A Self-Consistent Multisubband Model for Calculation of Scattering Rates in Quantum Well Structures *

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Abstract

A new efficient self-consistent multisubband model for calculation of scattering rates of electrons in the quantum well structures is presented. Yokoyama and Hess[1] previously presented a field-dependent model for calculation of electron mobility in $Al_{1-x}Ga_xAs/GaAs$ single well heterostructures by using a self-consistent Monte-Carlo simulator, which provides an accurate estimation of carriers mobility, but with very high computational expense. We previously reported a self-consistent Schrodinger-Poisson solver[2,3] in a two-dimensional numerical model for High Electron Mobility Transistor. In this paper we have used our Schrodinger-Poisson solver and have calculated the field-dependent, energy-dependent scattering rates of electrons in the five lowest subbands in the quantum well of an $Al_{1-x}Ga_xAs/GaAs$ heteroface. Our model predicts the scattering rates with almost the same accuracy, but with considerably less computation efforts. In our simulations we have applied external bias and computed the two-dimensional mobilities throughout the structure. The mobilities are calculated from the scattering rates due to polar optical phonons and ionized impurities. Intersubband scattering as well as intrasubband scattering mechanisms are included in the model.

The results obtained agree well with those reported by Yokoyama and Hess[1]. The scattering rates calculated have been used in a two-subband two-dimensional self-consistent numerical model for High Electron Mobility Transistor which is reported elsewhere in this Proceedings.[4]

I. Introduction

To accurately model the behavior of a High Electron Mobility Transistor (HEMT), one must use a field-dependent energy-dependent mobility model. The variations in the electric field throughout the channel (as governed by Poisson equation) and existence of different subbands with different eigenenergies (as governed by Schrodinger equation) necessitate a self-consistent calculation of the electron mobility in the HEMT structure. Further complications arise when electrons are scattered from one subband to another. Other researchers have undertaken the task of studying the carriers transport in HEMT, mainly, and most accurately, by Monte-Carlo simulation of one kind or another. Wang and Hess[5] have studied the distribution of electron velocity at high fields using a three-dimensional Monte Carlo, neglecting the quantum effects. Yokoyama and Hess[1] have self-consistently

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[1] K. Yokoyama and K. Hess, *Phys. Rev. B*, Vol. 33, pp. 5595-5606, 1986.

[2] Z. H. Ng, and R. Khoie, *IEEE Trans. on Electron Devices*, Vol. 38, No. 4, pp. 852-861, April 1991.

[3] Z. H. Ng, and R. Khoie, *Computational Electronics, Semiconductor Transport and Device Simulation*, edited by: K. Hess, J. P. Leburton, and U. Ravaioli, Kluwer Academic, pp. 55-58, January 1991.

[4] R. Khoie and H. Arman, *Elsewhere in this Proceedings*, May 1992.

[5] T. Wang and K. Hess, *J. Appl. Phys.*, vol. 57, pp. 5336-5339, 1985.

included the quantum effects in their Monte Carlo simulator and studied the electronic transport in a single well heterostructure. The Monte Carlo method they used is very computationally intensive. The computations involved can greatly be reduced, without significant loss of accuracy, by employing a two-dimensional model based on the moments of Boltzmann Transport Equation. We[2,3]previously extended Widiger's[6] work to include the effect of the quantization of the electrons in the quantum well by means of a self-consistent treatment of Schrödinger's and Poisson's equations.

In this paper we have used our previous Schrodinger-Poisson solver to evaluate the scattering rates due to polar optical phonons and remote ionized impurities. The results obtained agree well with those reported by Yokoyama and Hess[1]. These scattering rates are used to calculate the mobilities which have been used in a two-subband two-dimensional self-consistent numerical model for High Electron Mobility Transistor which is reported elsewhere in this Proceedings[4].

II. Self-Consistent Calculation of Scattering Rates

Our Schrodinger-Poisson solver consists of a simultaneous solution of Poisson equation:

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = -\frac{q}{\epsilon}[N_D(x,y) - n(x,y)], \tag{1}$$

and Schrodinger equation:

$$-\frac{\hbar^2}{2m_x}\frac{d^2\psi_i(x)}{dx^2} - qV(x,y)\psi_i((x) = E_i\psi_i(x) \tag{2}$$

Together with the two higher moments of Boltzmann Transport Equation:

$$\frac{\partial[n_i(x,t)]}{\partial t} = \nabla.[-\mu_i n_i(x,t)\nabla V(x) + \nabla(D_i n_i(x,t))] + G_i \qquad i = 1,...,5 \tag{3}$$

$$\frac{\partial(n_i(x,t)E_i(x,t))}{\partial t} = -J.\nabla V(x) + \nabla.(-\mu_{E,i} n_i(x,t)E_i(x,t)\nabla V(x) + \nabla(D_{E,i} n_i(x,t)E_i(x,t))) + F_i \quad i = 1,...,5 \tag{4}$$

In these equations n and J are the electron concentration and current, respectively. μ_i, D_i, $\mu_{E,i}$, and $D_{E,i}$ are the mobility, and diffusivity of carriers, and energy flux, respectively. The terms G_i and F_i account for the transfer of electrons and their energies among the subbands.

The polar optical-phonon scattering and the ionized impurity scattering are the main scattering mechanisms encountered in III-V compound semiconductors. For independent scattering mechanisms, the total scattering rate is defined by:[7]

$$\frac{1}{\tau_{tot}^{all}} = \frac{1}{\tau_{tot}^{I}} + \frac{1}{\tau_{tot}^{pop}} = \sum S(\mathbf{K_1}, \mathbf{K_2}) \tag{5}$$

where the subscript I denotes impurity scattering and *pop*, the polar optical-phonon scattering, τ is the relaxation time, and $S(\mathbf{K_1}, \mathbf{K_2})$ is the probability of an electron being scattered. The polar optical phonon scattering rate is given by:[8]

$$S_{mn}^{pop} = \frac{e^2\omega_0}{8\pi\epsilon_0}\left[\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s}\right](N_q + \frac{1}{2} \pm \frac{1}{2}) \times \int \frac{H_{mn}(Q)}{Q}\delta(E(\mathbf{k_2}) - E(\mathbf{k_1}) \pm \hbar\omega_0)d\mathbf{k_2} \tag{6}$$

[6]D. J. Widiger, I. C. Kizilyalli, K. Hess, and J. J. Coleman, *IEEE Trans. Electron Devices*, vol. ED-32, 1092-1102, 1985.

[7]K. Hess, *Advanced Theory of Semiconductor Devices*, Englewood Cliffs, New Jersey, Prentice Hall, 1988.

[8]K. Yokoyama and K. Hess, *The American Physical Society*, Vol.31, no. 10, pp. 6872-6874, May 1985.

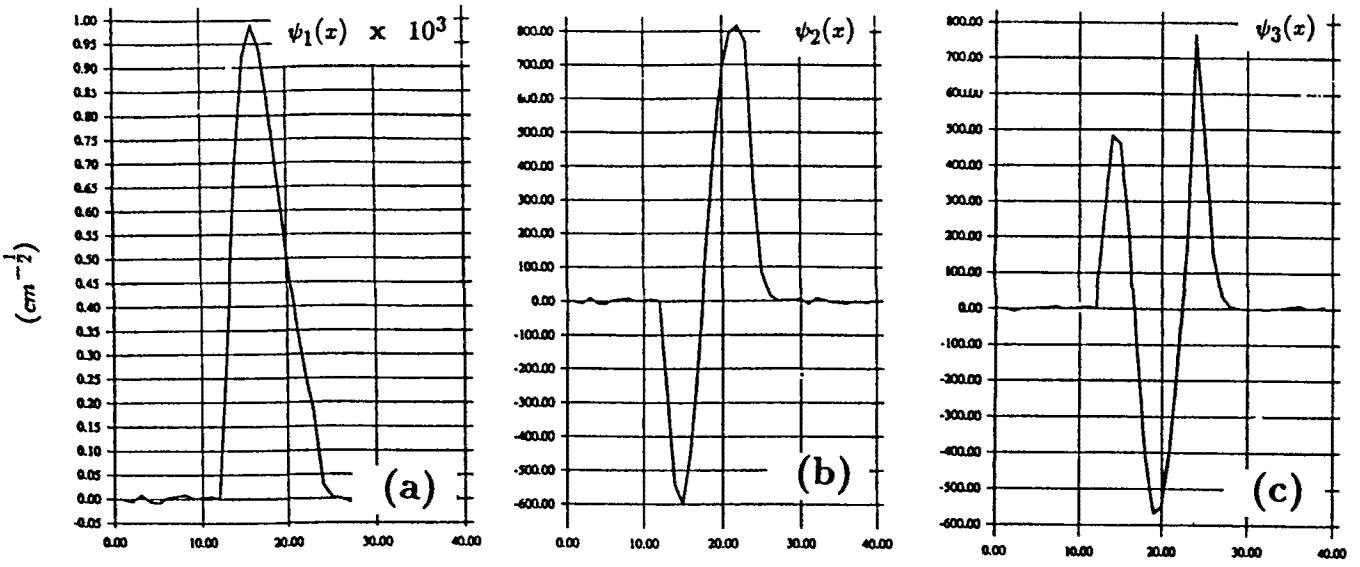

Figure 1: Wavefunction for (a) first, (b) second, and (c) third subbands.

where, ϵ_∞ and ϵ_s are the optical and static dielectric constant, $\hbar\omega_0$ is the polar-optical-phonon energy, Q is the phonon wave-vector component parallel to the interface, k_1 and k_2 denote the initial and final state wave vectors. N_q is the phonon occupation number, and $E(\mathrm{k}_1)$ and $E(\mathrm{k}_2)$ are the initial and final state energy. $H_{mn}(Q)$'s are the multisubband coupling coefficients.

The ionized impurity scattering rate is given by:[1]

$$S_{mn}^{imp} = \frac{1}{2\pi\hbar}\int |M_{mn}(Q)|^2 \delta(E(\mathrm{k}_2) - E(\mathrm{k}_1))d\mathrm{k}_2 \tag{7}$$

The matrix elements $M_{mn}(Q)$ account for the electron-impurity interactions.

III. Results and Conclusions

The wavefunctions, ψ_i, for the first three subbands are shown in Fig. 1. The wavefunction for the first subband peaks at a distance of about $17nm$ from the heterojunction, to a value of about $1000/\sqrt{cm}$. The highest peak for the second subband is located at 22 nm, and for the third subband at 24 nm. The multisubband coupling coefficients $H_{1n}(Q)$ are shown in Fig. 2 along with those reported by Ref. [1]. The agreement between the two sets of data is good. The polar optical-phonon scattering rates as a function of energy for the first subband at 300°K are shown in Fig. 3. Again, the agreement between the results of our model and those calculated by Ref [1] is very good.

The calculated values of $|M_{mn}(z_0)|^2$ vs location z_0 (a generalized position coordinate; in our case x_0) at 300°K with $Q = 1.86\ x\ 10^6$ for (1,1) transitions, and $Q = 1.84\ x\ 10^6$ for (1,2) transitions, and $Q = 8.22\ x\ 10^6$ for (3,3) transitions are shown in Fig. 4, with the results reported by Yokoyama and Hess[1] being shown in Fig. (4d). As it was predicted by Ref [1], the peak locations for intrasubband transitions coincide with the z_i's. For example, for the (1,1) transitions, that is, the transitions from the first subband back to the first subband, the peak is at $z_0 = 17nm$, as shown in Fig. 4, which is the same as the peak of the wavefunction shown in Fig. 1. The ionized impurity scattering rates for the first subband are shown in Fig. (5a), and the results obtained by Ref. [1] are shown in Fig. (5b), and they are in good agreement.

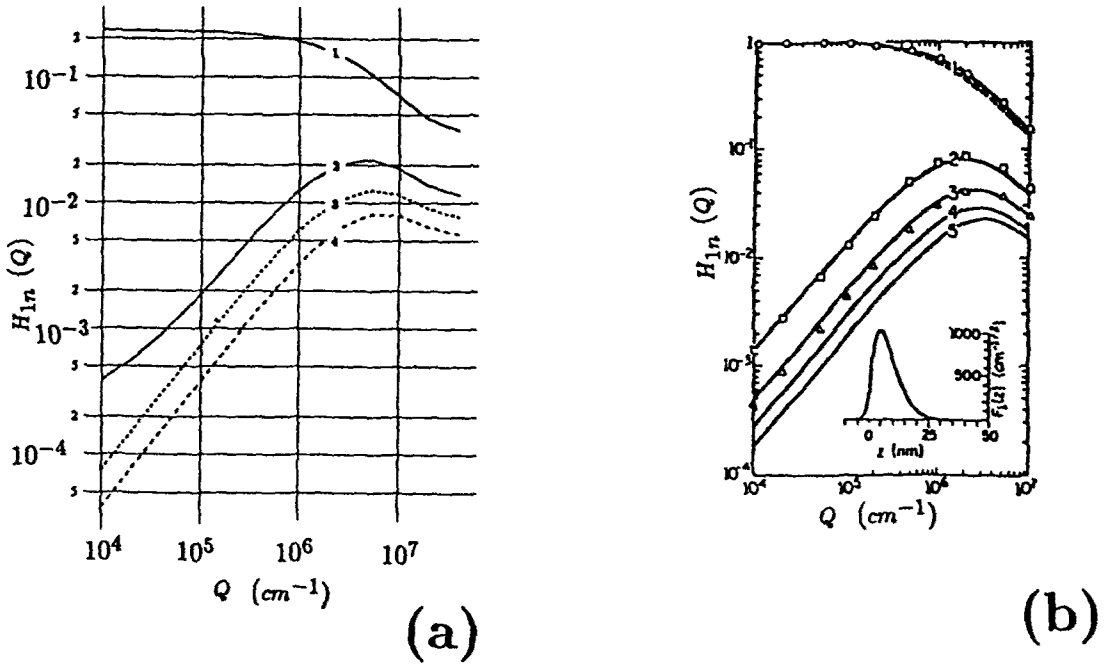

Figure 2: Multisubband coupling coefficients $H_{1n}(Q)$, for transfer of electrons from the first subband to the other subbands as a function of Q, the phonon wave vector, (a) our model, (b) Yokoyama and Hess [1].

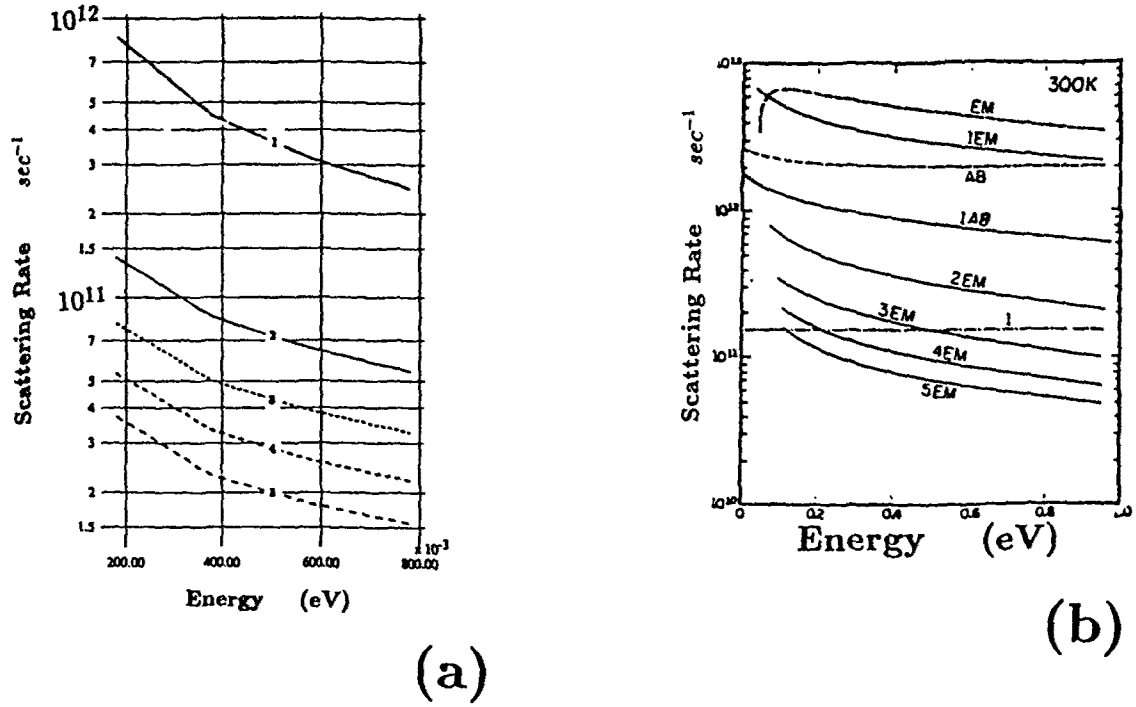

Figure 3: Polar optical-phonon scattering rates vs energy from first subband to the other subbands, (a) our model, (b) Yokoyama and Hess [1].

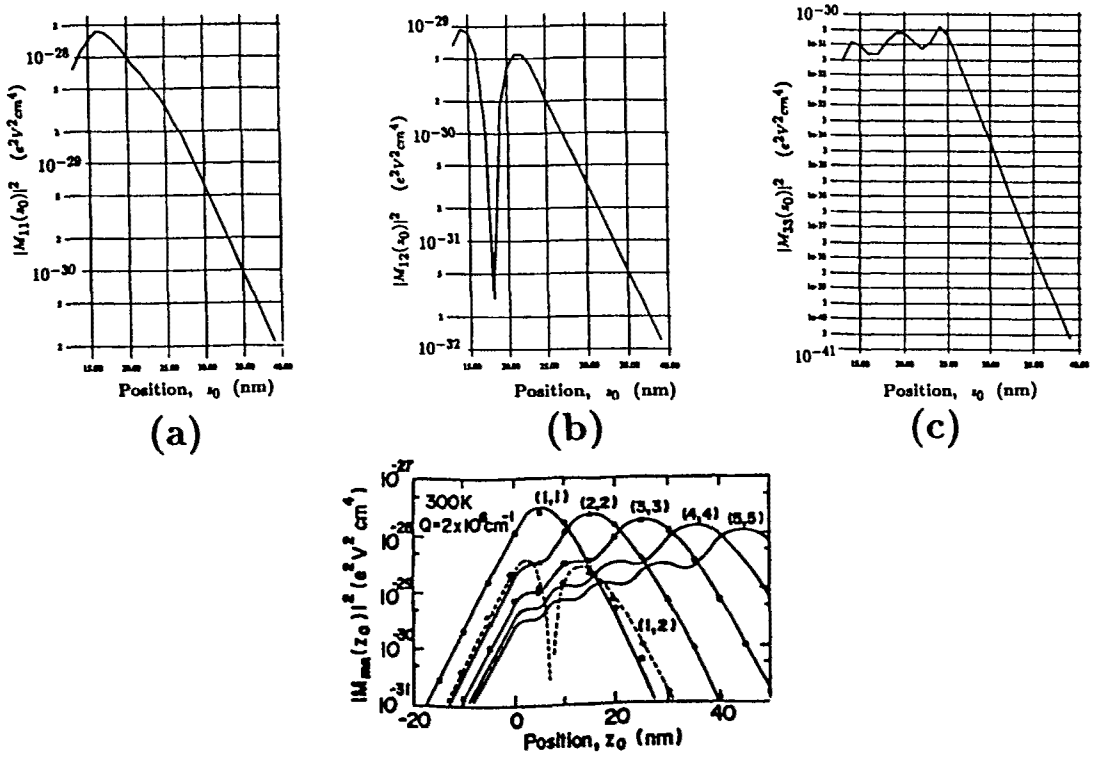

Figure 4: Calculated values of $|M_{mn}(z_0)|^2$ vs location z_0 for (a) (1,1) (b) (1,2), (c) (3,3) intrasubband transitions. The results reported by Yokoyama and Hess [1] are shown in (d).

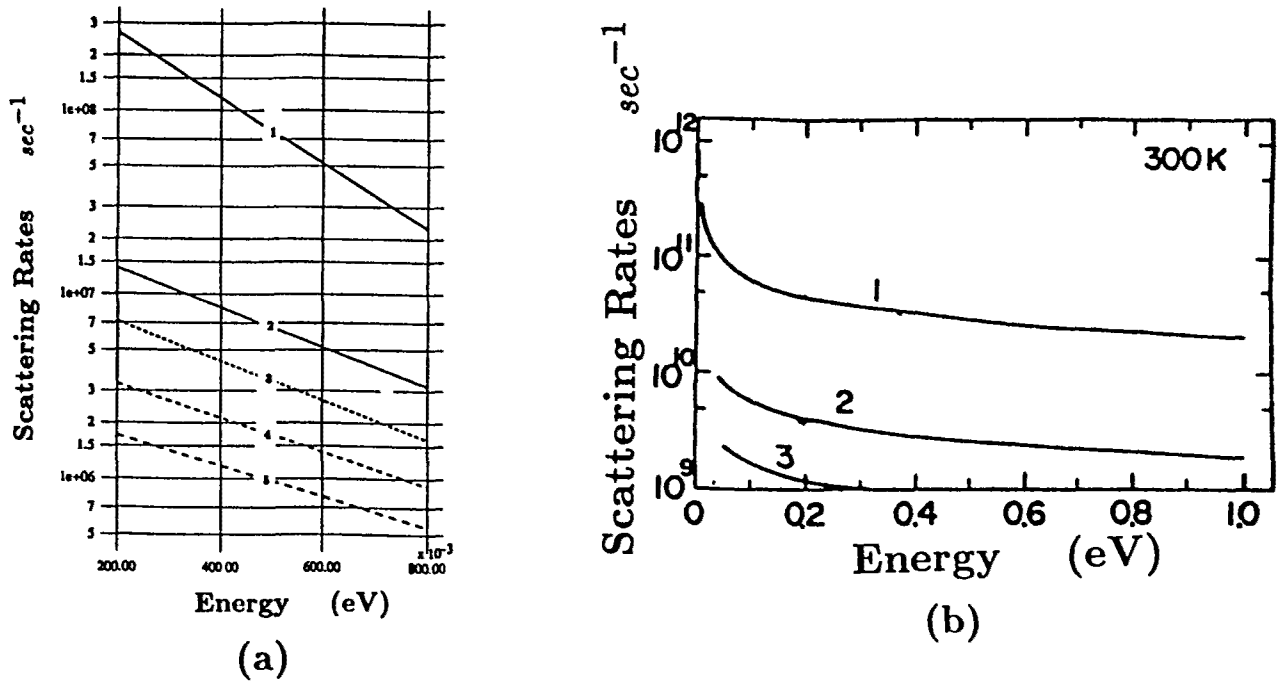

Figure 5: Ionized impurity scattering rates vs energy for the first subband at 300 K calculated by (a) our model, (b) Yokoyama and Hess [1].