Electron mobility in $Ga_{1-x}Al_xAs$ alloys

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Hall mobilities in high-purity epitaxial layers of n-type $Ga_{1-x}Al_xAs$ with room-temperature electron concentration in the range $(5-10) \times 10^{15}$ cm^{-3} have been measured for alloy compositions x in the range $0 \leq x \leq 0.78$ and in the temperature interval $15 \lesssim T \lesssim 300$ K. Models for the variation of various material parameters with x are developed and it is shown that the alloy scattering potential is ~ 0.3 eV and is weakly dependent on x. The data have been analyzed and it has been shown that alloy, space charge, and intervalley scatterings play an important role in limiting the electron mobility. The data suggest that the deep energy levels in $Ga_{1-x}Al_xAs$ behave as space-charge scattering centers.

I. INTRODUCTION

It is well known that $Ga_{1-x}Al_xAs$ is a potentially important semiconductor material for many optical and microwave devices because of the continuous variability of the band gap and band structure with alloy composition and a good control over the energy levels and the electrical properties.[1-4] The electron mobility in this material and its dependence on the alloy composition are very important device parameters but they have received considerably less attention in the past as compared to other material parameters. Particular attention has been paid to the study of $Ga_{1-x}Al_xAs$ properties as compared to other ternary alloys because of the lowest lattice mismatch ($\sim 0.16 \%$) between the end compounds GaAs and AlAs.[5]

The task of evaluating the electron mobility in $Ga_{1-x}Al_xAs$ is more difficult as compared to any binary compound because of the continuous variation of the band structure and material properties with alloy composition. Before an attempt is made to calculate the electron mobility, it is rather imperative to exploit the band structure and electrical properties in this alloy. The second major problem arises from the fact that although some mobility data is available in the literature, either the Al distribution is inhomogeneous in the layers[6] or the data are limited to too small a range of x values[7-9] to make any reasonable study of the mobility behavior. Neumann and Flohrer[10] have investigated the composition dependence of the electron mobility at 300 K in liquid-phase epitaxial crystals over the composition range $0 \leq x \leq 0.78$. Special growth conditions were chosen to overcome the problem of inhomogeneous Al distribution over the layer thickness. However, they did not make any measurements on crystals with x values in the range $0.35 \lesssim x \lesssim 0.45$, where the intervalley scatterings may be significant due to the close proximity of the direct and various indirect

minima.[1-4] In the light of the new assignment of the band structure of $Ga_{1-x}Al_xAs$ on a three-band Γ, L, X model as established by Saxena,[1-4] there is a reason to doubt the results of analysis of mobility data in Ref. 10, where a two-band Γ, X model was considered for this alloy, as proposed by Casey and Panish.[11] For low-alloy compositions $0 \leq x \leq 0.32$, the Γ minimum is the lowest-energy minimum and the effect of electrons in the L and X minima on the measured Hall mobility can be neglected to a good approximation. Similarly for high-alloy compositions $0.60 \leq x \leq 1.0$, the X minima are the lowest in energy and the contributions from the Γ and L minima electrons can be ignored. For intermediate alloy compositions $0.32 < x < 0.60$, the contributions from all three minima are to be considered, since they lie close to each other in energy. For three-valley conduction, the Hall-to-drift mobility ratio (which will be referred to here as the scattering factor) peaks near the direct (Γ)-indirect (X) crossover composition $x \simeq 0.43$ (Refs. 1–4) and can be as large as a factor of ~ 4 at this composition.[12] Due to the lack of knowledge of exact variation of the scattering factor with x, it is not justified to compare the measured Hall mobilities with the calculated drift mobilities. However, this condition could be safely overlooked for the alloy compositions in the ranges $0 \leq x \leq 0.32$ and $0.60 \leq x \leq 1.0$, since for these compositions the scattering factor is found to lie between 1.0 and 1.1.[4] The last problem arises due to the fact that the strength of the intervalley scattering is found to vary with the alloy composition from the pressure dependence of the Hall mobility in $Ga_{1-x}Al_xAs$.[13] Unless the various coupling constants are known as a function of x, it will not be worthwhile to explain the mobility data for the alloy compositions in the range $0.32 < x < 0.60$, where the contributions from the intervalley scatterings will be significant. Also for these alloy compositions, the analysis of the mo-

bility data should include the effect of electrons in
the L minima. At present not much is known about
the various parameters of the L minima in
$Ga_{1-x}Al_xAs$. Recently Lee et al.[14] have reported
the measurement and analysis of temperature de-
pendence $(296 \leqslant T \leqslant 503$ K$)$ of conductivity and Hall
coefficient in Te-doped $Ga_{1-x}Al_xAs$ $(0.08 \leqslant x \leqslant 0.95)$
with room-temperature electron concentration in
the range 8.5×10^{16} to 1.5×10^{18} cm^{-3} over most of
the composition range. To our knowledge, no data
on the composition dependence of mobility at room
temperature and its variation with temperature
are available for intentionally undoped $Ga_{1-x}Al_xAs$
over the entire composition range of the alloy.

In the present paper, we report the results on
the variation of the Hall electron mobility for alloy
compositions in the range $0 \leqslant x \leqslant 0.78$ and in the
temperature interval $15 \leqslant T \leqslant 300$ K on high-purity
epitaxial samples. Particular attention is paid to
the measurements on the samples with x values
near the direct-indirect crossover composition.
Models describing the variation of various mater-
ial parameters with composition are developed.
The experimental procedure is described in Sec.
II and the experimental results in Sec. III. Section
IV reviews the major scattering mechanisms. The
results are discussed in Sec. V and the conclusions
drawn from the present work are presented in
Sec. VI.

II. EXPERIMENTAL PROCEDURE

The high-purity $Ga_{1-x}Al_xAs$ layers used in these
experiments were grown on Cr-doped semi-insul-
ating GaAs substrates by liquid-phase epitaxy and
had thicknesses of 5–10 μm and room-temperature
electron concentrations of $(5-10) \times 10^{15}$ cm^{-3},
which are approximately two orders of magnitude
lower than in the samples used in Refs. 6–10 for
most of the compositions. The alloy compositions
were determined from a measurement of the ca-
thodoluminescence band-gap energy and converted
to compositions by using the energy-gap-composi-
tion curve given by Panish.[15] The compositions
were also cross-checked by electron-beam micro-
probe analysis and were found to be consistent
with the previous measurements to within $\pm 0.5\%$.
The Al composition was found to be fairly con-
stant over the layer thickness.

Standard van-der Pauw samples were used for
the Hall measurements. The Ohmic contacts were
made with Sn and subsequent alloying at 550°C
for 2 min in H_2 atmosphere. Before making any
measurements, the contacts were checked for
Ohmic characteristics. A correction was made to
the measured Hall mobilities for the finite size of
the contacts relative to the sample.[16] For low-
temperature measurements a liquid-He cryostat

(Air product DE-202) was used which could stabil-
ize the temperature of the sample within ± 0.1 K.
All the measurements were done in a magnetic
field strength of 5 kgauss and with the samples in
the dark since these were found to be highly pho-
tosensitive at low temperatures. Care was taken
to eliminate the spurious effects of the contact re-
sistances.

III. EXPERIMENTAL RESULTS

The experimentally measured Hall mobilities
μ_h at 300 K and as a function of alloy composition
x are shown in Fig. 1. Also shown by the full
square is the Hall mobility for epitaxial AlAs.[17]
Qualitatively, the mobility variation can be ex-
plained as follows: It is known that the electron
mobility μ_Γ in the Γ minimum of GaAs is limited
by polar optical scattering[18] and varies inversely
as $m_\Gamma^{*3/2}$, where m_Γ^* is the electron effective mass
in the Γ conduction-band minimum. With increas-
ing x $(0 \leqslant x \leqslant 0.3)$, the energy of the Γ minimum
and hence m_Γ^* increases. This reduces μ_Γ and,
therefore, μ_h with increasing x. As x is further
increased $(0.3 < x \leqslant 0.45)$, the energy separations
between the high mobility and low density-of-
states Γ minimum, and the low mobility, high
density-of-states subsidiary L and X minima de-
crease.[1-4] Thus with increasing x more electrons
are transferred to the subsidiary minima from
the Γ minimum, which causes μ_h to decrease
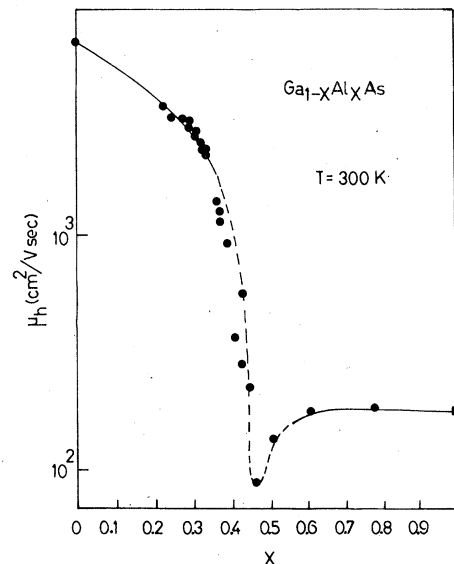sharply with x. For higher values of x $(x > 0.6)$,

FIG. 1. The Hall mobility μ_h of $Ga_{1-x}Al_xAs$ as a
function of alloy composition x. The full circles are the
measured values and the continuous lines show the cal-
culated results.

the electron transfer to the X minima is almost complete and μ_h saturates with x to the value characteristic of the electron mobility in the X minima. It will be shown that the minimum in μ_h at $x \simeq 0.47$ occurs due to intervalley, alloy, and space-charge scatterings. The temperature variation of μ_h for various alloy compositions has been measured and the results for a typical composition $x = 0.32$ are shown in Fig. 2 by full circles.

IV. ANALYSIS

In the analysis, the following assumptions are made:

(a) Each scattering process is described by a relaxation time $\tau_i(y)$ which depends upon the electron energy y in kT.

(b) The electrons are scattered in a parabolic band. This allows the use of simpler formulations for the various scattering processes.

(c) For each scattering process an average relaxation time $\langle \tau_i \rangle$ is calculated from the equation

$$\langle \tau_i \rangle = \frac{4}{3\sqrt{\pi}} \int_0^\infty \tau_i(y) y^{3/2} e^{-y} dy . \tag{1}$$

The electron mobility is then calculated from the equation

$$\mu_i = e\langle \tau_i \rangle / \overset{*}{m} , \tag{2}$$

where e is the electronic charge and $\overset{*}{m}$ the electron effective mass in one minimum.

(d) The various scattering mechanisms are independent of each other. The resultant mobility is defined as

$$\frac{1}{\mu} = \sum_i \frac{1}{\mu_i} . \tag{3}$$

For alloy compositions in the ranges $0 \leqslant x \leqslant 0.32$ and $0.60 \leqslant x \leqslant 1.0$, since the scattering factor is nearly unity, the nonequivalent intervalley scattering has been neglected in the analysis. The following scattering mechanisms have been considered:

A. Optical polar scattering

The temperature dependence of the electron mobility due to polar optical scattering follows the analysis of Fortini[18] and is given by the expression

$$\mu_{\text{PO}} = \frac{16\hbar\epsilon_s(2\pi kT)^{1/2}(e^{\xi_l} - 1)}{3ew_l(\overset{*}{m})^{3/2}(1/\epsilon_\infty - 1/\epsilon_0)} \int_0^\infty \gamma(\xi, \xi_l) d\xi , \tag{4}$$

where $\xi_l = T_{\text{LO}}/T$ and $w_l = kT_{\text{LO}}/\hbar$, T_{LO} being the optical phonon temperature. ϵ_0 and ϵ_∞ are the low- and high-frequency dielectric constants of the material, respectively, and ϵ_s the permittivity of free space. The infrared reflection spectra of
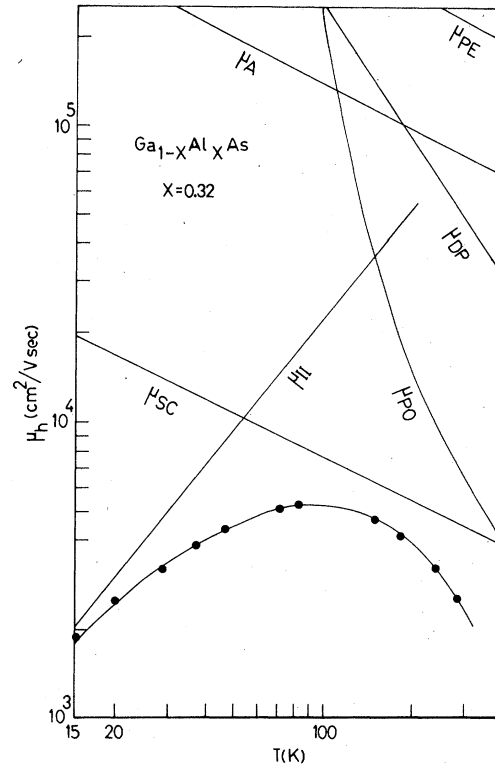

FIG. 2. Temperature dependence of the mobilities for a $Ga_{1-x}Al_xAs$ crystal with $x = 0.32$. The full circles are the measured Hall mobilities and the continuous lines show the calculated results. The unlabeled solid curve is the Hall mobility. Labeled solid curves are for ionized-impurity scattering only (μ_{II}), optical-phonon scattering only (μ_{PO}), piezoelectric scattering only (μ_{PE}), deformation potential scattering only (μ_{DP}), alloy scattering only (μ_A), and space-charge scattering only (μ_{SC}).

$Ga_{1-x}Al_xAs$ mixed crystals at the Γ point have been given by Ilegems and Pearson[19] and contain two branches, one due to GaAs-like and the other due to AlAs-like crystals. The term $T_{\text{LO}}/(e^{T_{\text{LO}}/T} - 1)$ in Eq. (4) is the average phonon energy $\bar{\epsilon}$ per mode. We have considered the total phonon energy as

$$\bar{\epsilon} = x\bar{\epsilon}_{\text{AlAs}} + (1 - x)\bar{\epsilon}_{\text{GaAs}} , \tag{5}$$

where $\bar{\epsilon}_{\text{AlAs}}$ and $\bar{\epsilon}_{\text{GaAs}}$ are the average phonon energies for the two phonons. Similarly, the integral in Eq. (4) is expressed as

$$G = xG_{\text{AlAs}} + (1 - x)G_{\text{GaAs}} . \tag{6}$$

Using Eqs. (5) and (6), we get from Eq. (4),

$$\mu_{\text{PO}} = \frac{25.54 T^{1/2} G}{(\overset{*}{m}/m_0)^{3/2}(1/\epsilon_\infty - 1/\epsilon_0)} \tag{7}$$

in units of cm^2/V sec.

The LO-phonon temperature at the X point (T_{LO}^X)

in GaAs (Ref. 20) and GaP (Ref. 21) are 345 and 580 K, respectively, and has been considered the same in AlAs as in GaP. To calculate the variation of T_{LO}^X with x, a linear extrapolation is assumed between its values in GaAs and GaP.

B. Deformation-potential scattering

The relaxation time for deformation-potential scattering based on the theory of Bardeen and Shockley[22] is given by Wolfe *et al.*[23] as

$$\frac{1}{\tau_{DP}} = 4.17 \times 10^{19}\left(\frac{E_1^2}{C_l}\right)\left(\frac{\overset{*}{m}}{m_0}\right)^{3/2} T^{3/2} y^{1/2} . \tag{8}$$

Using Eqs. (1), (2), and (8), we get,

$$\mu_{DP} = 3.17 \times 10^{-5} \frac{C_l T^{-3/2}}{E_1^2(\overset{*}{m}/m_0)^{5/2}} \tag{9}$$

again in cm^2/V sec, where $C_l = \rho u_l^2$, ρ and u_l being

the material density and sound velocity, respectively. E_1 is the deformation potential in eV. The values of ρ for GaAs and AlAs are given by Rode[24] and Mead and Spitzer[25] as 5.37 and 3.60 gm/cm^3, respectively. For calculating ρ as a function of x, a linear extrapolation between these values has been assumed. The potential E_1 of 8.6 eV for the Γ minimum in GaAs is taken the same for compositions $0 \le x \le 0.32$, as the majority of the electrons occupies this minimum. For compositions in the range $0.60 \le x \le 1.0$, since most of the electrons stay in the X minima the value of E_1 of 13.0 eV has been taken from GaP.[21]

C. Equivalent intervalley scattering (X-X)

Fawcett and Paige[26] have given the following expression for the scattering rate for scattering from state k in valley i to a state in valley j:

$$\lambda(k) = \frac{(N_j - 1)(\overset{*}{m_j})^{3/2}D_{ij}^2}{\sqrt{2}\pi\rho w_{ij}\hbar^3} \begin{cases} N_{ij}[\epsilon(k) + \hbar w_{ij}]^{1/2} \text{ absorption} \\ (N_{ij} + 1)[\epsilon(k) - \hbar w_{ij}]^{1/2} \text{ emission,} \end{cases} \tag{10}$$

where w_{ij} and D_{ij} are the frequency of the phonon and the intervalley coupling constant, respectively, and $N_{ij} = 1/(e^{\hbar w_{ij}/kT} - 1)$. N_j is the number of equivalent minima with $\overset{*}{m_j}$ as the mass in a single minimum. In the approximation $\epsilon \simeq \frac{3}{2}kT$ and using Eqs. (1), (2), and (10), we get

$$\mu_{IV} = \frac{2\pi e\hbar\sqrt{kT_c}}{\sqrt{3}(N_j - 1)(\overset{*}{m_j})^{3/2}D_{ij}^2}\left(\frac{(T/T_c + \frac{2}{3})^{1/2}}{(e^{T_c/T} - 1)} + \frac{(T/T_c - \frac{2}{3})^{1/2}}{(1 - e^{-T_c/T})}\right)^{-1}, \text{ for } \frac{T}{T_c} > \frac{2}{3}$$

$$= 0 \text{ for } \frac{T}{T_c} < \frac{2}{3} , \tag{11}$$

with μ_{IV} in units of cm^2/V sec where $\hbar w_{ij} = kT_c$. According to Birman *et al.*,[27] only LO phonons are considered for X-X scattering ($M_V > M_{III}$) and, therefore, $T_c = T_{LO}^X$. The coupling constant D_{ij} of 1.2×10^9 eV/cm has been considered the same as in GaP.[21]

D. Piezoelectric scattering

The relaxation time for piezoelectric scattering as determined by Zook[28] is given by the expression

$$\frac{1}{\tau_{PE}} = 1.05 \times 10^7 x h_{14}^2\left(\frac{4}{C_t} + \frac{3}{C_l}\right)\left(\frac{\overset{*}{m}}{m_0}\right)^{1/2} T^{1/2} y^{-1/2}, \tag{12}$$

where $h_{14}(= e_{14}/\epsilon_s\epsilon_0)$ is the piezoelectric constant in volt/cm and C_t, C_l the transverse and longitudinal elastic constants in dynes/cm^2, respectively, and are given by the equations[23]

$$C_t = \frac{1}{5}(C_{11} + 3C_{44} - C_{12})$$

and

$$C_l = \frac{1}{5}(3C_{11} + 2C_{12} + 4C_{44}) .$$

Rode[24] has given $e_{14} = 0.16$ C/m^2 and Fletcher and Butcher[29] quote the following values for the elastic constants in GaAs: $C_{11} = 1.188 \times 10^{12}$, $C_{12} = 0.538 \times 10^{12}$, and $C_{44} = 0.594 \times 10^{12}$ dynes/cm^2. From Eqs. (1), (2), and (12), we get

$$\mu_{PE} = 43.0\left(\frac{300}{T}\right)^{1/2} \frac{\epsilon_0^2}{(\overset{*}{m}/m_0)^{3/2}} \tag{13}$$

in units of cm^2/V sec. All the elastic constants have been considered independent of x since these are not known for Ga$_{1-x}$Al$_x$As except for $x = 0$. Since the contribution of this scattering mechanism to the resultant mobility is found to be appreciably smaller than that due to other scattering processes considered here, the uncertainty in the material parameters involved results in a negligibly small error.

E. Ionized-impurity scattering

It has been shown that deep energy levels are present in the band gap of Ga$_{1-x}$Al$_x$As.[1-4] As the

temperature decreases, the thermal energy of the electrons decreases linearly while the density of ionized impurities decreases exponentially with temperature. As the temperature approaches zero, the density of conduction electrons approaches zero and the density of the ionized donors N_D^+ approaches the acceptor density N_A^-. Under these conditions, the electron potential remains finite and large at low temperatures. Falicov and Cuevas[30] have derived an expression for the electron mobility in this limit as

$$\mu_{II} = \frac{2^{7/2}\pi^{-3/2}(kT)^{3/2}\epsilon_0^2 e^{-3}(\overset{*}{m})^{-1/2}(2N_A)^{-1}}{[\ln(1+n_0) + n_0(1+n_0)]} \quad (14)$$

where

$$n_0 = \frac{6kT\overset{*}{m}}{\pi^{2/3}\hbar^2(N_D - N_A)^{2/3}} .$$

The value of the net impurity concentration ($N_D - N_A$) for each composition to be analyzed here was determined from the analysis of temperature dependence of the Hall electron concentration.[1] For alloy compositions where the multiconduction band transport becomes significant, the net impurity concentration was determined experimentally from the measurement of the Hall electron concentration at high pressure where only the X minima are involved in the transport mechanism and the deep energy levels are almost ionized.[3]

F. Space-charge scattering

Weisberg[31] has discussed the mobility due to space-charge scattering which is given by the equation

$$\mu_{SC} = \frac{3.2 \times 10^9 \, T^{-1/2}}{\sqrt{\overset{*}{m}/m_0}(N_s A)} , \quad (15)$$

where N_s and A are the density and area of cross section of scattering centers, respectively.

G. Alloy scattering

The relaxation time due to alloy scattering is given by Hauser et al.[32] as

$$\frac{1}{\tau_A} = \frac{3\pi}{4} \frac{1}{8\sqrt{2}\hbar^4} (\overset{*}{m})^{3/2} x(1-x)a^3$$
$$\times (\Delta Ea)^2 \gamma(\epsilon)^{1/2} \frac{d\gamma(\epsilon)}{d\epsilon}(kT)^{1/2} , \quad (16)$$

where $\gamma(\epsilon) = \epsilon + \epsilon\alpha^2$ (α is the nonparabolicity of the band). The lattice constants (a) for GaAs and AlAs (Ref. 5) at 300 K are 5.6419 and 5.6611 A°, respectively. Taking a mean value for the lattice constant and assuming $\alpha = 0$, Eqs. (1), (2), and (16) give in units of cm^2/V sec,

$$\mu_A = \frac{52.83 T^{-1/2}}{(\overset{*}{m}/m_0)^{5/2} x(1-x)(\Delta E_a)^2} \quad (17)$$

In Ga$_{1-x}$Al$_x$As the variation of the alloy scattering potential ΔE_a with x is given by the equation (Appendix A)

$$\Delta E_a = 0.3 + 0.0011x .$$

Rode[24] has given ϵ_0 and ϵ_∞ for GaAs as 12.91 and 10.91, respectively, and Fern and Onton[33] for AlAs as 10.06 and 8.16, respectively. The values of ϵ_0 and ϵ_∞ as a function of x have been calculated taking a linear extrapolation for ϵ_0 and ϵ_∞ in GaAs and AlAs.

Since the variation in the X-minima energy with x is negligible compared to the Γ minimum,[1-4] the electron mass in the X minima has been considered independent of x. For alloy composition 0.6 $\leqslant x \leqslant 1.0$, three equivalent X minima[3] and the mass in a single minimum 0.35m_0^4 are considered, assuming it to be the same as in the X minima of GaP.[34] The variation of electron mass in the Γ minimum as a function of x is calculated from the standard $\vec{k} \cdot \vec{p}$ theory and is given by the expression[35]

$$\left(\frac{m_0}{\overset{*}{m}_\Gamma}\right) = 1 + E_{p\Gamma}\left(\frac{2}{E_\Gamma} + \frac{1}{E_\Gamma + \Delta O}\right). \quad (18)$$

The energy E_Γ of the Γ minimum at a particular temperature has been obtained from the data of Dingle et al.[36] at 2 K and the Varshini equation.[35] Here $E_{p\Gamma}$ and ΔO are the energies related to the momentum matrix element and the spin-orbit splitting of the valence band, respectively. In the present work the values for $E_{p\Gamma}$ and ΔO are taken as 7.51 and 0.341 eV, respectively, as given by Aspnes[35] for GaAs, and have been kept constant as a function of x.

V. DISCUSSION

The comparison between experimental and calculated Hall mobilities μ_h as a function of alloy composition x is shown in Fig. 1. The temperature dependence (15 $\leqslant T < 300$ K) of the Hall mobility for alloy compositions in the range 0 $\leqslant x < 0.32$ and 0.60 $< x < 1.0$ has also been successfully explained and the results for a typical sample with $x = 0.32$ are shown in Fig. 2. The agreement between the experimental and calculated results is satisfactory. In Fig. 3, we have plotted the ($N_s A$) product due to the space-charge scattering and the ratio of mobilities μ_A/μ_{SC} due to alloy and space-charge scattering, which resulted in the best agreement of the calculated and measured Hall mobilities. It is evident that the contribution of the alloy scattering compared to the space charge increases with the alloy composition. In other words, for low alloy compositions 0 $\leqslant x < 0.32$, the alloy scattering is relatively less important than for composition $x \geqslant 0.61$. The ($N_s A$) product increases
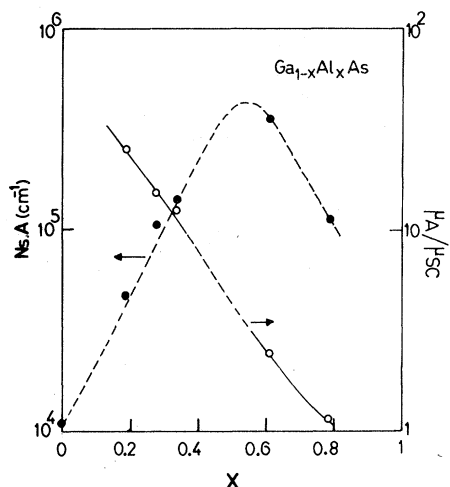
FIG. 3. The variation of density, area product $(N_s A)$ of space-charge scattering centers, and the ratio of mobilities (μ_A/μ_{SC}) due to alloy and space-charge scatterings as a function of alloy composition x.

with the composition in the range $0 \leqslant x < 0.32$ and is found to decrease for alloy compositions $x \geqslant 0.61$. It may, therefore, be expected to show a peak at a composition $x \simeq 0.5$ as is shown in Fig. 3. The electron mobility due to alloy scattering has been found to vary inversely with $[(\overset{*}{m})^{5/2}x(1-x)]$ for alloy compositions investigated in the present work and, therefore, may have a minimum value in the composition range $0.32 < x < 0.60$. Kaneko et al.[8] also found it necessary to include the space charge and alloy scatterings in their analysis in order to explain the temperature dependence $(80 \leqslant T < 300\text{ K})$ of Hall mobility for Sn-doped $Ga_{1-x}Al_x$ As $(0 < x \leqslant 0.15)$. We have compared our results for compositions $0.19 \leqslant x \leqslant 0.32$ with the extrapolated results for these compositions as suggested by Kaneko et al.[8] A comparison shows that the mobilities μ_A and μ_{SC} are in good agreement with those suggested by Kaneko et al.,[8] although the mobilities in the crystals studied here are approximately a factor of two higher. Stringfellow[9] has also reported that the space-charge scattering must be considered in order to explain the mobilities in Te-doped $Ga_{1-x}Al_x$As $(0 \leqslant x < 0.35)$.

Kaneko et al.[8] and Stringfellow[9] have concluded that in $Ga_{1-x}Al_x$As, the product (N_s, A) increases with the alloy composition in the ranges $0 \leqslant x \leqslant 0.15$ and $0 \leqslant x \leqslant 0.35$, respectively, and has almost the same value for compositions in the range $0 \leqslant x \leqslant 0.15$. They, however, could not analyze the data for higher compositions due to multi-conduction-band transport. The results in Fig. 3 also show that the product (N_s, A) increases with the alloy composition in the range $0 \leqslant x \leqslant 0.32$, but

the value of this product is lower than reported by Kaneko et al.[8] and Stringfellow.[9]

It has been shown that the electrical properties of $Ga_{1-x}Al_x$As are strongly controlled by the presence of complexes involving defects in the crystals.[1-4] The result that (N_s, A) product is higher for crystals studied by Kaneko et al.[8] and Stringfellow[9] than obtained in the present work may be due to the fact that the impurity and hence the defect concentration in the crystals studied here is much lower. It is not very surprising that the defect concentration may show a maximum at $x \simeq 0.5$ due to the random distribution of Ga and Al atoms, which may effectively increase the scattering area. We can, therefore, suggest that the electron scattering by the deep energy states also results in the space-charge scattering, showing a maximum (N_s, A) product at $x \simeq 0.5$ (Fig. 3). This product is found to be approximately an order of magnitude larger for AlAs-like crystals $(x = 0.78)$ than for GaAs $(x = 0)$, which reflects the present state of art of crystal growth.

From measurements of the Hall mobility as a function of pressure for various alloy compositions and the Monte Carlo simulations of the results, it has been shown that the minimum in μ_h occurs at a pressure corresponding to the direct (Γ)-indirect (L) crossover.[4] Since the contributions from alloy and space-charge scatterings are not expected to change with pressure for a fixed composition, the minimum primarily occurs due to intervalley scatterings as the various minima come close in energy to each other. Since varying the pressure on a crystal with a particular value of x is equivalent to varying the apparent composition of the crystal, it has been suggested that the minimum in μ_h at $x \simeq 0.47$ (Fig. 1) occurs due to the combined effects of alloy, space-charge, and intervalley scatterings.[13] A minimum in the Hall mobility as a function of alloy compositions has also been found in $GaAs_{1-x}P_x$ (Ref. 37) and $Ga_{1-x}In_xAs$ (Ref. 38) alloys at $x \simeq 0.55$, but the data remained unexplained.

Lee et al.[14] could explain their data without including the space-charge scattering in their analysis. For compositions $0 < x < 0.4$, they used the acoustic deformation potential for the Γ minimum as given by the equation $E_1 = 16.1 - 13.5\ x$ eV. Thus the extrapolated value in GaAs should be 16.1 eV, which is larger than the accepted value of 8.6 eV.[39] Since for alloy compositions in the range $0 \leqslant x < 0.32$, the band structure is similar to that of GaAs, it is expected that there will not be any appreciable change in the value of E_1 for these compositions. Secondly the mobilities at 295 K measured by Lee et al.[14] are much lower than those reported in the present work over most of

the composition range, partially due to large impurity concentration in their samples. For example, we have determined $N_D = 2.37 \times 10^{16}$ cm^{-3} and $N_A = 8.30 \times 10^{15}$ cm^{-3} for $x = 0.32$ from a rigorous analysis of the temperature dependence of the Hall electron concentration,[1] and used these values to calculate the mobility due to ionized impurities for the same sample (Fig. 2). Thus the total impurity concentration N_I for $x = 0.32$ is 3.2×10^{16} cm^{-3}. We have estimated from the data of Lee et al.[14] that for $x = 0.32$ the free-electron concentration should be $\sim 2.7 \times 10^{17}$ cm^{-3}, with $N_A \simeq 6.7 \times 10^{17}$ cm^{-3}, using a linear extrapolation for their values for the neighboring compositions. This means that $N_D \simeq 9.4 \times 10^{17}$ cm^{-3}, giving $N_I \simeq 1.6 \times 10^{18}$ cm^{-3} for $x = 0.32$. Using these values and $E_1 = 11.8$ eV for $x = 0.32$ as reported by Lee et al.,[14] we calculated the resultant mobility as 1090 cm^2/V sec at 300 K without considering the space-charge scattering. The calculated mobility is very close to the measured value of ~ 1080 cm^2/V sec as measured by Lee et al.[14] It thus appears that in the crystals studied by Lee et al.,[14] the effect of space-charge scattering is overshadowed by the large contributions from the impurity and acoustic-mode scatterings. It is evident from the results shown in Fig. 3 that compared to space-charge scattering, which is found mainly to limit the electron mobility in Ga$_{1-x}$Al$_x$As, the alloy scattering is relatively unimportant for low alloy compositions. The contributions from the alloy scattering become comparable to that due to space-charge scattering for high alloy compositions ($x > 0.6$). This result is in agreement with that of Lee et al.,[14] since they also found it necessary to consider the alloy scattering for compositions in the range $0.5 < x < 1.0$ only, and not for crystals with $x < 0.5$.

Although the band structure of Ga$_{1-x}$Al$_x$As alloy has been established,[1-4] we have not tried to explain the mobility data for compositions in the range $0.32 < x < 0.60$ due to the various parameters involved in the calculations, which are unknown for the L minima. Although Lee et al.[14] could explain their results with good consistency, they had many adjustable parameters which could fit their data over the entire composition range. For alloy compositions $0.32 < x < 0.6$, the band structure of the alloy had to be assumed as precisely known because of the large contributions from the intervalley scatterings. However, the various subband gaps proposed by Lee et al.,[14] do not agree well with the results obtained by Saxena.[1-4] For example, at $x = 0.43$, Lee et al.[14] suggest that the X minima lie 32 meV below the Γ and L minima. This does not agree with the band structure obtained by Saxena, who finds that at this composition the L minima lie 33 meV above the Γ and X min-

ima.[1-4] Such significant differences in the band structure may lead to large errors in the interpretation of the experimental results.

VI. CONCLUSIONS

The electron mobility in Ga$_{1-x}$Al$_x$As is drastically reduced near the direct-indirect crossover composition due to alloy, space-charge, and intervalley scatterings. To explain the Hall mobility data for compositions in the range $0.32 < x < 0.60$, further work is necessary to evaluate the various coupling constants and the Hall-to-drift mobility ratio as a function of alloy composition. The alloy-scattering potential in this alloy is found to be ~ 0.3 eV, which is weakly dependent on the alloy composition. It is suggested that deep energy states in Ga$_{1-x}$Al$_x$As act as space-charge scattering centers.

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APPENDIX: CALCULATION OF ALLOY-SCATTERING POTENTIAL IN Ga$_{1-x}$Al$_x$As

In past studies the alloy potential was considered to be either the band-gap difference[40] or the difference in the electron affinity[41] of the unalloyed components. The band gap and electron affinity can be considered as the properties determined for a bulk material. It is hard to justify that the misoccupation of Ga and Al atoms due to the disorder causes the difference in the bulk-material properties near the misoccupied lattice site.

Here the alloy-scattering potential is considered that which is due to the polarization deviation caused by the deviation of Callen's effective charge due to the deviation in electronegativity of atoms caused by the deviation of the covalent radius. III–V group semiconductors have ionic bonding and have a net charge Q. In GaAs and AlAs (Ref. 42) this is given in units of eV by

$$Q_{\text{GaAs}} = 0.46$$

$$Q_{\text{AlAs}} = 0.47 \ . \tag{A1}$$

The net charge in Ga$_{1-x}$Al$_x$As can be approximated as

$$Q_{\text{Ga}_{1-x}\text{Al}_x\text{As}} = (1 - x)Q_{\text{GaAs}} + xQ_{\text{AlAs}} \ . \tag{A2}$$

Putting Eq. (A1) in (A2), we get

$$Q_{Ga_{1-x}Al_xAs} = 0.46 + 0.01x . \qquad (A3)$$

The energy which is needed to take away one electron from the atom in such ionic-bonded crystals is given by the integral α. For Al and Ga atoms these integrals are given by the equations[37]

$$\alpha_{Al} = -6.67 - 6.81Q ,$$

$$\alpha_{Ga} = -6.93 - 6.90Q , \qquad (A4)$$

respectively. Then in $Ga_{1-x}Al_xAs$, we have from

Eqs. (A3) and (A4)

$$\alpha_{Al} = -9.80 - 0.0681x$$

$$\alpha_{Ga} = -10.10 - 0.059x . \qquad (A5)$$

Therefore, the alloy-scattering potential ΔEa, the difference between α_{Al} and α_{Ga}, is given by the equation,

$$\Delta Ea = \alpha_{Al} - \alpha_{Ga} = 0.3 + 0.0011x$$

which is weakly dependent on x.

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