Solution of the Boltzmann equation for calculating the Hall mobility in bulk GaN_xAs_{1-x}

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The ladder method for solving the linearized Boltzmann equation is developed to deal with a nonparabolic conduction band. This is applied to find the low field Hall mobility of electrons in bulk GaN_xAs_{1-x} using the band-anticrossing model, which predicts highly nonparabolic energy dispersion relations. Polar optical, acoustic phonon, piezoelectric, ionized impurity, neutral impurity, and nitrogen scattering are incorporated. In finding an exact solution to the linearized Boltzmann equation, we avoid the unrealistic assumption of a relaxation time for inelastic scattering via polar optical phonons. Nitrogen scattering is found to limit the electron mobility to values of the order 1000 $cm^2 V^{-1} s^{-1}$, in accordance with relaxation time approximation calculations but still an order of magnitude higher than measured values for dilute nitrides. We conclude that the nonparabolicity of the conduction band alone cannot account for these low mobilities.

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I. INTRODUCTION

In recent years, there has been growing interest in the use of dilute nitrides for optoelectronic applications. Since the early 1990s, fabrication techniques have been developed[1–3] that allow the incorporation of nitrogen in dilute concentrations into III-V semiconductors. This leads to a large reduction of the energy gap with N content,[4] making the dilute nitrides attractive candidate materials for long wavelength vertical cavity surface emitting lasers (VCSELS) for telecommunications[5] and efficient solar cells operating in the infrared.[6]

Although considerable attention has been given to theoretical models of the band-structure in dilute nitrides,[7–10] until recently there has been very little development in the theory of carrier transport.[11,12] Studies that have been carried out[11] suggest that there may be intrinsic limits on electron mobility, which will be an important consideration for device applications. These calculations, however, have only addressed nitrogen scattering in isolation, based on a relaxation time approximation for the mobility. The effect of the high degree of nonparabolicity in the energy dispersion relations predicted by the band-anticrossing (BAC) model[10] has not been addressed. Furthermore, the incorporation of polar optical scattering, which limits the room temperature mobility in most semiconductors, cannot be treated using a relaxation time approximation due to the highly inelastic nature of the interaction. Hence we have developed the ladder method[13,14] for solving the Boltzmann equation to deal with a nonparabolic, spherical conduction band. Using the BAC model to calculate the modified effective mass and density of states, we have calculated the low field Hall mobilities for bulk GaN_xAs_{1-x}.

II. THE LADDER METHOD

In the absence of any temperature gradient, the steady state Boltzmann equation governing the dynamics of the electron distribution function $f(\mathbf{k})$ for a driving force $\mathbf{F}$ is[15]

$$\frac{\mathbf{F}}{\hbar} \cdot \nabla_{\mathbf{k}} f(\mathbf{k}) = \left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_{scat}. \tag{1}$$

The right-hand side of Eq. (1) is the temporal rate of change of $f(\mathbf{k})$ due to scattering and can be written

$$\left(\frac{\partial f(\mathbf{k})}{\partial t} \right)_{scat} = \int s(\mathbf{k}',\mathbf{k}) f(\mathbf{k}')[1 - f(\mathbf{k})] - s(\mathbf{k},\mathbf{k}') f(\mathbf{k})[1 - f(\mathbf{k}')] d^3\mathbf{k}', \tag{2}$$

where $s(\mathbf{k}',\mathbf{k})$ and $s(\mathbf{k},\mathbf{k}')$ are the intrinsic scattering rates from $\mathbf{k}'$ to $\mathbf{k}$ and vice versa. If Eqs. (1) and (2) can be solved for $f(\mathbf{k})$ when $\mathbf{F}$ includes the magnetic field, then the Hall mobility can be calculated from the components of the conductivity tensor σ_{ij} found from

$$\sigma \mathbf{E} = \frac{e}{4\pi^3} \int \mathbf{v}(\mathbf{k}) f(\mathbf{k}) d^3\mathbf{k}, \tag{3}$$

where $\mathbf{E}$ is the electric field, e is the electronic charge, and $\mathbf{v}$ is the electron group velocity.

To find an exact solution of the Boltzmann equation, we must linearize the problem. Here, we follow the lead of Fletcher and Butcher.[14] Assuming a vanishingly small electric field $\mathbf{E}$, we expand $f(\mathbf{k})$ to first order about the equilibrium distribution $f_0(E)$ (E is energy), putting

$$f(\mathbf{k}) = f_0(E) + f_1(E) = f_0(E) - \frac{\partial f_0(E)}{\partial E} \mathbf{\Phi}(E) \cdot \mathbf{E}, \tag{4}$$

where the vector $\mathbf{\Phi}(E)$ is given by

$$\mathbf{\Phi}(E) = -e\{\tau_1(E)\mathbf{v}_t + \tau_2(E)(\hat{\mathbf{z}} \times \mathbf{v}_t) + \tau_3(E)\mathbf{v}_z\} \tag{5}$$

$\mathbf{v}_t = (v_x, v_y, 0)$, $\mathbf{v}_z = (0,0,v_z)$, and the $\tau_i(E)$ are effective relaxation times. The nonparabolicity of the energy bands is incorporated by defining the dispersion relations in terms of an as unyet specified function $\gamma(E)$

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$$\gamma(E) \equiv \frac{\hbar^2|\mathbf{k}|^2}{2m^*} \quad (6)$$

so that the group velocity is now given by

$$\mathbf{v} = \frac{dE}{d\gamma}\frac{\hbar\mathbf{k}}{m^*} \quad (7)$$

and the density of (single spin) states is

$$N(E) \equiv \frac{(2m^*)^{3/2}\gamma^{1/2}(E)}{4\pi^2\hbar^3}\frac{d\gamma(E)}{dE}. \quad (8)$$

Taking the driving force $\mathbf{F}$ to be given by

$$\mathbf{F} = -e(\mathbf{E} + \mathbf{v}\times\mathbf{B}) \quad (9)$$

with the magnetic field $\mathbf{B}$ taken to be in the z direction, we arrive, after some algebraic manipulation, at the set of equations

$$L(\tau_1(E)) = 1 + \frac{dE}{d\gamma}\frac{eB}{m^*}\tau_2(E),$$

$$L(\tau_2(E)) = -\frac{dE}{d\gamma}\frac{eB}{m^*}\tau_1(E),$$

$$L(\tau_3(E)) = 1, \quad (10)$$

where

$$L(\tau_i(E)) = \int s(\mathbf{k}',\mathbf{k})\frac{f_0(E')}{f_0(E)}\left(\tau_i(E) - \tau_i(E')\frac{v'}{v}\cos\alpha\right)d^3\mathbf{k}' \quad (11)$$

and α is the angle between $\mathbf{v}$ and $\mathbf{v}'$. For elastic processes, the τ_i emerge from Eq. (11) as simple momentum relaxation times. The situation changes for the inelastic process of scattering by optical phonons. We consider, for simplicity, the case where there is just one optical mode with energy $\hbar\omega$. We can put

$$s(\mathbf{k}',\mathbf{k}) = s_A\delta(E' - E - \hbar\omega) + s_E\delta(E' - E + \hbar\omega), \quad (12)$$

where s_A and s_E are the intrinsic scattering rates for absorption and emission, respectively. When Eq. (12) is inserted into Eq. (11), the effect of the delta functions is to introduce values of the τ_i at energies $E-\hbar\omega$, E, and $E+\hbar\omega$, which can then be taken outside the integrals. The result is an expression of the form

$$L(\tau_i(E)) = A(E)\tau_i(E - \hbar\omega) + B(E)\tau_i(E) + C(E)\tau_i(E + \hbar\omega) \quad (13)$$

where

$$A(E) = -\theta(E - \hbar\omega)\int s_E\frac{f_o(E')}{f_0(E)}\frac{v'}{v}\cos\alpha\,\delta(E' - E + \hbar\omega)d^3\mathbf{k}',$$

$$B(E) = \int s_A\frac{f_o(E')}{f_0(E)}\delta(E' - E - \hbar\omega)d^3\mathbf{k}' + \theta(E - \hbar\omega)\int s_E\frac{f_o(E')}{f_0(E)}\delta(E' - E + \hbar\omega)d^3\mathbf{k}'$$

$$C(E) = -\int s_A\frac{f_o(E')}{f_0(E)}\frac{v'}{v}\cos\alpha\,\delta(E' - E - \hbar\omega)d^3\mathbf{k}'. \quad (14)$$

Here, we have introduced the step function

$$\theta(E) = \begin{cases} 0, & E \leqslant 0 \\ 1, & E > 0 \end{cases} \quad (15)$$

since there can be no phonon emission when the electron energy $E<\hbar\omega$. We can start to see here how the scattering rate at any particular energy E is correlated with the rates at $E\pm\hbar\omega$. This suggests the picture of a phonon energy "ladder" with rungs $\hbar\omega$ apart. We can make this more explicit by writing the energy as ε, where $0\leqslant\varepsilon<\hbar\omega$, and rewriting Eq. (10) as a system of linear equations in terms of $E=\varepsilon+n\hbar\omega$.

To find τ_i at a particular level E, we need to solve for all the values of τ_i separated by integral multiples of $\hbar\omega$. In practice, we may only solve for a finite number of rungs, which we may do by using a matrix inversion technique. In order to minimize any truncation error incurred from only solving for a finite number of rungs, it is assumed that as $n\to\infty$, $\tau_i(E+n\hbar\omega)\to\tau_i(E+[n+1]\hbar\omega)$. Hence for the last rung N, we put

$$B(E + N\hbar\omega) \to B(E + N\hbar\omega) + C(E + N\hbar\omega). \quad (16)$$

It remains to solve the integrals in Eq. (14) when the forms of the scattering rates for s_A and s_E are inserted. The exact expressions can be found in, for instance, Ridley (Ref. 15). Our principle concern here is that these expressions introduce a factor $1/q^2$, where $q=|\mathbf{k}-\mathbf{k}'|$ is the magnitude of the phonon wave vector. To deal with this, we expand $1/q^2$ in terms of Legendre polynomials P_n

$$\frac{1}{q^2} = \frac{1}{2k'k}\sum_{n=0}^{\infty}(2n+1)Q_n(K)P_n(\cos\alpha),$$

$$K = \frac{k'^2 + k^2}{2k'k}, \quad (17)$$

where the Q_n are Legendre functions of the second kind. After performing the angular integrations, we can turn the remaining integration over k into an integration over E using Eqs. (6) and (8). The final result gives us

$$A(E) = -\theta(E - \hbar\omega)I^2(\mathbf{k}',\mathbf{k})W_0(\hbar\omega)^{1/2}n(\omega) \times\frac{f_0(E - \hbar\omega)}{f_0(E)}\frac{d\gamma(E)}{dE}\frac{\gamma^{1/2}(E - \hbar\omega)}{\gamma(E)} \times\left\{\frac{\gamma(E - \hbar\omega) + \gamma(E)}{2\gamma^{1/2}(E - \hbar\omega)\gamma^{1/2}(E)}\tanh^{-1}\left(\frac{\gamma(E - \hbar\omega)}{\gamma(E)}\right)^{1/2} - \frac{1}{2}\right\},$$

$$B(E)=I^2(\mathbf{k}',\mathbf{k})W_0\left(\frac{\hbar\omega}{\gamma(E)}\right)^{1/2}\left[\theta(E-\hbar\omega)n(\omega)\frac{f_0(E-\hbar\omega)}{f_0(E)}\times\tanh^{-1}\left(\frac{\gamma(E-\hbar\omega)}{\gamma(E)}\right)^{1/2}\frac{d\gamma(E-\hbar\omega)}{dE}+\{n(\omega)+1\}\times\frac{f_0(E+\hbar\omega)}{f_0(E)}\coth^{-1}\left(\frac{\gamma(E+\hbar\omega)}{\gamma(E)}\right)^{1/2}\frac{d\gamma(E+\hbar\omega)}{dE}\right], \quad (18)$$

$$C(E)=-I^2(\mathbf{k}',\mathbf{k})W_0(\hbar\omega)^{1/2}\{n(\omega)+1\}\times\frac{f_0(E+\hbar\omega)}{f_0(E)}\frac{d\gamma(E)}{dE}\frac{\gamma^{1/2}(E+\hbar\omega)}{\gamma(E)}\times\left\{\frac{\gamma(E+\hbar\omega)+\gamma(E)}{2\gamma^{1/2}(E+\hbar\omega)\gamma^{1/2}(E)}\times\coth^{-1}\left(\frac{\gamma(E+\hbar\omega)}{\gamma(E)}\right)^{1/2}-\frac{1}{2}\right\},$$

where

$$W_0=\frac{e^2}{4\pi\hbar\varepsilon_0}\left(\frac{2m^*\omega}{\hbar}\right)^{1/2}\left(\frac{1}{\kappa_\infty}-\frac{1}{\kappa_0}\right), \quad (19)$$

ε_0 is the permittivity of free space and κ_∞ and κ_0 are the high and low frequency dielectric constants, respectively. The factor $I^2(\mathbf{k}',\mathbf{k})$ represents the overlap integral of the wave functions of the initial and scattered states over the unit cell and is of order unity.

III. THE BAC MODEL

The ladder method can now be applied to calculate Hall mobilities in GaNAs. According to the BAC model, the presence of localized nitrogen impurity levels strongly affects both the effective mass and the density of states. These relations can be found from the secular equation describing the splitting of the conduction band[10]

$$\begin{vmatrix} E-E_M & \beta x^{1/2} \\ \beta x^{1/2} & E-E_N \end{vmatrix}=0, \quad (20)$$

where E_M and E_N are the energies of the unperturbed matrix semiconductor states and the nitrogen impurities and x is the nitrogen concentration. Assuming E_M is parabolic in the electron wave vector k, we can put

$$E_M=E_c+\frac{\hbar^2k^2}{2m_M^*}, \quad (21)$$

where E_c and $m_M{}^*$ are the conduction band edge and effective mass of the matrix semiconductor, respectively. E_c is also taken to have an x dependence[16]

$$E_c=E_{c0}-\alpha x \quad (22)$$

and a temperature dependence given by the Varshni relation

$$E_{c0}=E_0-\frac{aT^2}{(b+T)}. \quad (23)$$

Using Eqs. (20) and (21) we can put

$$\frac{\hbar^2k^2}{2m_M^*}=\frac{\beta^2x}{E_N-E}+E-E_c\equiv\gamma(E) \quad (24)$$

and hence obtain for the density of states $N(E)$[17]

$$N(E)dE=\frac{(2m_M^*)^{3/2}}{4\pi^2\hbar^3}\gamma^{1/2}(E)\frac{d\gamma(E)}{dE}dE=\frac{(2m_M^*)^{3/2}}{4\pi^2\hbar^3}\left(\frac{\beta^2x}{E_N-E}+E-E_c\right)^{1/2}\left(\frac{\beta^2x}{(E_N-E)^2}+1\right). \quad (25)$$

Note that it is more usual to give $\gamma(E)$ in terms of the energy relative to the conduction band edge $E_{\mathrm{CBE}}(x)$. Putting $E'=E-E_{\mathrm{CBE}}(x)$, we can rewrite Eq. (24) as

$$\gamma(E')\equiv\frac{\Delta E_c(x)}{\Delta E_N(x)}\frac{E'}{1-E'/\Delta E_N}+E', \quad (26)$$

where ΔE_c is the shift in the conduction band edge $E_c-E_{\mathrm{CBE}}(x)$ and $\Delta E_N=E_N-E_{\mathrm{CBE}}(x)$.

For a spherical energy band, the effective mass in the perturbed energy bands is given by

$$\frac{1}{m_\pm^*}=\frac{1}{m_M^*}\left(\frac{dE_\pm}{d\gamma}+2\gamma(E_\pm)\frac{d^2E_\pm}{d\gamma^2}\right)=\frac{1}{2m_M^*}[1\pm(E_N-E_M)G(E)]\pm\frac{\gamma(E)}{m_M^*}\times[(E_N-E_M)^2G^2(E)-1]G(E), \quad (27)$$

where

$$G(E)\equiv\{(E_N-E_M)^2+4\beta^2x\}^{-1/2}. \quad (28)$$

Note that the second term in Eq. (27) is actually proportional to $1/m_M{}^{*2}$, since $\gamma(E)$ contains a factor of $1/m_M{}^*$. Close to $k=0$, Eq. (27) reduces to[18]

$$\frac{1}{m_\pm^*}=\frac{1}{2m_M^*}[1\pm(E_N-E_M)G(E)] \quad (29)$$

or

$$m_\pm^*=m_M^*\frac{d\gamma(E_\pm)}{dE_\pm} \quad (30)$$

IV. ELASTIC SCATTERING PROCESSES

Polar optical scattering has already been incorporated into the ladder method via Eqs. (18). Under the assumption that the different scattering processes are independent, it is straightforward to extend the method to deal with additional elastic processes by simply adding the rates to $B(E)$ in Eq. (13). Here, we further include acoustic phonon, piezoelectric, ionized impurity, neutral impurity, and nitrogen scattering. The following formulas for the scattering rates have been derived quite generally, although a possible ambiguity arises in the case of dilute nitrides since we have been discussing two effective masses: that of the unperturbed matrix semi-

conductor m^*_M and the mass associated with the perturbed energy bands $m^*_\pm$. Using the definition of $\gamma(E)$ in Eq. (24), the effective masses given below should be taken to be those of the *matrix* semiconductor m^*_M.

The rates for acoustic phonon and piezoelectric scattering are derived from the intrinsic scattering rates given in Ridley;[15] the rate for ionized impurity scattering is based on the Brooks-Herring approach;[19] neutral impurity scattering on the Erginsoy formula,[20] and nitrogen scattering on the scattering matrix due to Fahy.[11]

A. Acoustic phonon scattering

$$w_{ac}(E) = 2\pi \frac{\Xi_d^2 k_B T}{\hbar c_L} I^2(\mathbf{k}', \mathbf{k}) N(E), \tag{31}$$

where Ξ_d is the deformation potential for pure dilation and c_L is the average elastic constant for longitudinal modes, given in terms of the components of the elastic stiffness constants c_{ij} by

$$c_L = c_{11} + \frac{2}{5}(c_{12} + 2c_{44} - c_{11}). \tag{32}$$

B. Piezoelectric scattering

$$w_{pe} = \frac{\pi e^2 K_{av}^2 \hbar\, k_B T}{2\varepsilon m^*} \frac{N(E)}{\gamma(E)} I^2(\mathbf{k}', \mathbf{k}) H(E), \tag{33}$$

where

$$H(E) = 1 - \frac{\hbar^2 q_0^2}{4m^* \gamma(E)} \log\left[\frac{8m^* \gamma(E)}{\hbar^2 q_0^2} + 1\right] + \frac{1}{8m^* \gamma(E)/\hbar^2 q_0^2 + 1}. \tag{34}$$

q_0 is the reciprocal Debye screening length and $\varepsilon = \kappa_0 \varepsilon_0$. K_{av}^2 is an average electromechanical coupling coefficient given in terms of the piezoelectric coefficient e_{14} and the average longitudinal and transverse elastic constants c_L and c_T by

$$K_{av}^2 = \frac{e_{14}^2}{\varepsilon}\left(\frac{12}{35c_L} + \frac{16}{35c_T}\right) \tag{35}$$

and

$$c_T = c_{44} - \frac{1}{5}(c_{12} + 2c_{44} - c_{11}). \tag{36}$$

C. Ionized impurity scattering

$$w_{ii} = \frac{\pi Z^2 e^4 N_{II} \hbar^3}{16\varepsilon^2 m^{*2} \gamma^2(E)} N(E) \left\{ \log\left[\frac{8m^* \gamma(E)}{\hbar^2 q_0^2} + 1\right] - \frac{1}{1 + \hbar^2 q_0^2 / 8m^* \gamma(E)} \right\}, \tag{37}$$

where Z is the ionization number (taken to be unity) and N_{II} is the number density of ionized impurities. From the hydrogenic impurity model, the donor ionization energy used to calculate N_{II} is given by

$$E_d(x) = \left.\frac{d\gamma}{dE}\right|_{k=0} E_d(\text{GaAs}) \tag{38}$$

(the acceptor impurities are all assumed to be occupied).

D. Neutral impurity scattering

$$w_{ni} = \frac{80\pi\varepsilon\hbar^3 N_{NI}}{e^2 (m^* d\gamma/dE)^2}, \tag{39}$$

where N_{NI} is the number density of neutral impurities.

E. Nitrogen scattering

For nitrogen scattering, we use the form of the scattering matrix derived by Fahy and O'Reilly[11]

$$\langle \psi_0 | \Delta U | \phi_0 \rangle = \frac{1}{V} \frac{dE_c}{dN_I}, \tag{40}$$

where ΔU is the perturbing potential, ψ_0 is the exact electron eigenstate, ϕ_0 is the eigenstate in the absence of the impurity, and E_c is the conduction band edge energy. The scattering rate is given by

$$w_N = N_I V \frac{2\pi}{\hbar} \int |\langle \psi_0 | \Delta U | \phi_0 \rangle|^2 (1 - \cos\alpha) \delta(E' - E) \frac{V}{8\pi^3} d^3\mathbf{k}' = \frac{\pi x a_0^3}{2\hbar}\left(\frac{dE_c}{dx}\right)^2 N(E), \tag{41}$$

where we have used $N_I = 4x/a_0^3$, for N concentration x and lattice constant a_0. Note that Eq. (41) is only valid for one type of N environment and would need to be modified to account for N—N pairs or H passivated sites.[12] For the E_- subband in the BAC model we have

$$\frac{dE_-}{dx} = -\frac{1}{2}\{\alpha + [\alpha(E_N - E_M) + 2\beta^2] G(E)\}. \tag{42}$$

V. RESULTS

For the temperature dependent calculations of the Hall mobility, the Fermi energy at each temperature was first calculated via the charge neutrality condition. Hence for given donor/acceptor concentrations, the ionized and neutral impurity concentrations were calculated. The parameters used in the calculations are listed in Table I (E_0 and E_N are given relative to the top of the valence band) and the overlap integral $I^2(\mathbf{k}', \mathbf{k})$ is taken to be unity. We assume n-type compensated GaNAs with a donor concentration of $N_D = 10^{17}\ \text{cm}^{-3}$ and $N_A/N_D = 0.5$.

A possible problem emerges here using the modified density of states in calculating the free carrier concentration. Due to the $1/(E_N - E)^2$ term, the integral of Eq. (25) does not converge near the nitrogen level. To examine the consequences of this, we assumed a Lorentzian broadening of the nitrogen level, chosen so that the integral of this density of

TABLE I. Parameters used in Hall mobility calculations.

Parameter	Value	Units	Source (Reference)
E_0	1.519	eV	25
a	5.405×10^{-4}	eV K^{-1}	25
b	204	K	25
E_N	1.65	eV	11
α	−1.45	eV	11
β	2.45	eV	11
m^*_M/m_0	0.067		14
a_0	5.65325	Å	25
ω	53.7	THz	14
κ_0	12.53		14
κ_∞	10.82		14
Ξ_d	7.0	eV	14
c_{11}	1.188×10^{-11}	Nm^{-2}	14
c_{12}	5.38×10^{-10}	Nm^{-2}	14
c_{44}	5.94×10^{-10}	Nm^{-2}	14
e_{14}	−0.16	Cm^{-2}	14
B	0.5	T	

states equaled the integral of the parabolic density of states plus the number of nitrogen states per unit volume. We found that for the temperature ranges we were considering (5–500 K), there was no significant difference in the calculated Fermi level from that calculated using the parabolic approximation.

Figure 1 shows the calculated relaxation times at 300 K. Shown here are the $\tau_3(E)$, which are independent of the magnetic field. The discontinuities at energy separations of the phonon energy are a characteristic feature of the ladder method. In general, the scattering rates at an energy E are correlated to the rates at energies $E\pm\hbar\omega$. However, for $E<\hbar\omega$ there is no possibility of phonon emission, so the rate

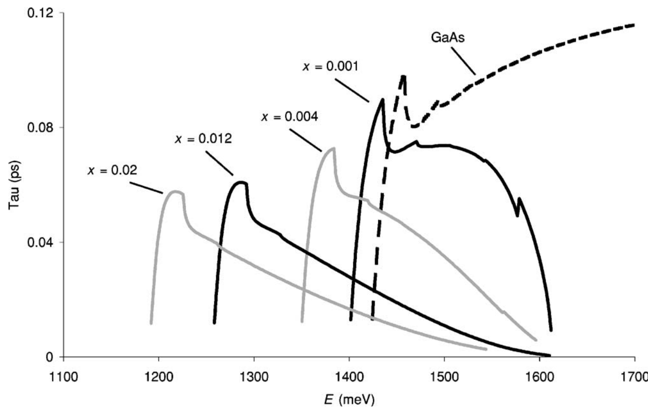

FIG. 1. Relaxation times (τ_3) for all scattering processes at different nitrogen concentrations. The jagged edges to these curves are due to the ladder nature of polar optical scattering. Note that the relaxation times all tend to zero near the nitrogen level. Also shown for comparison is the relaxation time for GaAs with the same donor and acceptor doping.

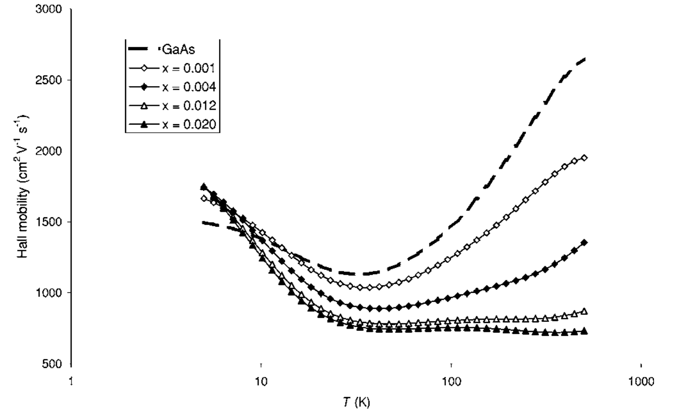

FIG. 2. Hall mobility for GaN_xAs_{1-x} for different nitrogen concentrations. In each case, the donor concentration is $N_D=10^{-17}$ cm^{-3} and the compensation ratio is $N_A/N_D=0.5$. The mobility for GaAs is shown for comparison (dashed line).

changes discontinuously at $E=\hbar\omega$ with the effect being propagated further up the ladder. The most obvious effect of the nonparabolicity is the tendency of the relaxation times towards zero near the nitrogen energy, where the electron becomes immobile.

In Fig. 2 we show the temperature dependence of the calculated Hall mobility for various nitrogen concentrations. At this level of doping, neutral and ionized impurity scattering tend to be dominant at low temperatures, with the mobility only curving over at high temperature (characteristic of polar optical limited transport) for low values of x. For $x>0.004$, the high temperature mobility becomes limited by nitrogen scattering.

The contributions of the individual processes are illustrated in Fig. 3 for $x=0.02$. At this nitrogen concentration, nitrogen scattering pins the high temperature mobility to around 720 cm^{-2} V^{-1} s^{-1}.

In Fig. 4, we show the x dependence of the mobility at 300 K and compare this to the relaxation time approximation due to Fahy and O'Reilly.[11] We see that for nitrogen scattering alone, there is little difference in the predicted mobility.

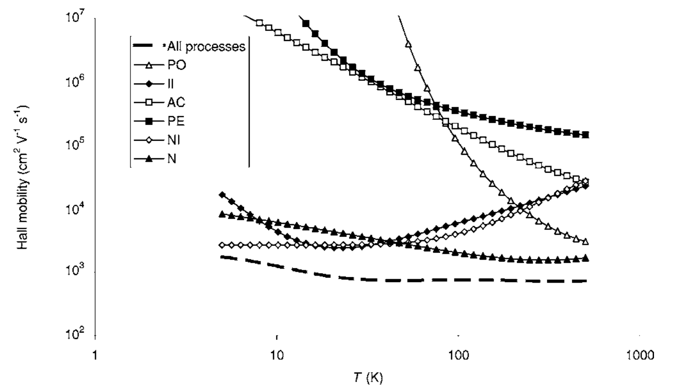

FIG. 3. The components of the mobility due to separate processes for a nitrogen concentration of $x=0.02$. Note that at low temperature, neutral impurity scattering dominates, while above about 40 K scattering from nitrogen centers is the dominant mechanism limiting the mobility.

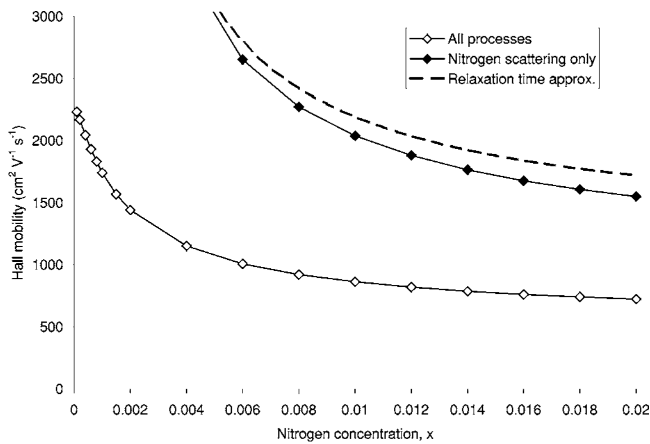

FIG. 4. Hall mobility at 300 K as a function of nitrogen concentration. Shown for comparison is the relaxation time approximation for nitrogen scattering alone due to Fahy and O'Reilly (Ref. 11).

VI. CONCLUSIONS

Despite the large reduction in mobility compared to GaAs, these results are still about an order of magnitude larger than many of the experimental determinations of the Hall mobility in compensated GaInNAs,[21,22] although electron mobilities of up to $2000\,\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$ have been reported.[23] Moreover, the results found here are of the same order of magnitude as the studies based on the relaxation time approximation for nitrogen scattering. This implies that the nonparabolicity of the conduction band predicted by the BAC model cannot on its own explain the very low mobilities observed in dilute nitrides.

It has been pointed out by Fahy and O'Reilly[24] that the scattering term in Eq. (41) $(dE_-/dx)^2$ may be inadequate as it stands to model the affect of nitrogen impurity states since it only applies to isolated N sites. In reality, there will be other types of nitrogen environments such as N-N pairs distributed at random throughout the crystal lattice. These environments introduce new resonant levels close to the conduction band edge. Consequently $(dE_-/dx)^2$ must be replaced by the sum of squares of derivatives[12] for each N environment, which will naturally increase the scattering rate.

This, of course, raises questions about the validity of the BAC model, which is based on a single N state mixing with the matrix semiconductor conduction band states. Some modification of the band structure, and hence expressions for the effective mass and density of states, may be required. As already pointed out, the density of states given in Eq. (25) is problematic due to the singularity at $E=E_N$. Essentially, however, this is an artifact of assuming spherical energy bands—an approximation that must break down as **k** approaches the edge of the Brillouin zone—and in our calculations has not proved too problematic since the electron population is limited to low energies in the Γ valley.

While these problems must be addressed, it is clear that the introduction of N into III-V semiconductors has a serious effect on the mobility. These calculations suggest that for $x > 0.001$, upper limits of $1000-2000\,\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{s}^{-1}$ may be imposed.

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