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Anisotropic mobility model for GaInAs covering full composition and strain range in the GaAs-InAs system

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Abstract. We propose a new model for the anisotropic mobility of GaInAs alloys with the independent parameters composition and strain. It is based on Monte Carlo transport calculation and relies on a formulation of the strained effective mass tensor which has been obtained by deformation potential and **k**·**p** formalism.

1. Introduction

Besides $Ga_xIn_{1-x}As$ which is nearly lattice-matched to GaAs and InP substrates both In-rich and highly strained alloys become increasingly important for heterojunction transistors and emitters also for room temperature applications. Since for layers exceeding a certain critical thickness partial strain relaxation by dislocations occurs [1], strain within the epilayer is no longer strictly coupled to composition via the lattice constants of epi- and neighboring layers. Therefore the electronic properties must be modeled as functions of the independent parameters composition and strain.

2. Calculation

2.1. Effective mass tensor

Based on deformation potential theory we first express the strain induced shifts of the conduction and valence band edges under biaxial stress over the envisaged range for (001) interfaces [2]. Using **k**·**p** theory we calculate the anisotropic effective mass tensor of the direct conduction band minimum [3]. The tetragonal distortion of the cubic crystal results in different masses $m_{\|}$, $m_{\perp}$ for in-plane and perpendicular directions, respectively. The obtained values compare well with the tight-binding calculations of [4]. The deviations from the unstrained mass m_0

$$\Delta m_{\mathrm{i}}(x, e_{\|}) = m_{\mathrm{i}}(x, e_{\|}) - m_0(x) \qquad \mathrm{i} = \|, \perp \tag{1}$$

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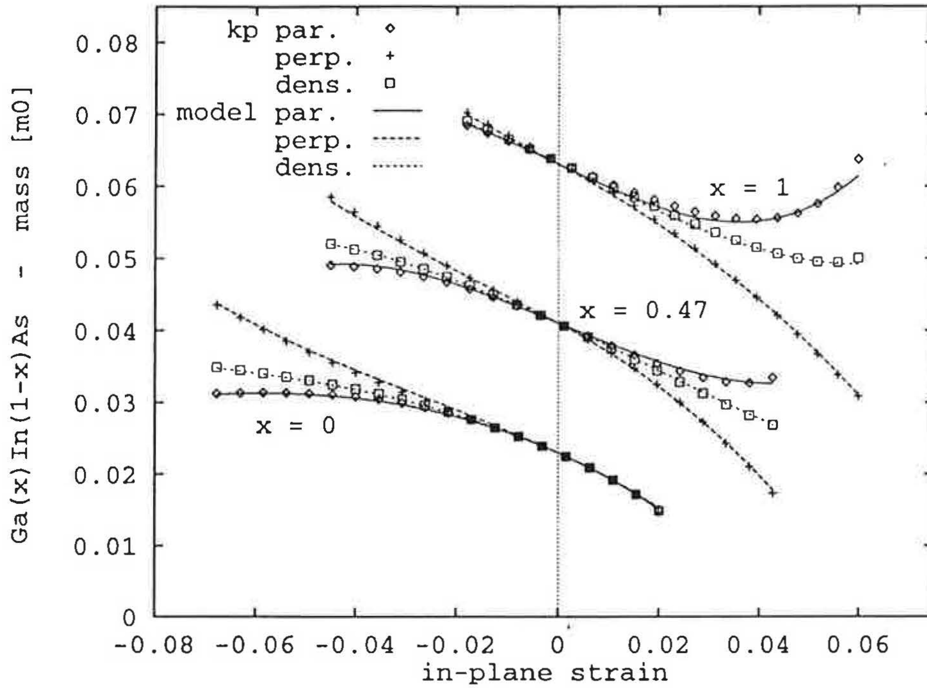

Figure 1. **k·p** calculated and fitted $m_{\|}$, $m_{\perp}$, and m_{d} versus $e_{\|}$.

we approximate by low-order polynomials in the in-plane strain $e_{\|}$ with composition dependent coefficients (Table 1). The density of states mass m_{d} can be fitted in the same way and is also shown in Fig. 1.

Table 1. Coefficients for strain shift of parallel, perpendicular and DOS mass of $Ga_xIn_{1-x}As$ for (001) interface orientation.

	$\Delta m_{\|}$			$\Delta m_{\perp}$			Δm_{d}		
	x^0	x^1	x^2	x^0	x^1	x^2	x^0	x^1	x^2
$e_{\|}^1$	−0.319	0.132	−0.147	−0.33	−0.168	0.104	−0.321	0.0235	−0.041
$e_{\|}^2$	−3.65	11.21	−7.60	−2.10	−0.593	1.692	−3.051	5.932	−3.128
$e_{\|}^3$	−10.50	164.0	−67.85	−25.86	−57.81	61.56	−12.95	74.47	−27.98

2.2. Electron mobility

We calculate the electron mobility using a steady-state single particle Monte Carlo (MC) procedure employing a nonparabolic ellipsoidal band structure including phonon and alloy scattering mechanisms. The used material properties and scattering parameters can be found in [5]. The resulting different parallel and perpendicular mobility components $\mu_{\|}$ and $\mu_{\perp}$ are shown in Fig. 2 and Fig. 3. Compressive strain decreases both values while tension enhances them significantly. The parallel component $\mu_{\|}$ is higher than $\mu_{\perp}$ in the first case and lower in the second.

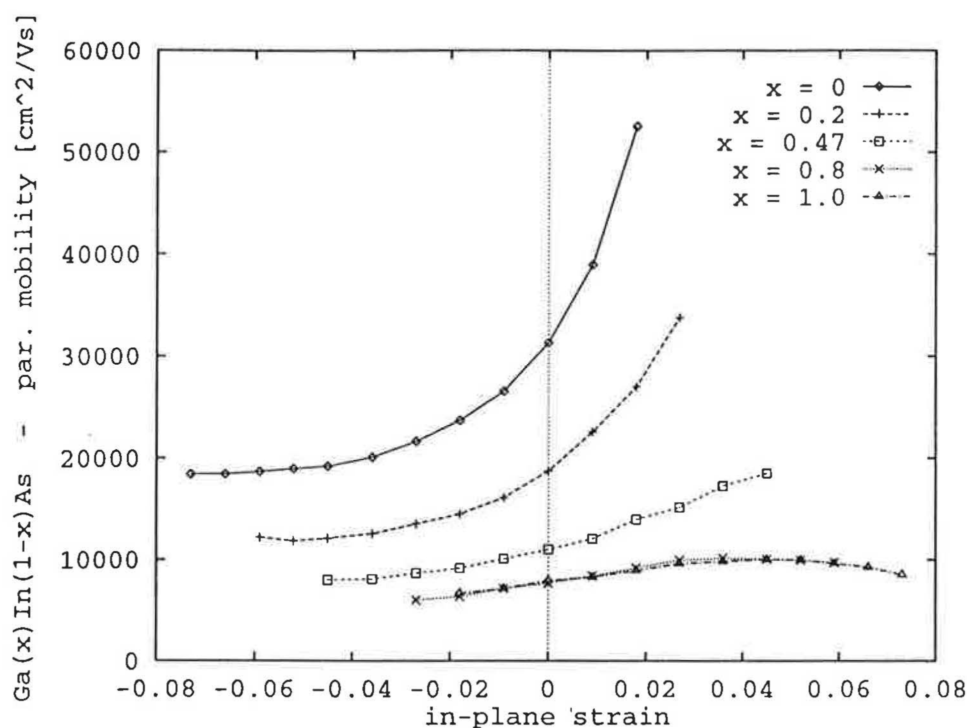

Figure 2. MC calculated $\mu_{\|}$ versus $e_{\|}$.

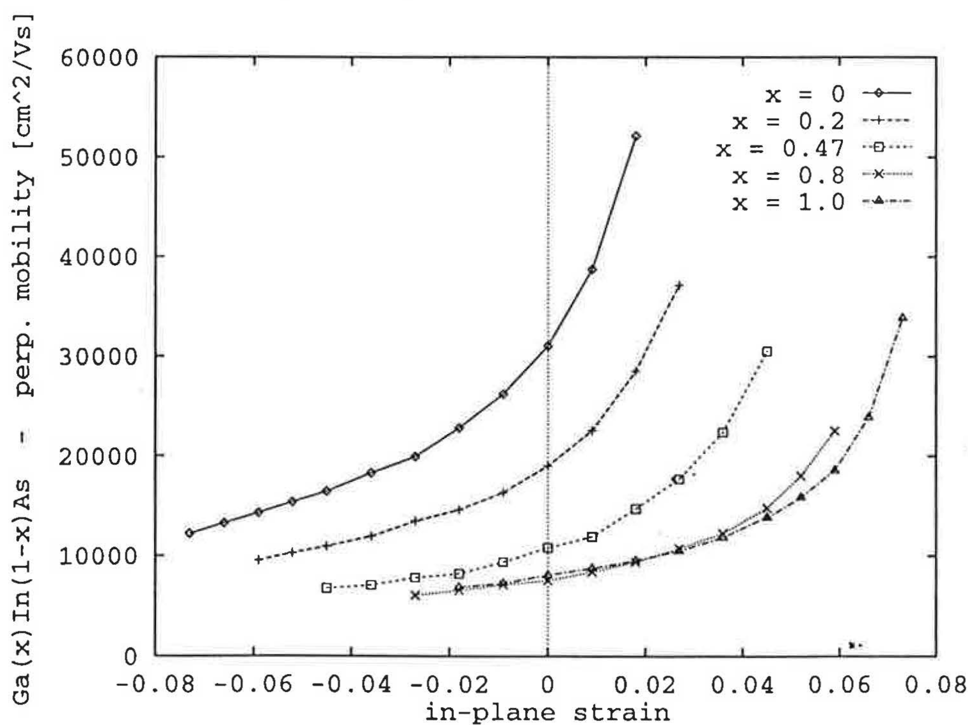

Figure 3. MC calculated $\mu_{\perp}$ versus $e_{\|}$.

Two features are striking. First, we observe that $\mu_{\|}/\mu_{\perp} = m_{\perp}/m_{\|}$ as one expects from a first-order perturbation calculation of the Boltzmann transport equation (BTE) for an ellipsoidal valley and isotropic relaxation rate. Second, defining an average mobility $\bar{\mu} = (\mu_{\perp} \cdot \mu_{\|}{}^{2})^{1/3}$ we find that it scales as $\bar{\mu} = \mu_0 \cdot (m_0/m_{\rm d})^{\beta}$, where β only weakly deviates from 3/2 over the entire composition range. This behavior justifies the assumption of an approximate relaxation time (with mass exponent $-1/2$) according to the BTE solution though the by far most important scattering process, polar optic phonon scattering, is both anisotropic and inelastic.

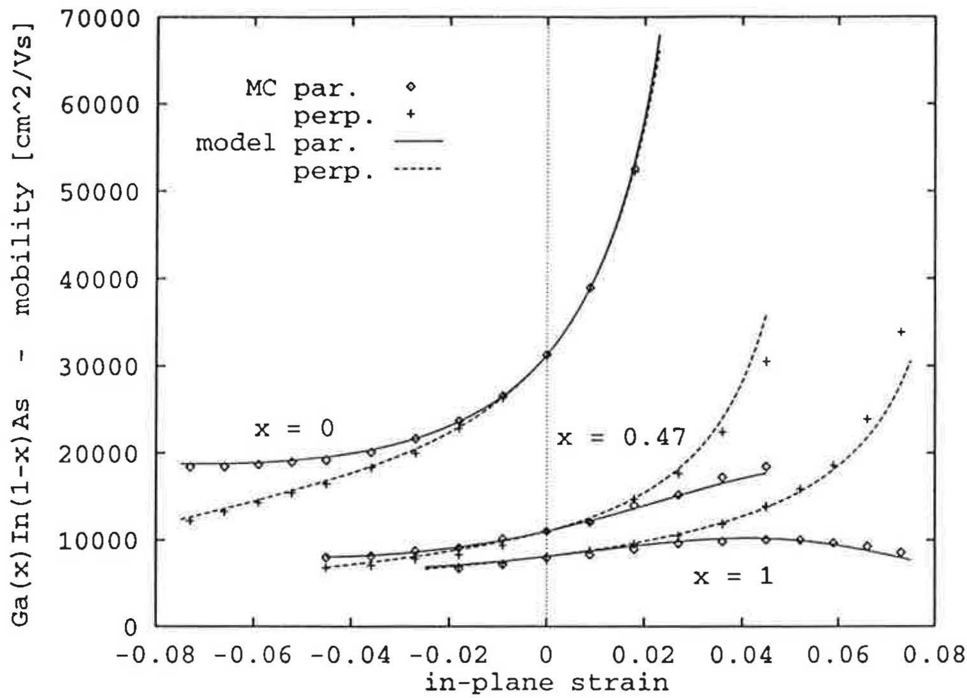

Figure 4. Comparison of $\mu_{\|}$ and $\mu_{\perp}$ versus $e_{\|}$ from the proposed model with MC data.

3. The new model

Based on the above mentioned observations we propose the following model which relates the strained mobilities to the unstrained mobility μ_0 virtually by use of the model for the strained masses (1)

$$\mu_{\mathrm{i}}(x,e_{\|}) = \frac{\mu_0(x)\cdot m_0(x)^{\beta}}{m_{\mathrm{i}}(x,e_{\|})\cdot m_{\mathrm{d}}(x,e_{\|})^{\beta-1}} = \frac{\mu_0(x)}{\left(1+\frac{\Delta m_{\mathrm{i}}(x,e_{\|})}{m_0(x)}\right)\cdot\left(1+\frac{\Delta m_{\mathrm{d}}(x,e_{\|})}{m_0(x)}\right)^{\beta-1}} \quad (2)$$

In Fig. 4 the proposed model is compared with the MC data. The correspondence over the whole composition and strain range is very good. Its computational simplicity makes it especially suitable for device simulation purposes.

Acknowledgments

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