Hole Transport in the Warped Band Model of GaAs

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Abstract
Hole transport in the warped band model of GaAs has been investigated using an Ensemble Monte Carlo approach. Scattering rates used in the simulations were derived for warped heavy and light hole bands and for a spherical split-off band. The obtained velocity-field characteristics are in better agreement with experimental data than recently published values where only the heavy and light hole bands were included in the model and warping was accounted for by an approximate overlap function. Simulations show that a better fit to the experiment and to results of a realistic band structure model can be attained with an optimal choice of valence band parameters.

I. Introduction

The performance of semiconductor devices, such as bipolar transistors, p-channel field-effect transistors and heterojunction bipolar transistors, is determined by hole transport proprieties. In some earlier studies, warping of the valence band has been either ignored[1] or taken into account by the use of an approximate overlap function[2]. The split-off band has also been mostly ignored due to its relatively low population. However, warping and the effect of the spin-orbit interaction on the heavy and light hole band cannot be overlooked if precise hole transport modeling is an issue. Brennan and coworkers[3, 4] used the Monte Carlo method in their investigation of hole transport in a realistic band structure. However, high precision is achieved that way at the expense of CPU time. Recently Brudevoll and coworkers[5] pointed to the fact that scattering rates often used in literature for ionized impurity scattering, inter-band polar optical phonon scattering and acoustic phonon scattering rates require corrections. Brudevoll and coworkers[2] studied the warm and hot hole drift velocity in GaAs using a valence band model made of a heavy and a light hole band, and warping of the valence bands was taken into account by the use of an approximate overlap function.

In this paper, hole transport in a warped valence band model of GaAs is investigated using an Ensemble Monte Carlo program. The scattering rate calculations for intra- and inter-band hole scattering take warping and the overlap integrals into account. Hole velocities were obtained for different sets of warping parameters and for fields up to 100kV/cm. Simulation results using this simple model are compared to the results of Brudevoll and coworkers[5], Brennan and coworkers[3], and to the experimental data of Holway and coworkers[6]. The Monte Carlo model used in this work is presented next. The results of the simulation are discussed in section III. Conclusions are given in section IV.

II. The Monte Carlo Model

The Monte Carlo approach is used in this work to investigate hole transport for fields applied along the $\langle 100 \rangle$ direction. The valence band model includes warped heavy and light hole bands and a parabolic split-off band. For the warped bands, the energy is given by:

$$E(k) = \frac{|A|\hbar^2 k^2}{2m_o}\left[1 \pm g(\theta, \phi)\right] \tag{1}$$

where

$$g(\theta,\phi) = \left[(B/A)^2 + (C/A)^2(\sin^2\theta\cos^2\theta + \sin^4\theta\cos^2\phi\sin^2\theta)\right]^{1/2} \tag{2}$$

Above, the +(-) sign correspond to the light(heavy) hole band, $\theta(\phi)$ is the polar(azimuthal) angle of $\mathbf{k}$, and A, B, and C are the inverse band mass parameters. The set of parameters (A=-6.98, B=-4.5, C=6.2) given by Madelung[7], and the sets (A=-7.98, B=-5.16, C=6.56) and (A=-7.65, B=-4.82, C=7.7) used by Brudevoll and coworkers[5] are adopted in simulations. The mass of the holes in the warped bands is direction dependent and is given by:

$$m_h = \frac{m_o}{A\,(1 \pm g(\theta,\phi))} \tag{3}$$

For the split-off band, a spherical equi-potential surface is assumed with a scalar effective mass. Scattering mechanisms included are the acoustic phonon, optical phonon scattering, screened polar optical phonon, with intra- and inter-band transfers for all three bands. Impurity scattering is not included for simplicity.

The scattering rates contain overlap factors which are approximated by functions derived by Wiley[8]. The resulting expressions become easy to use in Monte Carlo calculations. In the particular case of ionized impurity scattering, Jacoboni and Reggiani[9] propose to neglect a weak warping in the process of scattering process determination, but use a corrected effective mass. Warping would be taken into account in final state determination. Such approach is justified as warping has a noticeable effect on next state determination rather than on the values of the scattering rates. Tiersten[10], for example, found that the valence band anisotropy can result in hole mobility variation of up to 20%, while the scattering rates vary by less than 1.%. In our Monte Carlo program, scattering rates are evaluated at each time step so that angular evolutions could be observed. The scattering rates for the acoustic and optical non-polar scattering are weighted by an overlap factor of 1/2 while the polar optical transition rates are integrated taking the overlap factor into account. The final states are determined by applying the rejection technique to the exact angular probability functions containing angular contributions from both warping and the overlap integral. The results of the simulations will be presented in the following section.

III. Results and Discussion

The velocity-field characteristics were calculated for the current model at 300K lattice temperature. Figure 1 shows the obtained velocities for the same parameters used by

Brudevoll and coworkers[2]. Also shown are the experimental results of Holway and coworkers[6]. The recent results of Brudevoll and coworkers overestimate the hole drift velocity at all fields. It is obvious from figure 1 that the current calculations, which take into account the direction dependence of the hole mass, are in better agreement with the experiment. The inclusion of the split-off band doesn't have a strong effect at low fields as its hole population is low. However, its contribution to the hole velocity becomes important at fields higher than 60kV/cm. It is also above that field that the current model and the model of Brudevoll and coworkers don't realize a complete velocity saturation. Figure 2 illustrates the dependence of the hole drift velocity on warping parameters. The shown simulation results were obtained using 3 sets of valence band parameters and GaAs parameters taken from reference [4]. The set (A=-6.98, B=-4.5, C=6.2) by Madelung[7] and (A=-7.65, B=-4.82, C=7.7) result in almost equal velocity curves and band warping. These results overestimate the velocity at high fields when compared to experimental data and the results of Brennan and coworkers[3] obtained using a more complete valence band model. However, for fields below 60kV/cm results closer to the experiment can be obtained by an optimal choice of valence band parameters.

IV. Conclusion

We have investigated hole transport in the warped band model of GaAs, using an Ensemble Monte Carlo program. The velocity-field characteristics for three recently reported valence band parameters have been shown to be between the recent results of Brudevoll and coworkers[5], the results of Brennan and coworkers[4] and the experimental data of Holway and coworkers[6]. The current model, though simple, coupled to an optimal choice of valence band parameters, results in velocity-field characteristics consistent with previously published data. This model could be useful in the study of anisotropy dependent phenomena, such as orientational relaxation of carrier momentum.

References

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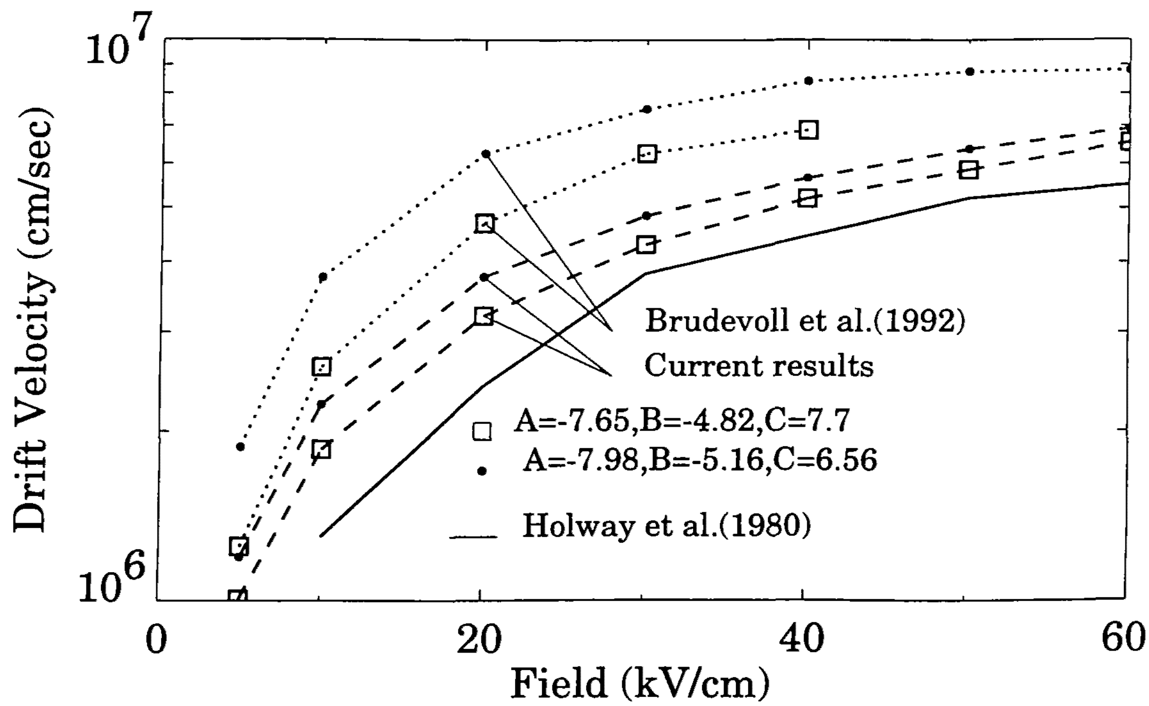

Fig.1. Velocity-Field characteristics for holes

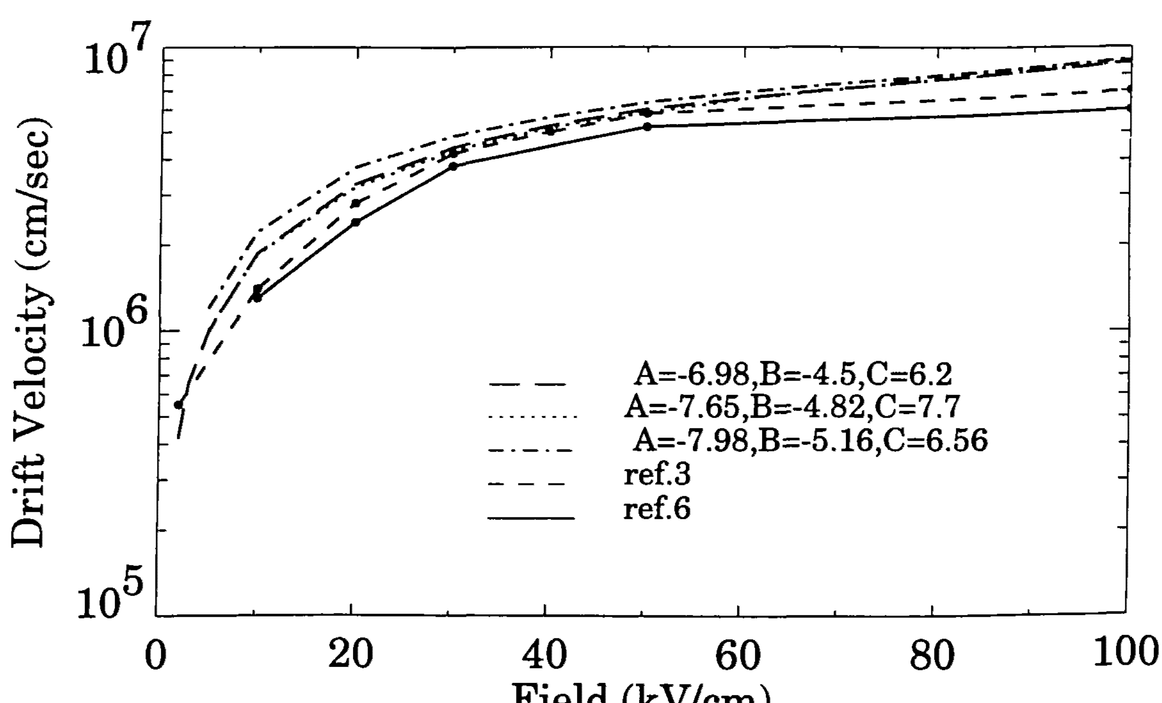

Fig.2. Velocity-Field characteristics for holes for different valence band parameters.