

Mobility model for III-V compounds suited for hydrodynamic device simulation

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Abstract. We propose an improved mobility model for hydrodynamic device simulation. The mobility is modeled as function of the total mean energy. Expressions for the individual valley mobilities are combined by means of the relative valley populations estimated by a modified Boltzmann distribution. Our model is based on steady-state Monte Carlo calculations and reflects the situation of intervalley transfer in III-V compounds. As an example the model is applied to $\text{Ga}_x\text{In}_{1-x}\text{As}$.

1. Introduction

Hydrodynamic device simulation is believed to be today's best suited tool for device characterization in the submicron regime in view of accuracy and computational effort. It bridges the gap between the classical drift-diffusion simulation tools, which run into difficulties if the characteristic length dimensions approach the thermal wavelength, and the computationally expensive Monte Carlo codes which are most accurate in describing non-local effects. The drift-diffusion (DD) and the hydrodynamic (HD) methods are approaches to solve the semiclassical Boltzmann equation via balance equations which are solved for the moments of the carrier distribution function. An important physical parameter governing electron transport in devices within the mentioned frameworks is the carrier mobility μ . The Monte Carlo (MC) technique calculates the distribution function by observing particle trajectories, the only input being basic physical quantities and scattering formulae [1].

2. Mobility modeling

Carrier mobility modeling is usually split into the characterization of the mobility at zero field, μ_0 , which takes into account all doping and temperature dependences and the deviation from this value at increasing fields. A usual approach in the DD framework is to assume mobility as a function of the local driving force \mathbf{F} , $\mu = \mu(\mu_0, \mathbf{F})$, which

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consists of the electric field and a diffusion term, $\mathbf{F} = \mathbf{E} - \frac{1}{n} \nabla \frac{nkT}{q}$. A summary of various formulations can be found in [2]. In the HD case a dependence on the local carrier energy w is commonly assumed, $\mu = \mu(\mu_0, w)$. This includes non-local dissipation since the electron energy is a solution of the energy balance equation.

3. Methods of calculation

In calculating μ_0 one usually assumes an equilibrium distribution function (Boltzmann or Fermi-Dirac) and calculates mobilities for the individual scattering mechanisms which implies that momentum relaxation times exist. These contributions are then combined by Mathiessen's rule. This is believed to be reasonably accurate in most cases of elemental and III-V semiconductors.

Different methods for the calculation of high-field mobility have been proposed in the literature [3]. The simplest one is based on the relaxation time approximation. The energy dependent relaxation times are averaged over the assumed distribution function. Though very crude, this gives analytic expressions for isotropic parabolic bands. The method of calculating the distribution function by a variational principle gives more accurate results. The most accurate method is the Monte Carlo technique. It removes the restrictions of the relaxation time approximation and allows full inclusion of the complex band structure of semiconductors [4]. This technique yields a self consistent distribution function, therefore we have used it in this work.

3.1. Monte Carlo calculation

Our simulation program incorporates a many-valley isotropic nonparabolic band structure representation (Γ, L, X valleys) and takes into account scattering by polar and non-polar optic phonons, acoustic phonons, ionized impurities, and alloy disorder. An interpolation routine for the basic material parameters is included both for ternary and quaternary alloys. The band edges are given by quadratic expressions in the composition ratio. In the ternary case we have

$$E_{A_x B_{1-x} C} = x E_{AC} + (1 - x) E_{BC} - x(1 - x) C_{ABC}. \quad (1)$$

The remaining parameters are interpolated linearly.

Fig. 1 and Fig. 2 show the calculated low-field mobility and velocity-field relation, respectively, with the typical negative differential resistivity, both as function of the composition x for $\text{Ga}_x\text{In}_{1-x}\text{As}$. Table 1 shows the material parameters used in the MC calculation.

4. The hydrodynamic mobility model

4.1. The conventional model

Hänsch [5] obtained the following expression for the momentum relaxation time τ_m from a series expansion of the distribution function into its first four moments,

$$\tau_m^{-1} = A + B \frac{\mathbf{j} \cdot \mathbf{S}}{j^2}, \quad (2)$$

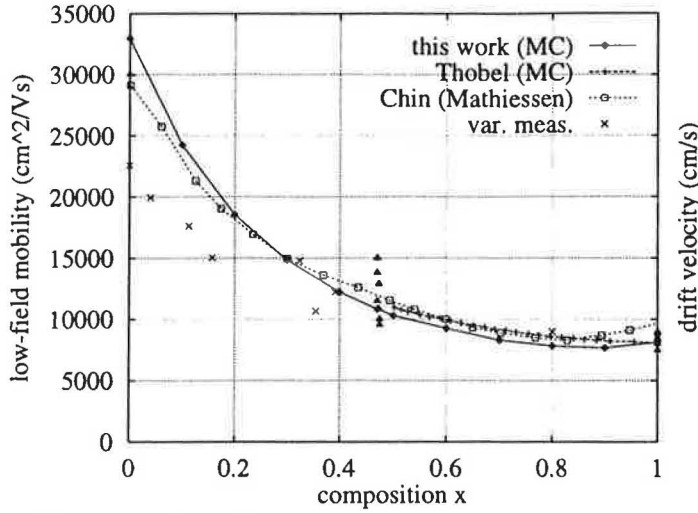


Figure 1. Low-field mobility for $\text{Ga}_x\text{In}_{1-x}\text{As}$ at 300K as function of the composition x .

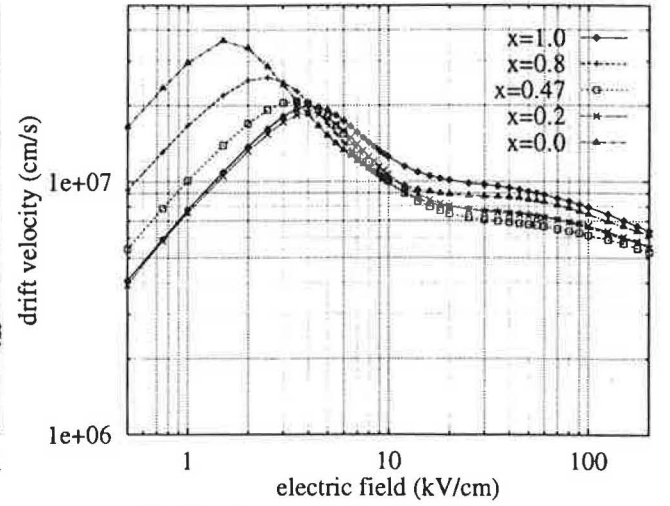


Figure 2. Electron velocity for $\text{Ga}_x\text{In}_{1-x}\text{As}$ at 300K as function of the electric field.

Table 1. Material parameters used in MC calculation.

Quantity	GaAs			InAs			Unit	
a	5.653			6.058			Å	
v_l	5.23			4.28			10^5cm/s	
v_t	2.47			2.65			10^5cm/s	
ϵ_s	12.9			15.15			ϵ_0	
ϵ_∞	10.92			12.75			ϵ_0	
ρ	5.36			5.67			g/cm^3	
$\hbar\omega_{LO}$	36.25			30.2			meV	
		Γ	L	X	Γ	L	X	
E		1.439	1.769	1.961	0.36	1.442	1.98	eV
m^*		0.063	0.22	0.41	0.023	0.29	0.64	m_0
α		0.61	0.461	0.204	1.39	0.536	0.90	eV^{-1}
D_{ac}		7.0	9.2	9.27	8.0	8.0	8.0	eV
D_o		—	3.0	—	—	3.0	—	10^8 eV/cm
D_{ij}	Γ	—	10.0	10.0	—	10.0	10.0	10^8 eV/cm
	L	10.0	10.0	5.0	10.0	10.0	9.0	10^8 eV/cm
	X	10.0	5.0	7.0	10.0	9.0	9.0	10^8 eV/cm
$\hbar\omega_{ij}$	Γ	—	27.8	29.9	—	27.8	29.9	meV
	L	27.8	29.0	29.3	27.8	29.0	29.3	meV
	X	29.9	29.3	29.9	29.9	29.3	29.9	meV
C_Γ				0.44			eV	
C_L				1.10			eV	
C_X				2.0			eV	
D_{all}				0.5			eV	

where j denotes the current density and S the energy flux. A and B are constants with respect to the moments. The balance equations for momentum and energy read in the

stationary homogeneous case

$$\mathbf{j} = q\mu n \mathbf{E} \quad \mathbf{j} \cdot \mathbf{E} = n \frac{w - w_0}{\tau_w}, \quad (3)$$

where w_0 is the equilibrium energy, and τ_w denotes the energy relaxation time which is assumed to be constant. This gives the mobility as function of w ,

$$\mu(w) = \frac{\mu_0}{1 + \eta(w - w_0)} \quad \eta = \frac{\mu_0}{q\tau_w v_s^2}. \quad (4)$$

This dependence represents the well-known saturation curve in silicon via the explicit $w(\mathbf{E})$ relation which can be obtained from (3).

4.2. The new model

However, because of the different band structure of compound semiconductors a different behavior is observed from MC results (Fig. 4). A much steeper decay is clearly evident, which can be related to intervalley transfer.

In principle two different approaches for dealing with the many-valley bands of compounds can be thought of. Firstly, one could introduce a carrier concentration for each valley and find models as functions of the average energy of that carrier types (measured from the valley minimum). The intervalley processes must be accounted for via energy dependent generation terms in the balance equations. This approach increases the number of PDEs, both the number of variables and the model complexity are increased too. Keeping in mind the rather poor convergence of the HD method itself, it is not often used. Secondly, one retains the single electron model in the calculation, where the different valleys are lumped together into the physical models, thus using a single energy variable. This approach is pursued in our work.

4.2.1. The valley mobilities. We propose a functional relation for each valley ($i = \Gamma, L, X$) which is a modified version of (4)

$$\mu_i(w) = \frac{\mu_{0,i} \left(\frac{w}{w_{0,i}} \right)^{\gamma_i}}{1 + \left(\frac{w - w_{0,i}}{\delta_i} \right)^{\beta_i}}. \quad (5)$$

The equilibrium energy $w_{0,i}$ in the nonparabolic case can be expressed as

$$w_{0,i} \cong \frac{3kT}{2} \left(1 + \frac{5}{2}z - 5z^2 \right) \quad z = \alpha_i kT, \quad (6)$$

where α denotes the nonparabolicity parameter. (6) results from series expansion of the integral representation of the average energy. The parameter γ describes the mobility at low energies i.e. when intervalley scattering does not play any significant role. γ is the energy exponent of the prevalent scattering process in this range. In direct compounds polar-optic phonon scattering yields a value of $\gamma \approx 0.5$. δ can be viewed as the energy at which intervalley transfer starts to be important (at the band edge difference), the exponent β reflects the amount of energy that an electron changes when it moves to a different valley.

Usually the total kinetic energy w is split into a drift and a thermal part, $w = \frac{m^* \langle v \rangle^2}{2} + \frac{3kT_c}{2}$. In parabolic valleys $w = \frac{m^* \langle v^2 \rangle}{2}$, in nonparabolic valleys w is generally higher. In the many-valley case the total energy consists of kinetic and potential energy, $w = w_{kin} + w_{pot} = \sum_i n_i (w_i + \Delta E_i) / \sum_i n_i$, where n_i is the population of the i th valley. Fig. 3 depicts the energy versus field relations.

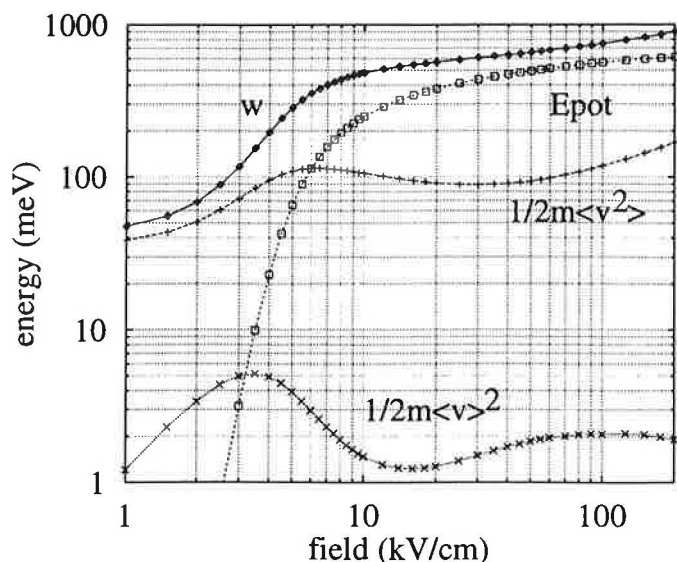


Figure 3. Energy vs. electric field for $\text{Ga}_{47}\text{In}_{0.53}\text{As}$.

4.2.2. *The combined mobility.* Having defined the valley mobilities, we can calculate the total mobility by weighing the valley contributions by the valley populations, $\mu(w) = \sum_i n_i(w) \mu_i(w) / \sum_i n_i(w)$. It is known that the distribution function in high fields deviates significantly from the drifted Maxwellian. However, we find it a useful approximation to assume a modified heated Maxwellian leading to a relative population of valley i with respect to the lowest one,

$$n'_i(w) = \frac{n_i}{n_1} = R_i \exp\left(-a \frac{\Delta E_i}{w}\right), \quad (7)$$

where a is a factor describing the different scaling in energy (the total energy w is used instead of the kinetic energy) and R takes into account valley degeneracy and the carrier masses.

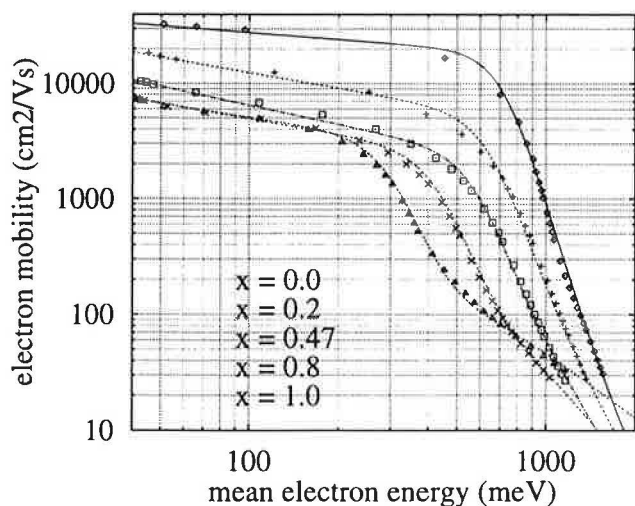


Figure 4. Total mobility for $\text{Ga}_x\text{In}_{1-x}\text{As}$ at 300K as function of the total energy w with material composition x as parameter.

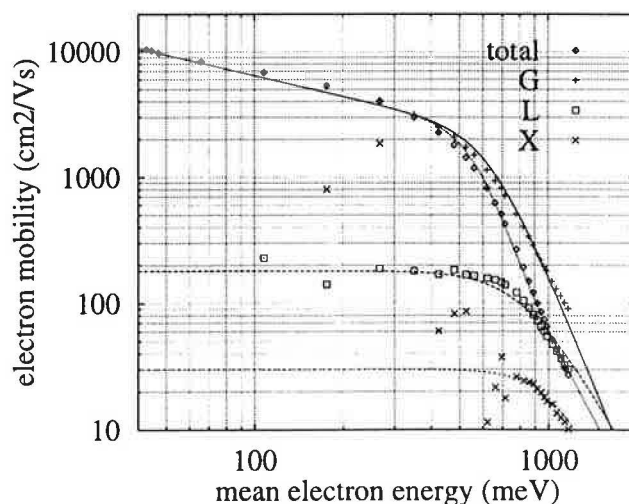


Figure 5. Valley specific mobilities for $\text{Ga}_{47}\text{In}_{0.53}\text{As}$ at 300K as function of the total energy w .

Table 2. Model parameters for $\text{Ga}_x\text{In}_{1-x}\text{As}$ obtained from MC calculation.

$\mu_{0,\Gamma}$ (cm^2/Vs)	$32900 - 101900x + 181820x^2 - 166910x^3 + 62270x^4$
$\mu_{0,L}$ (cm^2/Vs)	$234.8 - 304.4x + 429.7x^2$
$\mu_{0,X}$ (cm^2/Vs)	$27.2 - 91.8x + 204.3x^2$
δ_Γ (meV)	$734.1 - 770.9x + 320.5x^2$
δ_L (meV)	$1108.5 - 1403.5x + 748.7x^2$
δ_X (meV)	$1604.2 - 2528.9x + 1475.8x^2$
β_Γ	$5.82 - 2.85x + 2.13x^2$
β_L	$7.0 - 5.2x + 0.2x^2$
β_X	$5.0 + 1.47x - 4.63x^2$
γ_Γ	$-0.23 - 0.98x + 0.83x^2$
γ_L	0
γ_X	0
a	4.0

5. Results

As an example the new mobility model is demonstrated for $\text{Ga}_x\text{In}_{1-x}\text{As}$, an important channel material used in heterostructure FETs. The parameters β , γ , δ are obtained by a nonlinear least-square fitting algorithm. The result at 300K is given in Table 2. A good correspondence between the new model (lines) and the MC results (symbols) is obtained (Fig. 4 and 5).

Acknowledgments

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References

- [1] Jacoboni C and Lugli P 1989 *The Monte Carlo Method for Semiconductor Device Simulation* (Vienna-New York: Springer)
- [2] Selberherr S 1984 *Analysis and Simulation of Semiconductor Devices* (Vienna-New York: Springer)
- [3] Nag B R 1980 *Electron Transport in Compound Semiconductors* (Berlin-Heidelberg-New York: Springer)
- [4] Fischetti M V 1991 *IEEE Trans. on Electr. Dev.* **38** 634–649
- [5] Hänsch W and Miura-Mattauch M 1986 *J. Appl. Phys.* **60** 650–656
- [6] Chin V W L and Tansley T L 1991 *Solid-State Electr.* **34** 1055–1063
- [7] Thobel J L *et al* 1990 *Appl. Phys. Lett.* **56** 346–348