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Monte Carlo simulation of bulk hole transport in $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{In}_{1-x}\text{Al}_x\text{As}$, and $\text{GaAs}_x\text{Sb}_{1-x}$

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We report a Monte Carlo study of hole transport in $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{In}_{1-x}\text{Al}_x\text{As}$, and $\text{GaAs}_x\text{Sb}_{1-x}$. The effects of alloy scattering are significant in all three cases, but mobilities are still high enough to be advantageous in particular device applications. We separately calculate the Hall r factors by a Boltzmann transport method and show that these factors are vitally important when attempting to compare Monte Carlo drift mobilities with experimental Hall data. © 1995 American Institute of Physics.

I. INTRODUCTION

While modeling of electron transport in III-V compounds and their alloys has been quite widespread in the last two decades, hole transport has received much less attention. However, interest in high-speed bipolar devices and complementary unipolar devices has prompted a recent increased interest in hole transport in these materials. Nevertheless, the general case is that Monte Carlo results are compared to experimental data in the form of Hall mobility while the simulation does not typically account for the Hall factor. While such practice is quite acceptable for the case of electron transport where this factor is typically close to unity, it is not acceptable for hole transport since this factor is on the order of 2 and its effect is often not negligible.

In this article, we simulate hole transport in $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{In}_{1-x}\text{Al}_x\text{As}$, and $\text{GaAs}_x\text{Sb}_{1-x}$ by using the Monte Carlo method and we determine the Hall mobility from the Hall factor which is calculated by solving the Boltzmann transport equation. This method is validated by comparing the resulting mobilities with measured Hall mobilities of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ over a range of compositions and the method is then applied to the other materials for which there are no data for comparison. This study illustrates the effects of the alloy scattering potential on the hole transport in various ternary semiconductors and the important role of the Hall r factor when comparing with experiment.

II. MONTE CARLO SIMULATION

The Monte Carlo simulation was performed using a single-particle approach assuming transport in both the heavy-hole and light-hole bands with scattering allowed between the bands. Both bands were assumed to be parabolic and symmetric, degenerate at $k=0$. The material constants used for the compounds are given in Table I. In the case of

alloys, parameters used were interpolated based upon the composition of the alloys following the method of Adachi.¹

Using these parameters, the mobilities for $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{In}_{1-x}\text{Al}_x\text{As}$, and $\text{GaAs}_x\text{Sb}_{1-x}$ were calculated using an applied electric field value of 5 kV/cm (well within the linear region). For the calculation of alloy scattering rates, the expression of Look *et al.* was used.² Since the alloy potential is largely an empirical parameter, the value of 0.53 eV, which was fitted to $\text{Al}_x\text{Ga}_{1-x}\text{As}$ data,² was used when appropriate and a range of values (from 0 eV to the difference in band gaps) was used for the other materials since there were insufficient data for fitting in these cases. Scattering rate expressions for the polar optical phonon, nonpolar optical phonon, and ionized impurity scattering mechanisms (a doping level of 10^{17} cm^{-3} was assumed) were taken from Brudevol *et al.*³ and the expressions for acoustic phonon scattering were taken from Costato and Reggiani⁴ using the equipartition approximation. The resulting drift mobilities are plotted in Figs. 1–3.

III. CALCULATION OF HALL r FACTOR

Calculation of hole scattering rates in semiconductors such as GaAs are very difficult because of the presence of two, coupled, degenerate hole bands. The Monte Carlo scheme accounts for this two-band nature in a straightforward manner but is slow to converge to an accurate solution. Further, the task of calculating a Hall mobility by Monte Carlo, instead of the usual drift mobility, is even worse because of the addition of a magnetic field requires many more scattering events to accurately characterize the effects which produce the Hall electric field. On the other hand, the Boltzmann transport equation, as solved by Rode's iterative method,² can effectively produce highly accurate single-band values of both drift (or conductivity) and Hall mobilities, but is of uncertain accuracy for two-band Hall mobilities, at least in most present implementations. Unfortunately, most experimental mobilities are Hall mobilities, so to employ Monte Carlo it is at least necessary to know approximately how

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TABLE I. Material parameters used for Monte Carlo Simulation.

	GaAs	GaSb	InAs	AlAs
m_{hh}/m_0	0.475 ^a	0.330 ^b	0.600 ^c	0.760 ^a
m_{lh}/m_0	0.087 ^d	0.046 ^e	0.027 ^a	0.150 ^a
ρ (g/cm ³)	5.36 ^f	5.61 ^g	5.67 ^h	3.76 ^e
ω_{LO} (rad/s)	5.30×10^{13i}	4.52×10^{13j}	4.58×10^{13h}	7.72×10^{13g}
ϵ_r	13.20 ^k	15.69 ^h	14.60 ^f	10.06 ^l
ϵ_∞	10.89 ⁱ	14.44 ^h	12.25 ^g	8.16 ^j
s_l (cm/s)	4.73×10^{5e}	3.97×10^{5e}	4.45×10^{5m}	5.55×10^{5n}
s_r (cm/s)	3.34×10^{5e}	2.77×10^{5e}	2.64×10^{5k}	3.95×10^{5n}
C_l (dyn/cm ²)	1.403×10^{12o}	1.038×10^{12e}	9.975×10^{11p}	1.340×10^{12n}
C_r (dyn/cm ²)	4.860×10^{11i}	3.550×10^{11e}	3.136×10^{11m}	4.490×10^{12n}
a (eV)	10.0 ^q	2.21 ^f	2.50 ^f	15.0 ^q
b (eV)	-1.70 ^q	-3.30 ^g	-1.80 ^f	-1.60 ^q
d (eV)	-4.40 ^q	-8.35 ^u	-3.60 ^f	-3.40 ^q

^aReference 8.^bReference 9.^cReference 10.^dReference 11.^eReference 12.^fReference 13.^gReference 14.^hReference 15.ⁱReference 16.^jReference 17.^kReference 18.^lReference 19.^mReference 20.ⁿReference 21.^oReference 22.^pReference 23.^qReference 24.^rReference 25.^sReference 26.^tReference 27.^uReference 28.

drift mobilities and Hall mobilities compare in cases of interest, e.g., as a function of alloy scattering strength, which is the subject of this article.

The ratio of Hall mobility, μ_H , to drift mobility, μ , is known as the Hall r factor; i.e., $\mu_H = r\mu$. (Here we will assume that the drift and conductivity mobilities are equal.) If we consider the light and heavy hole bands individually, their separate Hall coefficients are given as $R_l = r_l/ep_l$ and $R_h = r_h/ep_h$, where p_l and p_h are the respective hole concentrations in the bands. Also, the conductivities are $\sigma_l = e\mu_l p_l$ and $\sigma_h = e\mu_h p_h$. Each r factor can be written as a product $r_i = r_{si}r_{ai}$ ($i=l$ or h), where r_{ai} is an anisotropy factor, reported in Ref. 2, and r_{si} is the scattering factor calculated from the Boltzmann equation. Interband scattering

FIG. 1. Drift mobility of holes in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ as a function of mole fraction of AlAs as simulated by the Monte Carlo method. An alloy potential of 0.53 eV was used as found by Look *et al.* (Ref. 2).

FIG. 2. Drift mobility of holes in $\text{GaAs}_x\text{Sb}_{1-x}$ as a function of mole fraction of GaAs as simulated by the Monte Carlo method. Alloy potentials ranging from none to 0.7 eV were chosen for the simulation since the actual value is unknown and this represents the range of difference in potentials between GaAs and GaSb.

is explicitly accounted for, with the modification $k_f = k_i(m_f/m_i)^{1/2}$ instead of $k_f = k_i$ in deriving the usual scattering formulas, as in Ref. 5. (Here k_f and k_i are the wave vector magnitudes in the final and initial states, respectively.)

At this point, we treat the bands as independent entities to calculate an overall conductivity and Hall coefficient

$$\sigma = \sigma_l + \sigma_h = e(\mu_l p_l + \mu_h p_h) = ep\mu, \quad (1)$$

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

where $p = p_l + p_h$. (The quantities p_l and p_h are found from the average residence times of the holes in the Monte Carlo simulation.) By definition, $\mu_H = R\sigma = r\mu$. Thus, within the confines of this approximate model, we can calculate r which should give us a means of comparing theoretical Monte Carlo results with experimental Hall data. Although

FIG. 3. Drift mobility of holes in $\text{In}_{1-x}\text{Al}_x\text{As}$ as a function of mole fraction of AlAs as simulated by the Monte Carlo method. Alloy potentials ranging from none to 1.6 eV were chosen for the simulation since the actual value is unknown and this represents the range of difference in potentials between InAs and AlAs.

FIG. 4. Calculated Hall r factor for $\text{Al}_x\text{Ga}_{1-x}\text{As}$, $\text{GaAs}_x\text{Sb}_{1-x}$, and $\text{In}_{1-x}\text{Al}_x\text{As}$ as a function of mole fraction of AlAs, GaAs, and AlAs, respectively, and using alloy potentials of 0.53, 0.5, and 0.4 eV, respectively. The Hall r factor is defined by $r = \mu_H / \mu$ where μ_H is the Hall mobility and μ is the drift mobility. Note the "bowing" of the r factor.

the absolute values of r may not be extremely accurate, because they depend on the relative strengths of several different scattering mechanisms, the trend as we change only one scattering parameter (in this case, the alloy strength) should be more accurate, as can be inferred from other studies. The r factors for an alloy potential of approximately 0.5 eV are shown in Fig. 4 for each of the three alloys considered here. Because, as stated above, the absolute accuracy of the r factors is unknown, we have normalized the Monte Carlo mobilities of Figs. 1–3 to Hall mobilities (Figs. 5–7) by using a multiplicative factor $r(x)/r(x=0)$. Also, experimental results for some available $\text{Al}_x\text{Ga}_{1-x}\text{As}$ data of approximately the same doping are shown in Fig. 5 for a comparison of the "bowing" of the curves with x , and the agreement is quite good.

FIG. 5. Normalized Hall mobility of holes in $\text{Al}_x\text{Ga}_{1-x}\text{As}$ as a function of AlAs mole fraction. This represents an adjustment of the Monte Carlo simulated drift mobilities to account for the Hall r factor by multiplying the drift mobility by $r/r(x=0)$. Measured Hall mobilities are included to show the agreement between simulation and measurement.

FIG. 6. Normalized Hall mobility of holes in $\text{GaAs}_x\text{Sb}_{1-x}$ as a function of GaAs mole fraction. This represents an adjustment of the Monte Carlo simulated drift mobilities to account for the Hall r factor by multiplying the drift mobility by $r/r(x=0)$.

IV. DISCUSSION

One of the prime conclusions of this study is that if Monte Carlo theoretical mobilities are compared with Hall experimental mobilities, the bowing with x will be stronger in the latter. The largest discrepancy will be for $\text{In}_{1-x}\text{Al}_x\text{As}$, then $\text{Al}_x\text{Ga}_{1-x}\text{As}$, and the smallest for $\text{GaAs}_x\text{Sb}_{1-x}$. Stated in other terms, it may be said that the decrease in mobility suffered when going from a binary to a ternary is never as bad as it may appear from Hall results. This fact can be very important in cases for which the low-field mobility is a critical factor, as, for example, in a heterojunction bipolar transistor which must have the lowest possible base resistance.

Irrespective of the Hall r factor, theoretical Monte Carlo results themselves should be of great use in selecting or comparing materials for device applications. For example, the simulation of $\text{GaAs}_x\text{Sb}_{1-x}$ shows that, for compositions near the lattice matching condition for InP (51% GaSb), the hole mobility is generally better than that of GaAs. This would

FIG. 7. Normalized Hall mobility of holes in $\text{In}_{1-x}\text{Al}_x\text{As}$ as a function of AlAs mole fraction. This represents an adjustment of the Monte Carlo simulated drift mobilities to account for the Hall r factor by multiplying the drift mobility by $r/r(x=0)$.

indicate that $\text{GaAs}_x\text{Sb}_{1-x}$ should be capable of producing superior p -channel transistors, as has been shown experimentally.⁶

Further, the simulation of $\text{In}_{1-x}\text{Al}_x\text{As}$ shows that its transport properties are similar to those of $\text{Al}_x\text{Ga}_{1-x}\text{As}$. Although this seems to do little to recommend $\text{In}_{1-x}\text{Al}_x\text{As}$ for device use, it should be noted that its high valence band-edge discontinuity with $\text{GaAs}_x\text{Sb}_{1-x}$ (Ref. 7) makes it very appealing for p -channel transistors.

In conclusion, the results given in this article should be useful in: (1) selecting new ternary materials on the basis of low-field mobility; (2) determining the effects of alloy scattering on the mobilities; and (3) estimating the true drift mobility from the experimental Hall mobility. Other ternary materials should be amenable to the same type of analysis presented here.

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