BIPOLAR MONTE CARLO - AN IMPROVED VALENCE BAND MODEL FOR GaAs

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Abstract

A novel Monte Carlo model of hole transport in GaAs intended for self-consistent device simulation is described. The model employs an isotropic effective mass representation of the valence band structure and energy dependent nonparabolicity factors. This comprises a simplification of numerical representations of the valence bands. Results are presented, and compare well with reported experimental and Monte Carlo data. Hole energy and momentum relaxation times are calculated and the effect of split-off holes on transport characteristics is shown to be negligible.

Introduction

The computer simulation of bipolar or p-type devices, such as the GaAs photodiode [1] which prompted this study, requires an accurate model of hole transport. In GaAs this poses a problem as hole transport is much less well characterised than that of electrons.

In the case of Monte Carlo simulations hole transport models depend upon the valence band energy/wave vector relationships - the *band structure*. These are highly complex, being both nonparabolic and anisotropic. Numerical techniques may be employed to characterise the band structure fully [2], but it is felt that this approach may be prohibitively time-consuming for inclusion into self-consistent device simulators, especially where anisotropic effects such as impact ionisation are unimportant, or where the crystallographic orientation of a device is unknown. Alternatively, one could model the band structure as a pair of isotropic, parabolic bands, each characterised by a single hole effective mass. Such an approach was attempted by the present authors, but saturated hole velocities calculated using this model were far outside the reported range of experimental results [3,4]. A compromise was therefore sought which aimed to represent the valence band structure of GaAs by a nonparabolic, isotropic effective mass approximation.

The Valence Band Model

An isotropic model for the valence band structure of GaAs has been developed following the work of Asche and von Borzeszkowski on silicon [5]. The following cubic equation is used to describe this structure:

$$a_3k^6 + a_2k^4 + a_1k^2 + a_0 = 0 \qquad (1)$$

where k is the hole wave number and the a_i depend on cyclotron resonance parameters A,B,C,N, the split-off energy Δ and hole energy below the degenerate heavy/light band maximum E thus:

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$$a_3 = -(A+2B)(A-B)^2 + \frac{3}{5}C^2(A-B) - \frac{1}{105}(N-3B)^2(2N+3B) \quad (2.a)$$

$$a_2 = -3\left[(A^2-B^2) - \frac{C^2}{5}\right]\left[E + \frac{\Delta}{3}\right] \quad (2.b)$$

$$a_1 = -3AE\left[E + \frac{2}{3}\Delta\right] \quad (2.c)$$

$$a_0 = E^2(E+\Delta) \quad (2.d)$$

and for GaAs [6,7]

$$\left.\begin{array}{l} A = -6.98 \\ B = -4.4 \\ C = -6.2 \\ N = -17 \end{array}\right\} \cdot \frac{\hbar^2}{2m_e} \qquad eV^2/m^2$$

$$\Delta = 0.34 \qquad eV$$

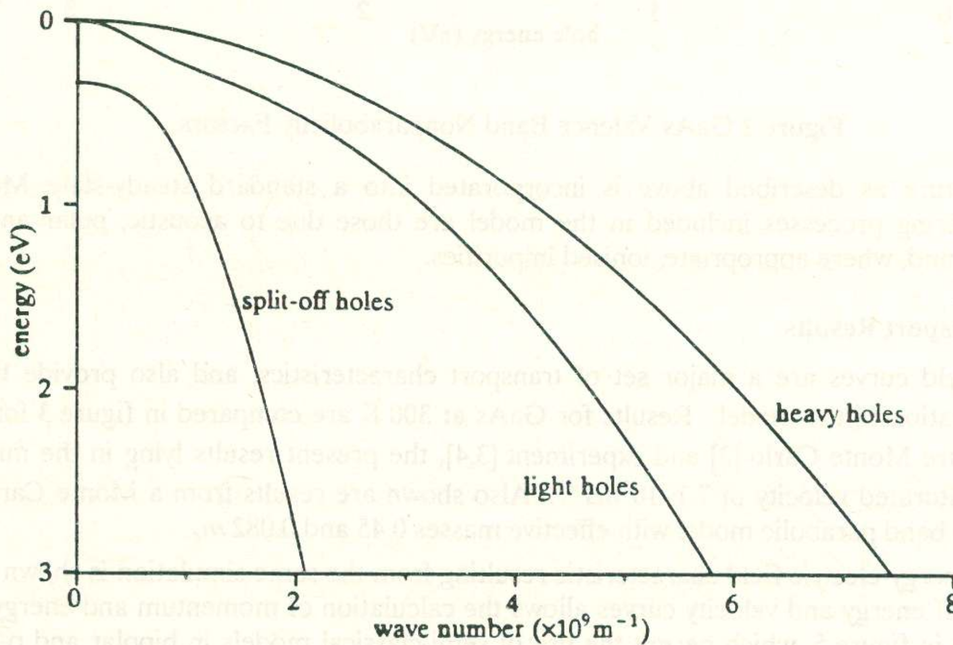

Figure 1 GaAs Valence Band Structure.

The solutions of equation 1 define the $E-k$ relationships for the heavy, light and split-off valence bands of GaAs and are shown in figure 1. This structure is incorporated into the Monte Carlo model via the expression

$$\xi(1+\alpha_i(\xi)\xi) = \frac{\hbar^2 k^2}{2m_i^*} \quad (3)$$

where energy ξ is measured from the ith band maximum. This expression has the same form as that commonly used to describe the structure of the conduction band, except that the nonparabolicity parameter α_i becomes an energy dependent factor, illustrated in figure 2. The effective masses m_i^* are obtained from the $\xi \rightarrow 0$ limit of equation 3 and are: for heavy holes $0.56m_e$, for light holes $0.082m_e$ and for split-off holes $0.14m_e$ where m_e is the free electron mass.

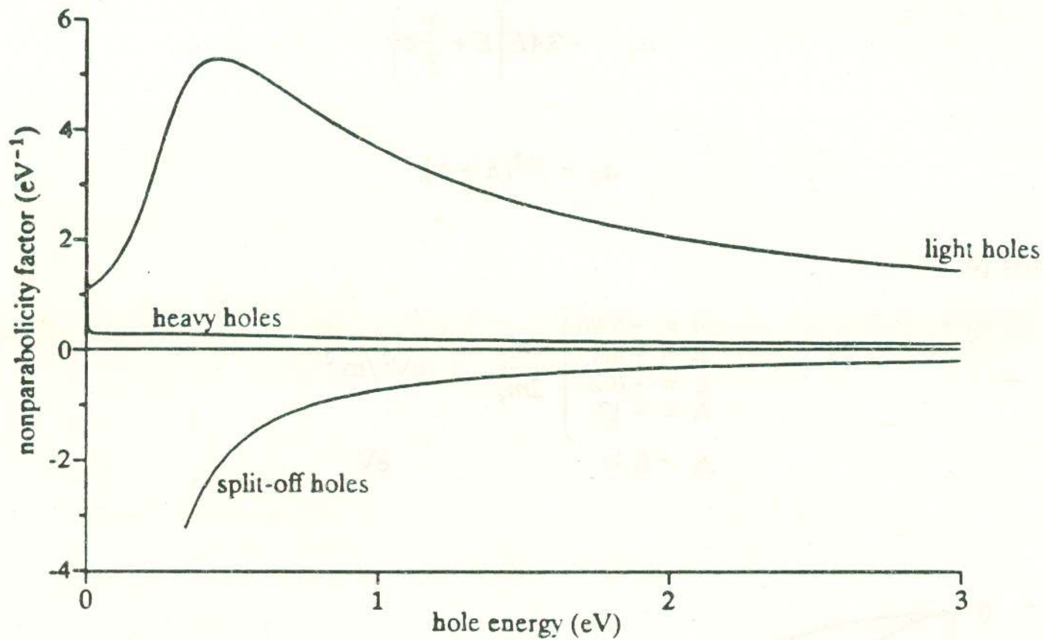

Figure 2 GaAs Valence Band Nonparabolicity Factors.

The band structure as described above is incorporated into a standard steady-state Monte Carlo program. Scattering processes included in the model are those due to acoustic, polar and nonpolar optical phonons and, where appropriate, ionised impurities.

GaAs Hole Transport Results

Hole velocity-field curves are a major set of transport characteristics, and also provide the primary means of verification of the model. Results for GaAs at 300 K are compared in figure 3 for this work, full band structure Monte Carlo [2] and experiment [3,4], the present results lying in the middle of the spread with a saturated velocity of $7.7\times10^4 \mathrm{ms}^{-1}$. Also shown are results from a Monte Carlo program employing a two band parabolic model with effective masses 0.45 and 0.082 m_e.

The total hole energy-electric field characteristic resulting from the same simulation is shown in figure 4. A combination of energy and velocity curves allows the calculation of momentum and energy relaxation times [8], shown in figure 5, which permit the use of semi-classical models in bipolar and p-type device simulators [9].

Distribution functions for holes in k-space are also available from the Monte Carlo program. Figure 6 details the relative population of each band versus electric field, suggesting that split-off holes have relatively little effect on overall hole transport. Indeed, one would expect a low occupancy of this band due to its displacement in energy and low density of states, although this effect may be compensated by the low effective mass and increased acceleration of split-off holes. Figure 7 compares results from the above, three band model with one incorporating only heavy and light holes. The split-off holes contribute little to the overall transport characteristics and one may safely assume their direct effect to be negligible, although the split-off band is important in determining the total band structure via equation 1.

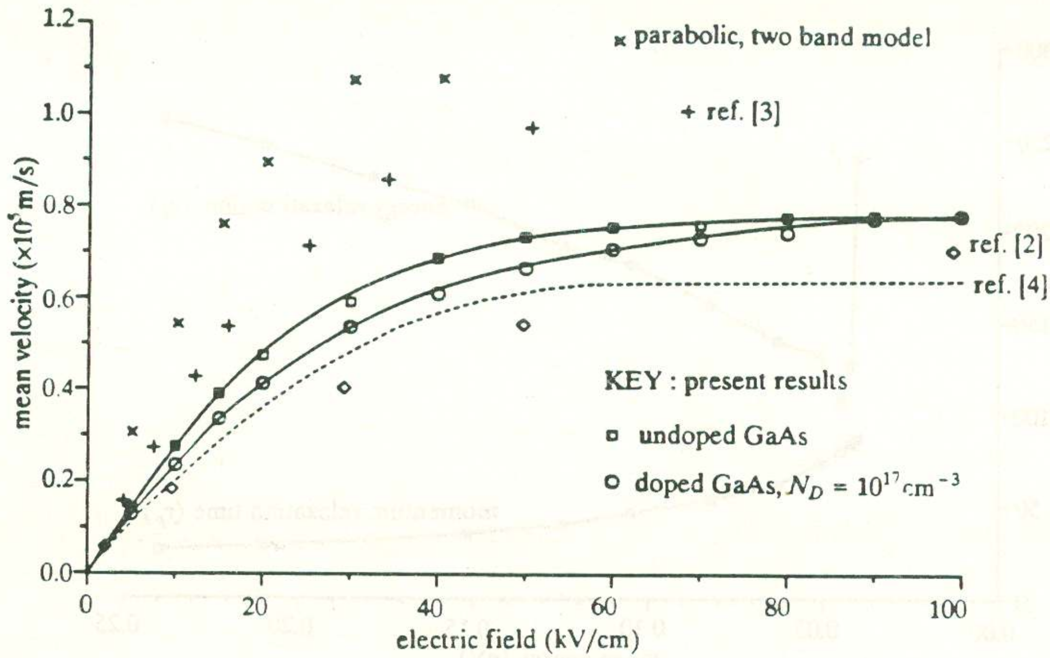

Figure 3 GaAs Hole Velocity-Field Characteristics.
The solid curves show the trend in the Monte Carlo results.

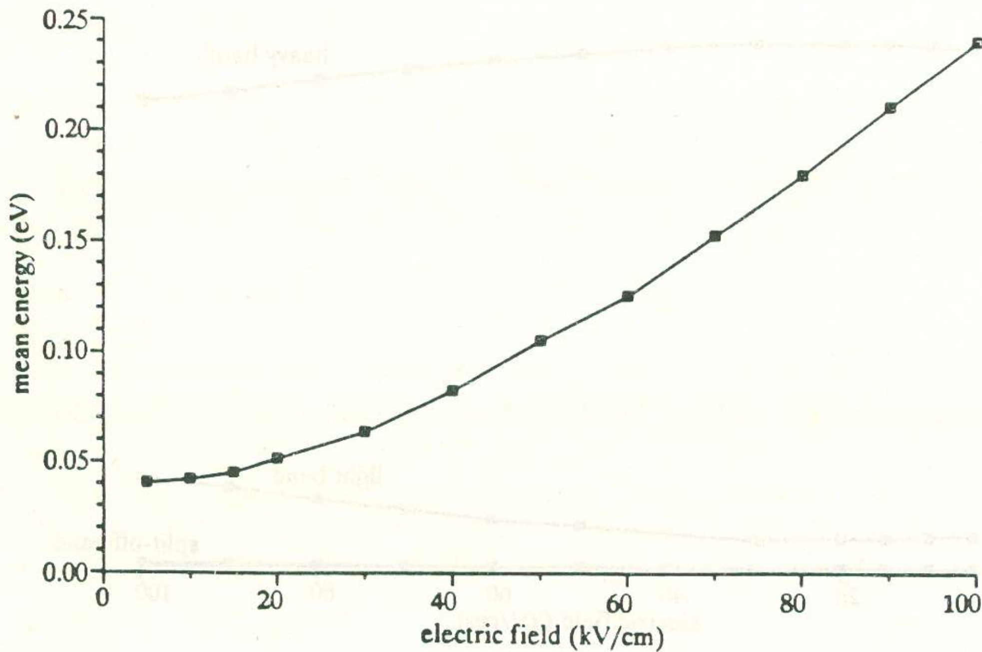

Figure 4 Undoped GaAs Hole Energy-Field Characteristics.

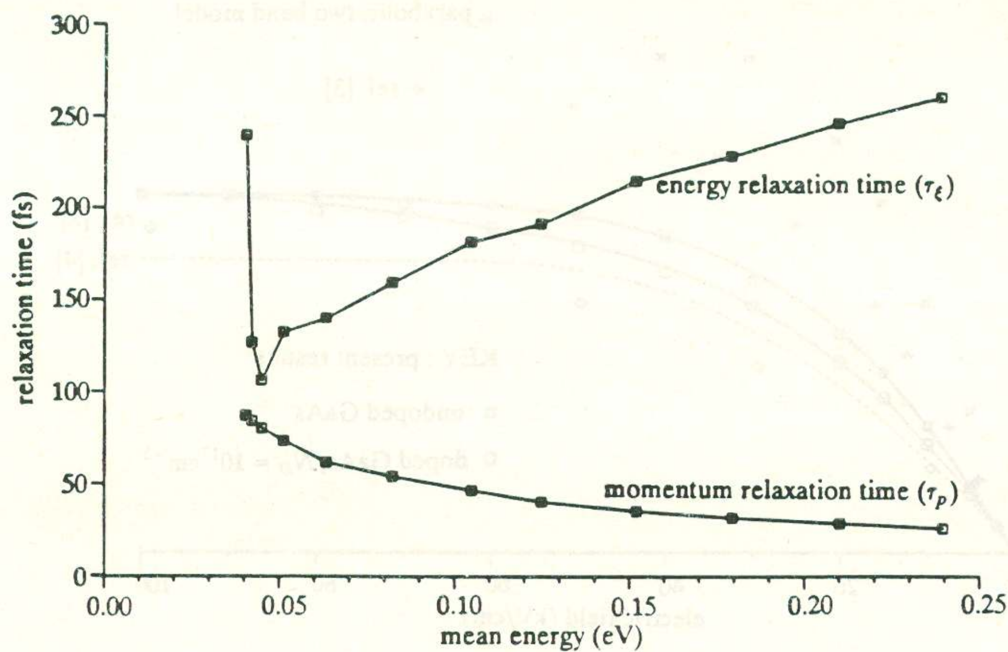

Figure 5 Undoped GaAs Hole Relaxation Times.

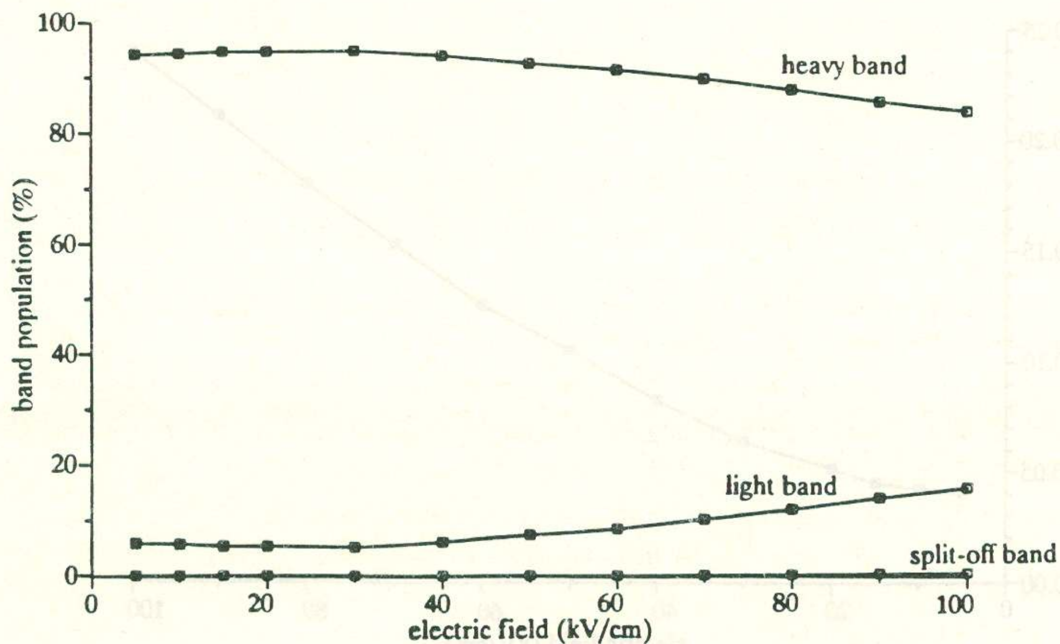

Figure 6 Undoped GaAs Valence Band Population-Field Characteristics.

Conclusion

In conclusion, a simplified model for the valence band structure of GaAs has been demonstrated. The model provides isotropic, nonparabolic expressions for the heavy, light and split-off bands, which may each be characterised via a band-edge effective mass and energy dependent nonparabolicity factor. The effect of split off holes is negligible, however, and this band may reasonably be ignored. Results of the

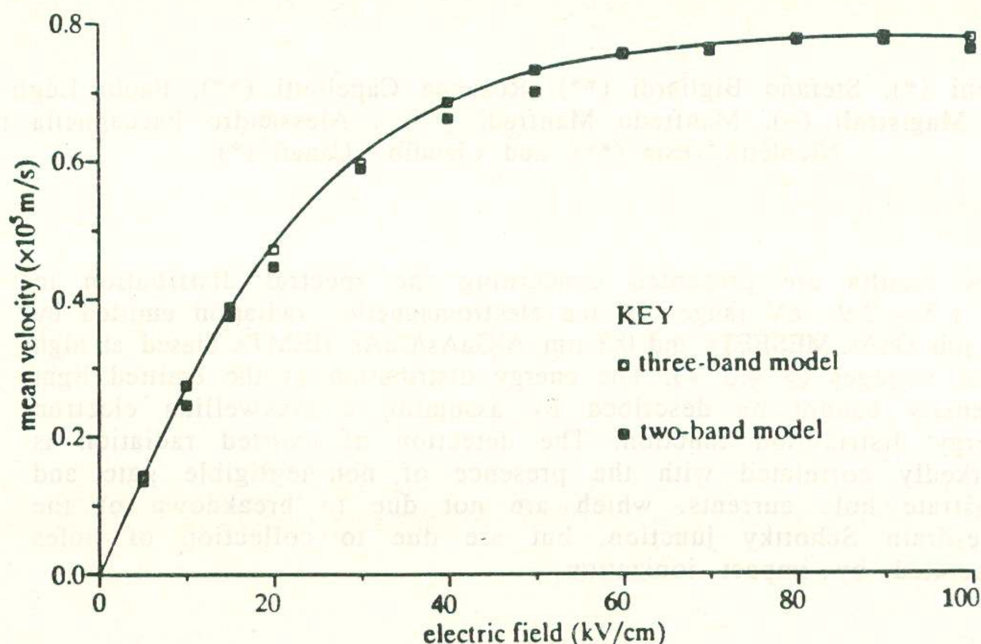

Figure 7 Undoped GaAs Hole Velocity-Field Characteristics - a comparison of two- and three-band model results.

model compare well with experimental and other simulated velocity field characteristics, and the availability of momentum and energy relaxation times permits their use in semiclassical, as well as Monte Carlo, device simulations.

References

[1] Parker, D.G., *Electronics Letters*, Vol. 21, No. 18, p 778, 1985.

[2] Brennan, K. and Hess, K., *Physical Review B*, Vol. 29, No. 10, pp 5581-5590, 1984.

[3] Dalal, V.L., Dreeben, A.B. and Triano, A., *Journal of Applied Physics*, Vol. 42, No. 7, pp 2864-2867, 1971.

[4] Holway, L.H., Steele, S.R. and Adlerstein, M.G., *Proceedings, 7th Biennial Cornell Electrical Engineering Conference*, pp 199-208, 1979.

[5] Asche, M. and von Borzeszkowski, J., *Physica Status Solidi*, Vol. 37, pp 433-438, 1970.

[6] Skolnick, M.S., Jain, A.K., Stradling, R.A., Leotin, J., Ousset, J.C. and Askenazy, S., *Journal of Physics C*, Vol. 9, pp 2809-2821, 1976.

[7] Kane, E.O., *Journal of Physics and Chemistry of Solids*, Vol. 1, pp 82-99, 1956.

[8] Snowden, C.M., *'Introduction to Semiconductor Device Modelling'*, World Scientific, 1986.

[9] Barry, D.M., *'Characterisation of Microwave-Optical Processes in Photodiodes'*, PhD Thesis, University of Leeds, 1989.