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High-Field Transport Properties of $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$

M. Deb Roy

Jadavpur University, Physics Department, Calcutta-700 032, India

B.R. Nag and D. Chattopadhyay

Institute of Radio Physics and Electronics 92, Acharya Prafulla Chandra Road, Calcutta-700 009, India

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Abstract. Monte-Carlo results on the velocity-field characteristics, ac diffusion-constant and thermal-noise voltages are presented for $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ at 300 K. Recently available values of physical constants have been used in the calculations. The values of diffusion constants are close to those of InP but the thermal noise voltages are found to increase faster with the field. The peak velocity is 1.9×10^7 cm/s and the threshold field for negative differential mobility is about 6 kV/cm.

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The quaternary compound $In_{1-x}Ga_xAs_yP_{1-y}$ is of great technical importance as its energy band-gap may be adjusted by choosing the composition to suit the low attenuation and low dispersion wavelength band (0.9–1.3 μm) of optical fibres. The lattice constant of the material may also be adjusted to match that of other commercially available substrate materials (InP or GaAs) and good crystals may be grown by liquid phase epitaxy. Some calculations [1] also predicted for this material a peak velocity substantially higher than that for other binary and ternary materials, so that it could be considered as a better material for high frequency FET's and for high-speed logic devices.

Early calculations of the transport coefficients of $In_{1-x}Ga_xAs_yP_{1-y}$ were based on interpolated values of the various physical constants. Recent experiments have produced values of some of these constants, which are not in full agreement with the interpolated values. Experimental low-field mobilities and the high-field characteristics do not also agree with the early calculations. The low-field mobility results have been examined [2] in detail in the light of the theory by using the revised values of the physical constants and reasonable agreement was found between theory and experiment.

In the present paper we report the velocity-field characteristic, the ac diffusion-constant and the thermal-noise voltage of $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ calculated with the latest values of the physical constants. The particular composition was chosen to match the lattice constant of InP. The band gap [3] for this composition corresponds to a wavelength of 1.25 μm which is within the band of interest for optical fibre communication. Low-field experimental results [4] are also available for this composition so that some of the unknown interaction parameters could be estimated by fitting theory with these experiments. The composition is also close to that for which early calculation predicted a high peak velocity.

1. Values of Physical Constants

The conduction band structure of $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, has been recently reviewed by Ferry [5] and he has given a plot of the $\Gamma-L$ and $\Gamma-X$ valley separation as a function of y considering all the available theoretical and experimental results. For the $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ system the $\Gamma-L$ and

$\Gamma - X$ separation are as follows:

$$\Delta E_{\Gamma L} = 0.5 \pm 0.05\,\text{eV} \quad \text{and} \quad \Delta E_{\Gamma X} = 1.01\,\text{eV}. \tag{1}$$

For this separation the X-valley will not be significantly populated within the range of fields of our interest and we have therefore excluded it in our calculations. It may also be pointed out that the above value of $\Delta E_{\Gamma L}$ is about 0.7 times the value used by Littlejohn et al. [1] in their calculations for a similar composition of the material. Littlejohn et al. obtained their value by interpolation, whereas the above value has been obtained by using the dielectric method [6], which gives results in agreement with the experimental results for many other alloy systems and may therefore be considered more likely.

For our calculations we need also the values of the direct band-gap which gives the non-parabolicity of the Γ-band, the values of effective masses for the two valleys, the various deformation potential constants and the phonon frequencies. The effective mass for the L-valleys and the intervalley deformation potentials are not known. In fact, these constants are not known for most of the semiconductors, and only estimated values are available. However, for not too high fields even when L-valleys are populated, the Γ-valley electrons determine the characteristics because of their lower effective mass. Errors in the L-valley parameters do not, therefore, significantly affect the characteristics. We have used for the L-valley effective mass, the intervalley deformation potential constants and the phonon frequencies, values estimated from those of GaAs, InAs and InP by interpolation.

There have been a number of experiments [3, 7–9] giving the Γ-valley effective mass and the direct band gap. Through these experiments the following formulae have been estiblished

$$m^*/m_0 = 0.077 - 0.05y + 0.014y^2, \tag{2}$$

$$E_g = 1.35 - 0.738y + 0.138y^2. \tag{3}$$

The two parameters have been obtained from these formulae.

The phonon spectra for the InGaAsP system has also been obtained from Raman studies [10]. It is found that there are effectively two modes corresponding to the InP and $In_{0.53}Ga_{0.47}As$ LO modes. The frequencies of these modes as obtained in the experiments have been used in our calculations. The coupling strengths S_1 and S_2 of the two modes have been obtained from the measured ratio of Raman intensities, R, using the formulae [11]

$$S_1/S_2 = R,\ S_1 + S_2 = K_\infty^2 (K_\infty^{-1} - K_s^{-1}). \tag{4}$$

The high-frequency and static dielectric constants K_∞ and K_s were obtained by interpolation from the values corresponding to InP and $In_{0.53}Ga_{0.47}As$. It may be mentioned that such a linear interpolation for the dielectric constant is supported by the model of Harrison and Hauser [12].

The mass density and the acoustic velocity were also obtained by interpolation and the acoustic phonon deformation potential constant was taken to be 7 eV, a value used for most of the compound semiconductors. Since the contribution from acoustic phonon scattering is not very significant, errors in the above values are not of much importance.

The remaining constant, the value of the alloy scattering potential Δu, was taken to be 0.66 eV, the value which has been found to give the best agreement with low-field mobility experiments [2]. There are three theoretical models for the calculation of this potential in the literature, the difference of band gaps, the difference of electron affinities and the difference in electronegativity. These give, respectively, the values of 0.51, 0.27, and 0.29 eV. The value of 0.66 eV used in our calculations is significantly higher. However, it may be noted that in addition to alloy scattering, two other scattering mechanisms, the cluster scattering and space-charge scattering also limit electron mobility in alloy semiconductors. The energy and temperature dependence of these two scattering mechanisms being identical to that of alloy scattering, their effect can not be distinguished from the analysis of temperature-dependence of mobility. The value of 0.66 eV chosen by us may therefore be considered to represent the effective value, including the effects of all the three scattering mechanisms.

The values of the various physical constants derived from the above considerations are given in Table 1.

2. Results and Discussion

The velocity-field characteristic, ac diffusion-constant and thermal-noise voltage have been calculated at 300 K for the field range 1–10 kV/cm. The calculations were done by the Monte-Carlo technique. The band non-parabolicity and the associated effects were included for the Γ-valley electrons. The L-valley was, however, assumed to be parabolic and isotropic. The drift velocity was obtained by the usual averaging over about 50,000 real collisions.

The ac diffusion coefficient $D(\omega)$ was obtained from the autocorrelation function using the formula

$$D(\omega) = \int_0^\infty C(s) \cos \omega s\, ds. \tag{5}$$

The autocorrelation function, $C(s)$ was calculated using the method described in [13, 14].

Table 1. Physical constants of $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$

Parameter	Symbol	Unit	L-Valley	L-Valley
Number of equivalent valley	–	–	1	4
Effective mass ratio	m^*/m_0	–	0.056	0.3
Energy band gap	Eg	eV	1.01	–
Acoustic deformation potential	E_1	eV	7	12
Alloy scattering potential		eV	0.66	0.66
Polar Optic Scattering				
(a) L valley Equivalent Temp	T_p	K	–	428
(b) Γ valley				
(i) InP mode Equivalent Temp	T_1	K	487	–
Mode Strength	S_1	–	0.98	–
(ii) InGaAs mode Equivalent Temp	T_2	K	370	–
Mode Strength	S_2	–	1.028	–
Intervalley scattering Equivalent temp	$T_{\Gamma L}$	K	349	349
Coupling const.	$D_{\Gamma L}$	10^8 eV/cm	10	10
Separation between valleys		eV	0.53	
Static dielectric const	K_s	–	13.04	
Optic dielectric const	K_α	–	10.56	
Density		gm/cm^3	5.15	
Velocity of sound		10^5 cm/s	4.9	
Lattice const		10^{-8} cm	5.869	

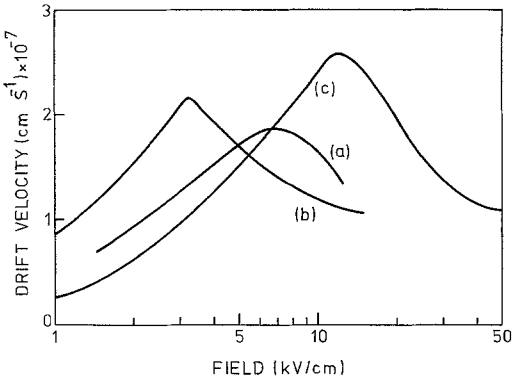

Fig. 1a–c. Velocity-field characteristics for, (a) $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$; (b) GaAs [17]; (c) InP [18]

The parallel and perpendicular components of the thermal noise voltages V_{Fp} and V_{Ft} were obtained from the relations given in [15],

$$V_{Fp}/V_0 = (\mu_0/\mu_d)[D_p(0)/D_0]^{1/2} \quad (6)$$

and

$$V_{Ft}/V_0 = (\mu_0/\mu_c)[D_t(0)/D_0]^{1/2}, \quad (7)$$

where V_0 is the noise voltage for low fields, μ_0 is the low field mobility, μ_c is the chord mobility, μ_d is the differential mobility, $D_p(0)$, $D_t(0)$ are the parallel and transverse components of diffusion constants, D_0 being the low-field diffusion constant.

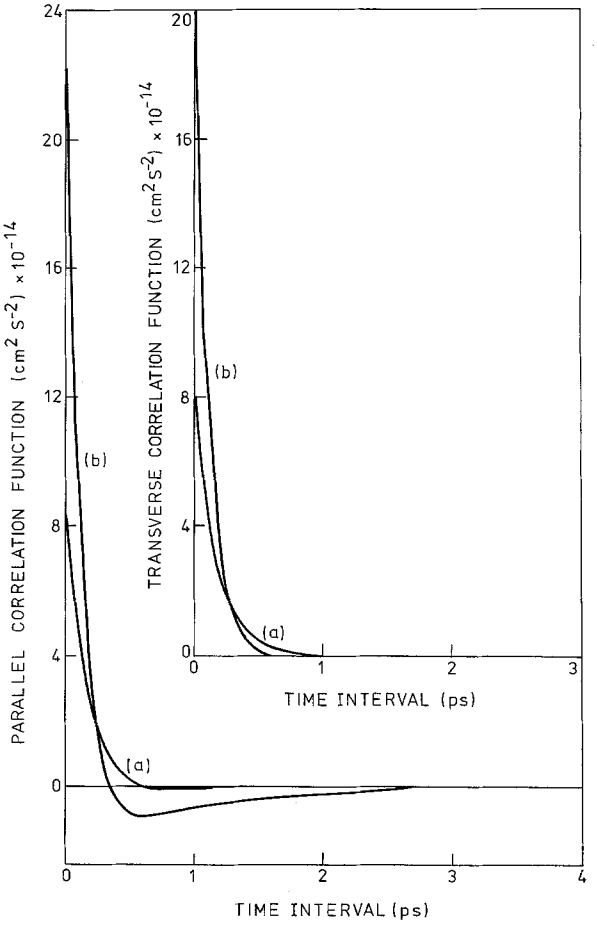

Fig. 2a and b. Velocity autocorrelation function for $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$; (a) 2 kV/cm; (b) 10 kV/cm

2.1. *Velocity-Field Characteristics*

The velocity-field characteristics are given in Fig. 1. The results are significantly different from those obtained in earlier calculations. The peak velocity is about 1.9×10^7 cm/s, which is very close to the experimental result [16]. The threshold field for negative differential mobility is about 6 kV/cm. It is 20% higher than that reported from experiments. However, considering that the threshold field is very difficult to determine accurately from pulse experiments, as inhomogeneities may cause instabilities and domains at low fields, the above agreement may be considered to be good.

We have also plotted in Fig. 1 the characteristics of GaAs [17] and InP [18]. It is seen that the peak velocity for $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ is smaller than that for either of these materials. Hence, it does not offer any advantages for high-speed devices.

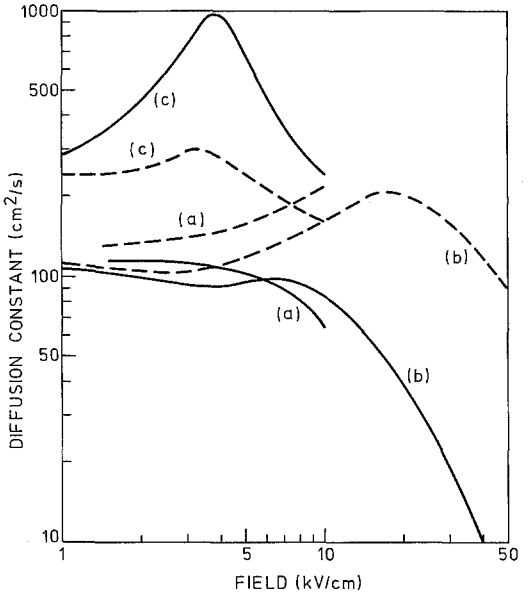

Fig. 3a–c. Diffusion constant vs field characteristics. (Solid line: Transverse component; Dotted line: Parallel component) (a) $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$; (b) InP [18]; (c) GaAs [17]

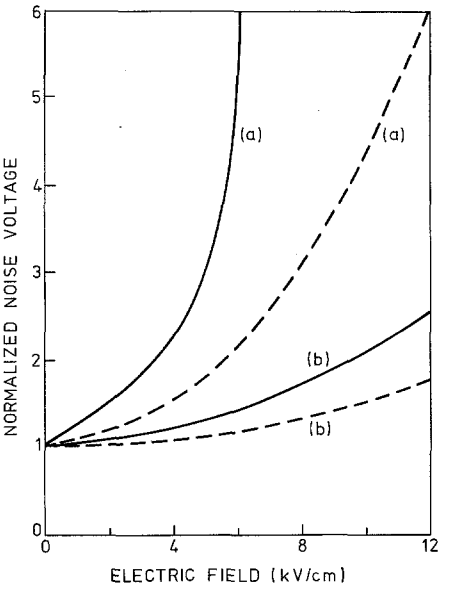

Fig. 5a and b. Normalized noise voltage-field characteristics. (Solid line: Parallel component; Dotted line: Transverse component) (a) $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ (b) InP

2.2. *Diffusion Constants*

The correlation coefficients are given in Fig. 2. We find that the shape of the curves are identical to those for InSb, InP, GaAs, HgCdTe and CdTe reported by us earlier [13–15, 19]. The transverse component of the correlation coefficient exponentially decreases to zero, while the parallel component becomes first negative and then increases to zero.

The low frequency diffusion constants are given in Fig. 3. For comparison we have also included plots of diffusion constant of GaAs and InP. We find that the diffusion constants for this material are close to those of InP. The thermal noise in $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ devices would therefore be similar to that in InP and much smaller than in GaAs. The ac diffusion constants are given in Fig. 4. As in other compound semiconductors, the transverse component remains constant up to about 250 GHz and then decreases monotonically, while the parallel component starts

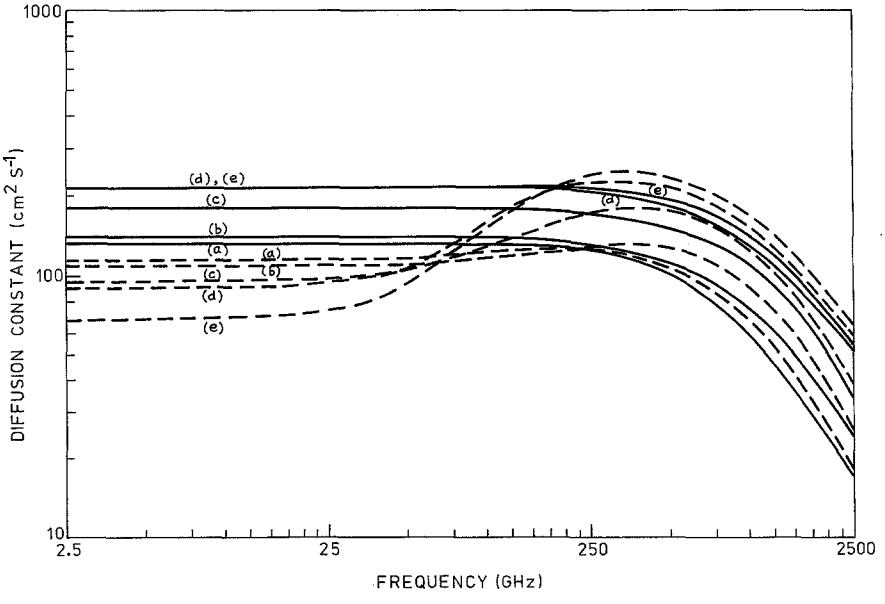

Fig. 4a–e. AC diffusion constant for different fields. (Solid line: Transverse component; Dotted line: Parallel component) (a) 2 kV/cm; (b) 4 kV/cm; (c) 6 kV/cm; (d) 8 kV/cm; (e) 10 kV/cm

with a much lower value, increases to a maximum around the same frequency and then decreases again.

Ternary compound semiconductors are also used as photoconductive detectors. The thermal noise voltage expected in such applications are given in Fig. 5. We have also included for comparison similar plots for InP obtained from the earlier calculated results [18]. In comparison, the voltages for $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ increase much faster than those for InP. In photoconductive detectors and for similar applications $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ would thus be more noisy.

3. Conclusion

We have presented the velocity-field characteristics, ac diffusion constants and thermal noise voltage of $In_{0.765}Ga_{0.235}As_{0.5}P_{0.5}$ calculated by the Monte-Carlo technique using the latest values of the physical constants. The velocity-field characteristic is found to be in close agreement with experiments. The diffusion constants are close to those of InP, but the thermal noise voltages are larger for high fields.

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