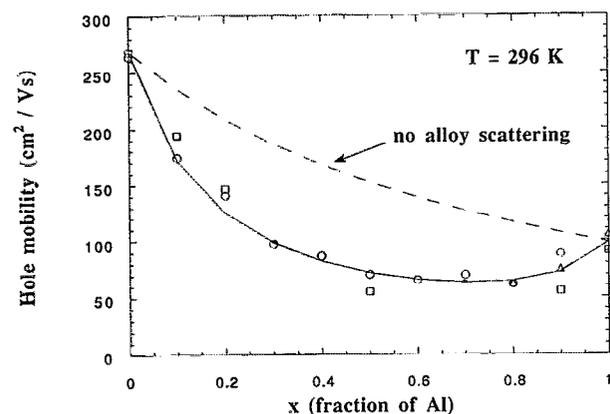

FIG. 2. The experimental (circles, squares, and triangles) and theoretical (solid line) Hall mobility as a function of x for p-type $Al_xGa_{1-x}As$. Also shown is the case of no alloy scattering (dashed line).

approximately 2.5×10^{17} cm^{-3}. The fitted N_D for $x=0$ (i.e., GaAs) was 1.5×10^{17} cm^{-3}. As seen in Fig. 2, the fit is excellent with the parameter $E_{al} = 0.53$ eV. Other parameters are given in Table I. This value of E_{al} should be compared to the value of 0.7 eV obtained by Masu et al.[8] Note that their raw μ vs x data are very similar to ours (within 15%: compare their Fig. 5 with our Fig. 2), so that we would have obtained an E_{al} quite close to our value of 0.53 eV had we fitted their data with our theory. The difference is not entirely in the much more approximate theoretical treatment which they employed, but also in their equation for μ_{al}, which differs from our Eq. (29) in the prefactor. (Theirs is $32\sqrt{2}/9\pi^{3/2} = 0.903$ whereas ours is $2^{3/2}\pi^{1/2}/3 = 1.671$.) Although we did not employ μ_{al} directly in our calculations, still it suggests that the scattering rate leading to their μ_{al} expression would also have been different. Furthermore, their use of Matthiessen's rule is questionable since the alloy scattering over much of the range of x is of similar magnitude to some of the other scattering mechanisms (e.g., see their Fig. 4). Under these circumstances, Matthiessen's rule is known to be inaccurate. However, it must again be remembered that both our E_{al} and that of Masu et al. are simply fitting parameters which are mainly useful for estimating the strength of the alloy scattering relative to the rest of the scattering. Although there should, of course, be a theoretical significance to E_{al}, we believe that the approximations leading to the scattering rate S_{al} [Eq. (27)], from which μ_{al} [Eq. (29)] is derived, seriously reduce the accuracy of E_{al}. For example, to speculate on whether E_{al} is more closely related to the band-gap difference (0.74 eV at 296 K), or the valence-band discontinuity (0.26 eV), seems highly questionable to us. However, the formalism we have offered here should be applicable to other III-V ternaries, and it should be possible to estimate the effects of alloy scattering in these systems by using reasonable values of E_{al}.

V. CONCLUSIONS

Alloy scattering is very important in p-type $Al_xGa_{1-x}As$, and can lower the hole mobility by close to a factor of 2, even in doped materials. We have presented a reasonably accurate formalism for calculating mobility in p-type, III-V semiconductors, and have applied it to relatively pure GaAs and to $Al_xGa_{1-x}As$ doped with about 2×10^{17} cm^{-3} Be. The alloy-scattering contribution is well described by an alloy potential term $E_{al} \simeq 0.53$ eV, which should be used when applying our formalism to other problems. Different values of E_{al} would in general be needed for other formalisms. From our results, it is clear that the analysis of electronic devices which depend on conduction in p-type $Al_xGa_{1-x}As$ will have to take alloy scattering into consideration.

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