Transport Coefficients For A GaAs Hydrodynamic Model Extracted From Inhomogeneous Monte Carlo Calculations

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Abstract
The validity of energy-dependent relaxation times often used in a GaAs hydrodynamic model has been carefully examined using the self-consistent Monte Carlo simulation. We have found that those transport coefficients associated with the intervalley transfer from the lower to the upper valley are not single-valued functions of the averaged electron energy in the valley. If, instead, the valley population ratio or the average energy weighted by the valley population ratio is used a substantial improvement in accuracy can be achieved.

I. Introduction

Conventionally, macroscopic (averaged) relaxation times such as τ_n, τ_p and τ_W appearing in the hydrodynamic (HD) transport equations are assumed energy-dependent and determined by performing Monte Carlo (MC) calculations under steady state and homogeneous field conditions. These expressions are often extended to the case of inhomogeneous fields without any justification. Sandborn et al. [1], using the MC simulation, found that both the energy and momentum relaxation times in an equivalent single-valley model under the transient condition differ very much from the steady state and homogeneous field values. Yamada [2] also observed the discrepancy in the relaxation times between the homogeneous and inhomogeneous field conditions. He suggested that the relaxation times should depend not only on the energy but also on the valley population. In this study, instead of a single-valley model, a three-valley HD model for GaAs has been developed. The transport coefficients appearing in the HD model for homogeneous and inhomogeneos field conditions are evaluated by a single particle MC simulation program and a multi-particle self-consistent MC simulation program, respectively. A one dimensional $N^+ - N - N^+$ GaAs ballistic diode was used as a test device. This approach allows us to rigorously examine the validity of the energy dependence of each relaxation time as well as provides us valuable information for a more appropriate description of the relaxation times.

II. Moments of the Boltzmann Transport Equation

The HD transport equations can be obtained by taking various moments of the Boltzmann transport equation (BTE) [3]. Extending the work of [4], [5] to a multi-valley system, we obtain the following steady-state conservation equations for the ith valley:

$$\nabla \cdot (n_i \vec{V}_i) = [-\frac{n_i}{\tau_{nij}} - \frac{n_i}{\tau_{nik}} + \frac{n_j}{\tau_{nji}} + \frac{n_k}{\tau_{nki}}], \quad (1)$$

$$\frac{1}{n_i}\nabla\cdot(n_i\hat{U}_i)-\vec{F}=-\frac{q\vec{V}_i}{\mu_{ii}}-\frac{q\vec{V}_i}{\mu_{ij}}-\frac{q\vec{V}_i}{\mu_{ik}}, \tag{2}$$

$$\frac{1}{n_i}\nabla\cdot(n_i\vec{S}_i)-\vec{V}_i\cdot\vec{F}=-\frac{W_i-W_0}{\tau_{Wii}}-\frac{W_i}{\tau_{Wij}}-\frac{W_i}{\tau_{Wik}}+\frac{n_j}{n_i}\frac{W_j}{\tau_{eji}}+\frac{n_k}{n_i}\frac{W_k}{\tau_{eki}}, \tag{3}$$

$$\frac{1}{n_i}\nabla\cdot(n_i\hat{R}_i)-(W_i\hat{I}+\hat{U}_i)\cdot\vec{F}=-\frac{q\vec{S}_i}{\mu_{sii}}-\frac{q\vec{S}_i}{\mu_{sij}}-\frac{q\vec{S}_i}{\mu_{sik}}, \tag{4}$$

where $\vec{V}_i=\langle\vec{v}_i\rangle, \hat{U}_i=\langle\vec{v}_i\hbar\vec{k}_i\rangle, W_i=\langle\varepsilon_i\rangle, \vec{S}_i=\langle\vec{v}_i\varepsilon_i\rangle$ and $\hat{R}_i=\langle\varepsilon_i\vec{v}_i\hbar\vec{k}_i\rangle$. In the conventional HD transport model, the transport coefficients (τ_n, μ, τ_W,etc.) are usually assumed to depend on the average energy,$W(\vec{r})$. This approach ignores the dependence of the transport coefficients on the shape of the distribution function.

III. Self-Consistent Monte Carlo Simulation

To examine the accuracy of energy-dependent transport coefficients, we begin with a rigous solution of the steady-state BTE by the MC method. The simulation program uses an analytical multi-valley, non-parabolic band. The following types of scattering are taken into account: acoustic phonon scattering, optical phonon scattering, polar optical phonon scattering, ionized impurity scattering, equivalent and nonequivalent intervalley scattering. The various scattering parameters are similar to those used in [6]. In this work, a one-dimensional N^+-N-N^+ GaAs structure with a 0.5 μm N-region was examined. The doping densities of the three layers were $N_d=1\times10^{17}cm^{-3}, 1\times10^{16}cm^{-3}$ and $1\times10^{17}cm^{-3}$, respectively. The applied bias was 2.0 volts. Fig. 1 displays the doping density and electric field profiles within the device as obtained from the self-consistent MC (SCMC) simulation. Fig. 2 shows the $\Gamma-$ valley velocity and energy profiles.

IV. Results and Discussions

At each position within the device we evaluated the transport coefficients and the average energy in each valley by the SCMC program. We found that these coefficients are generally a function of the local average energy in the valley except for those due to the intervalley transfer from the lower to the upper valley (i.e. $\Gamma\rightarrow L$, $\Gamma\rightarrow X$, and $L\rightarrow X$.). Figs.3,5 and 7 respectively display the $\Gamma\rightarrow L$ intervalley transfer coefficients, $\tau_{n\Gamma L}, \mu_{\Gamma L}$ and $\tau_{W\Gamma L}$ versus the average $\Gamma-$valley energy, W_Γ, for both the homogeneous and the inhomogeneous field calculation. The "hysteresis" loops clearly indicate that none of them can be described as a single-valued function of W_Γ. For these cases, the energy-dependent transport coefficients which were obtained from the homogeneous field calculation always underestimate the actual one in the increasing field region and overestimate the same in the decreasing field region. If, instead, W_Γ is weighted by the valley population ratio (i.e., $\frac{n_L}{n_\Gamma}W_\Gamma$) then the hysterisis loop for $\tau_{n\Gamma L}$ can be significantly reduced (see Fig. 4). This is motivated by the fact that the valley population ratio more or less reflects the fraction of electron population which have sufficient energy to transfer from the lower to the upper valley. We also found that using the valley population ratio alone (i.e., $\frac{n_L}{n_\Gamma}$) the hysterisis loop can be considerably reduced for $\mu_{\Gamma L}$ and $\tau_{W\Gamma L}$ as seen in Figs.6 and 8,respectively.

The result for $\tau_{e\Gamma L}$ is very similar to $\tau_{W\Gamma L}$ and that for $\mu_{s\Gamma L}$ is similar to $\mu_{\Gamma L}$. Once the hysterisis loop is reduced, these transport coefficients can now be modelled empirically as single-valued functions of the valley population ratio or the energy weighted by the valley population ratio.

V. Conclusions

A SCMC simulation program was used to examine the conventional assumption of energy-dependent transport coefficients in a multi-valley system. We found that the transport coefficients related to the intervalley transfer from the lower to the upper valley (i.e., $\Gamma \rightarrow L$, $\Gamma \rightarrow X$ and $L \rightarrow X$) are not a single-valued function of the average energy in the valley. A substantial improvement in the accuracy can be achieved if the valley population ratio or the average energy weighted by the valley population ratio is used.

Acknowledgement

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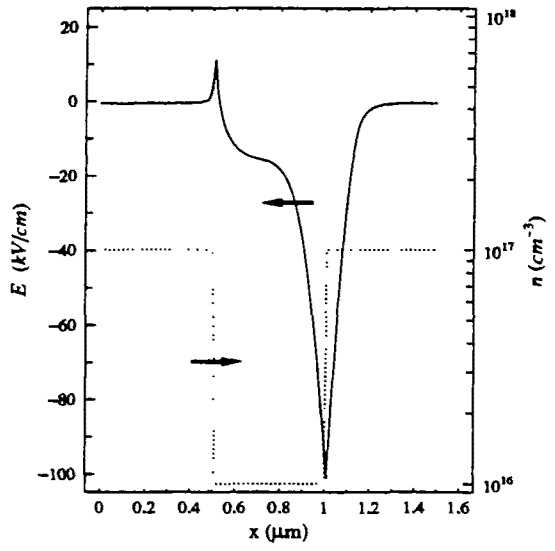

Figure 1: Impurity doping profile and its self-consistent electric field for an abrupt $N^+ - N - N^+$ structure with an applied bias of 2.0 volts.

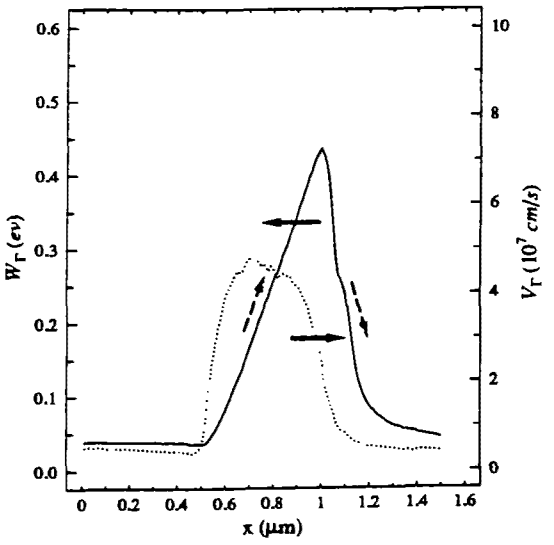

Figure 2: Average electron energy and velocity in the $\Gamma-$valley.

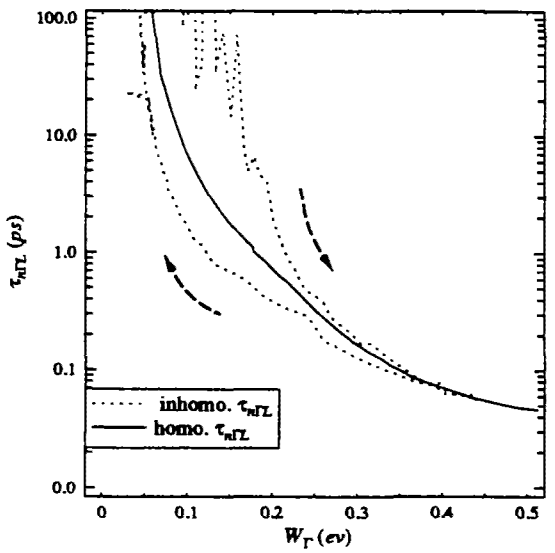

Figure 3: Carrier relaxation time , $\tau_{n\Gamma L}$, versus the average $\Gamma-$valley energy,W_Γ.

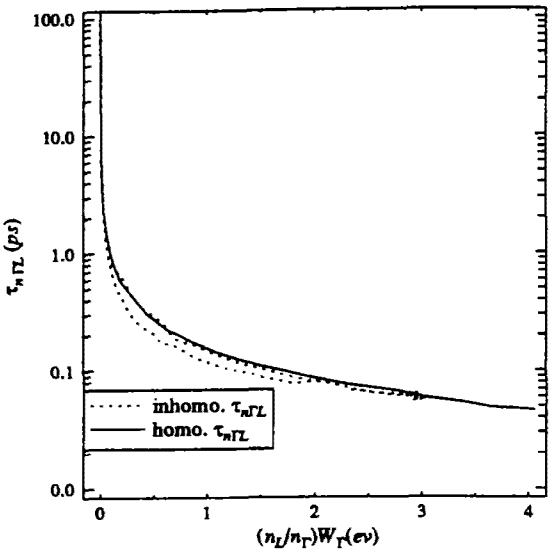

Figure 4: Carrier relaxation time , $\tau_{n\Gamma L}$, versus $(\frac{n_L}{n_\Gamma})W_\Gamma$.

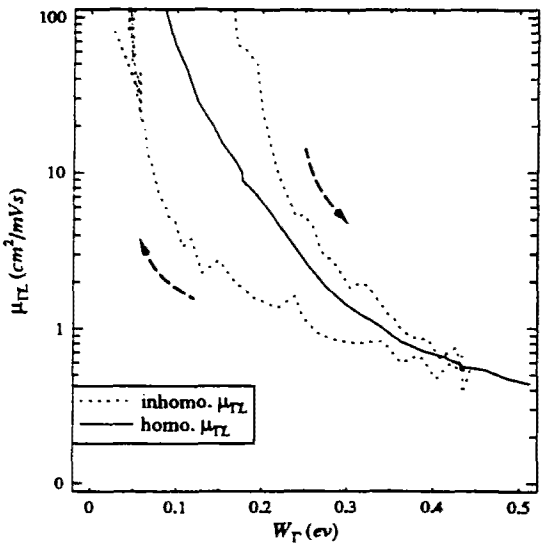

Figure 5: Carrier mobility , $\mu_{\Gamma L}$, versus the average $\Gamma-$valley energy,W_Γ.

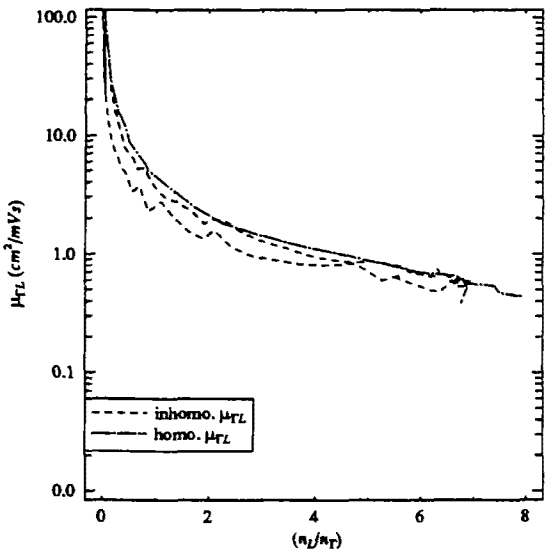

Figure 6: Carrier mobility , $\mu_{\Gamma L}$, versus $(\frac{n_L}{n_\Gamma})$.

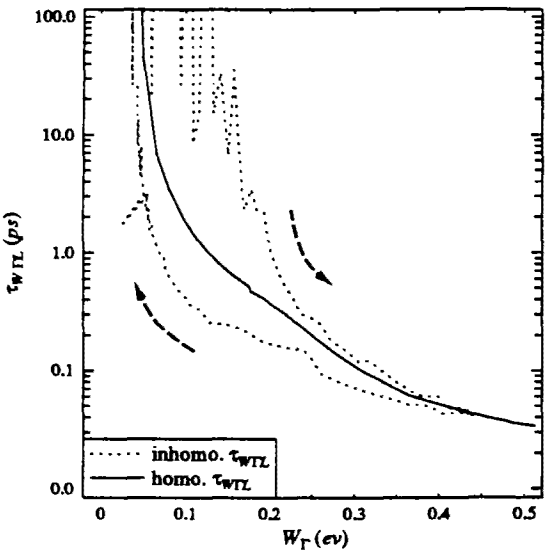

Figure 7: Energy relaxation time , $\tau_{W\Gamma L}$, versus the average $\Gamma-$valley energy,W_Γ.

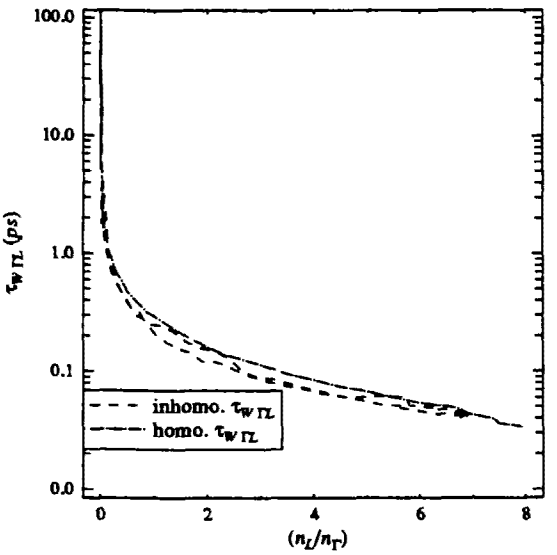

Figure 8: Energy relaxation time , $\tau_{W\Gamma L}$, versus $(\frac{n_L}{n_\Gamma})$.