Comparison of Hydrodynamic Formulations for Non-Parabolic Semiconductor Device Simulations

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Abstract

This paper presents two non-parabolic hydrodynamic model formulations suitable for the simulation of inhomogeneous semiconductor devices. The first formulation uses the Kane dispersion relationship, $(\hbar k)^2/2m = W(1 + \alpha W)$. The second formulation makes use of a power law, $(\hbar k)^2/2m = xW^y$, for the dispersion relation. Hydrodynamic models which use the first formulation rely on the binomial expansion to obtain closed form coefficients. The power law formulation produces closed form coefficients similar to those under the parabolic band approximation.

1. Introduction

Current hydrodynamic models consist of a set of conservation equations derived by taking moments of the Boltzmann transport equation. During the derivation of the conservation equations the parabolic band approximation is used to obtain rather simple coefficients on the forcing terms in the flux equations. By relying on the parabolic band approximation higher order energy transport effects due to variations in the band structure are neglected. Accounting for band structure effects in hydrodynamic device simulation is important because parabolic models can not adequately account for high energy effects in semiconductors with non-parabolic band structures.

Non-parabolic hydrodynamic models have been reported for homogeneous material systems [1-4] using the Kane dispersion relationship [5]. The general functional form obtained is similar to parabolic hydrodynamic models with first order corrections on the diffusion term. However, the non-parabolic coefficient in the field term and the forcing terms due to non-uniform band structure are neglected in the other moment equations. Cassi and Riccò [6] introduced an alternative to the Kane relation in the form of a power law for the dispersion relationship. Instead of using a classical Kane dispersion law relating the energy and momentum, the band was fit over a

specified energy range using two adjustable parameters. The approximations and assumptions implied by assuming the power law formulation were absent. It will be shown below that the power law dispersion relation leads to a more simplistic and compact formulation than the classical Kane expression.

2. Dispersion relations, concentrations, flux equations

The three dispersion relations considered in the derivation of the hydrodynamic conservation equations are; parabolic, Kane dispersion, and power law

$$\frac{(\hbar k)^2}{2m_e} = W \qquad \frac{(\hbar k)^2}{2m_e} = W(1+\alpha W) \qquad \frac{(\hbar k)^2}{2m_e} = xW^y \tag{1}$$

where α is the non-parabolicity factor and x, y are fitting parameters over a specified energy range. If the power law is fit over the energy range $1.5 \leq W \leq 3.0$ eV as suggested in [6] the deviation in carrier concentration from the parabolic case and the Kane formulation is greater than 80% at most reduced energy values. However, when fit over the energy range $0 \leq W \leq 0.2$ eV the deviation is ~2%, as seen in Figure 1 (α = 0.4789). The case of the Kane dispersion relation using a binomial approximation is also included in the figure. Using the parabolic dispersion relation the particle flux equation is

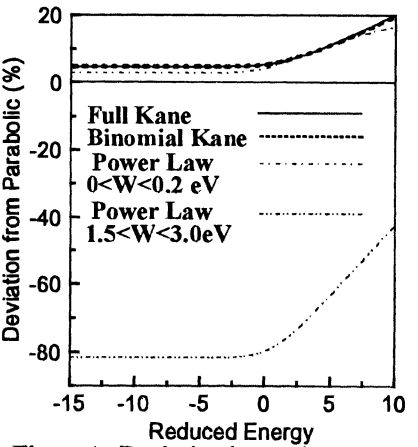

Figure 1. Deviation in carrier concentration from the parabolic case using different dispersion relations

$$-n\bar{v} = \mu KT\left[\frac{\mathcal{F}_{\frac{1}{2}}}{\mathcal{F}_{-\frac{1}{2}}}\right]\nabla n + \mu n\nabla\epsilon_c + \frac{5}{2}\mu nKT\frac{\mathcal{F}_{\frac{3}{2}}}{\mathcal{F}_{\frac{1}{2}}}\left[1-\frac{3}{5}\frac{\mathcal{F}^2_{\frac{1}{2}}}{\mathcal{F}_{-\frac{1}{2}}\mathcal{F}_{\frac{3}{2}}}\right]\frac{\nabla T}{T} \tag{2}$$

The flux equation for the Kane dispersion using a binomial expansion is

$$-n\bar{v} = \mu KT\left[\frac{\mathcal{F}^2_{\frac{1}{2}} + \frac{10}{4}\alpha KT\mathcal{F}_{\frac{3}{2}}\mathcal{F}_{\frac{1}{2}}}{\mathcal{F}_{\frac{1}{2}}\mathcal{F}_{-\frac{1}{2}} + \frac{15}{4}\alpha KT\left(\mathcal{F}^2_{\frac{1}{2}} + \frac{\mathcal{F}_{-\frac{1}{2}}\mathcal{F}_{\frac{3}{2}}}{2}\right)}\right]\nabla n + \mu\left[\frac{\mathcal{F}_{\frac{1}{2}} - \frac{21}{4}\alpha KT\mathcal{F}_{\frac{3}{2}}}{\mathcal{F}_{\frac{1}{2}} + \frac{15}{4}\alpha KT\mathcal{F}_{\frac{3}{2}}}\right]n\nabla\epsilon_c \tag{3}$$

$$+\frac{\mu nKT}{\left(\mathcal{F}_{\frac{1}{2}} + \frac{15}{4}\alpha KT\mathcal{F}_{\frac{3}{2}}\right)\left(\mathcal{F}_{-\frac{1}{2}} + \frac{15}{4}\alpha KT\mathcal{F}_{\frac{1}{2}}\right)}\left[\frac{5}{2}\mathcal{F}_{-\frac{1}{2}}\mathcal{F}_{\frac{3}{2}} - \mathcal{F}^2_{\frac{1}{2}} - \frac{\mathcal{F}^3_{\frac{1}{2}}}{2\left(\mathcal{F}_{\frac{1}{2}} + \frac{15}{4}\alpha KT\mathcal{F}_{\frac{3}{2}}\right)}\right]\frac{\nabla T}{T}$$

The flux equation obtained using the power law dispersion relation is

$$-n\bar{v} = \frac{2\mu}{3xy^2}(KT)^{2-y}\frac{\left(\frac{y}{2}+1\right)\Gamma\left(\frac{y}{2}+1\right)\mathcal{F}_{\frac{y}{2}}}{\left(\frac{3}{2}y-1\right)\Gamma\left(\frac{3}{2}y-1\right)\mathcal{F}_{\frac{3}{2}y-2}}\nabla n + \frac{(2-y)\,\mu}{xy^2}(KT)^{1-y}\frac{\Gamma\left(\frac{y}{2}+1\right)\mathcal{F}_{\frac{y}{2}}}{\Gamma\left(\frac{3}{2}y\right)\mathcal{F}_{\frac{3}{2}y-1}}n\nabla\epsilon_c \quad (4)$$
$$+\frac{\mu n}{xy^2}(KT)^{2-y}\left[\frac{-y\left(\frac{y}{2}+1\right)\Gamma\left(\frac{y}{2}+1\right)\mathcal{F}_{\frac{y}{2}}}{\left(\frac{3}{2}y-1\right)\Gamma\left(\frac{3}{2}y-1\right)\mathcal{F}_{\frac{3}{2}y-2}} - \frac{(4+y)\Gamma\left(\frac{y}{2}+2\right)\mathcal{F}_{\frac{y}{2}+1}}{3\Gamma\left(\frac{3}{2}y\right)\mathcal{F}_{\frac{3}{2}y-1}}\right]\frac{\nabla T}{T}$$

The derivation of all these three equations is given in reference [7]. Similarly the electron energy flux equations using the three dispersion relations can also be formulated [7]. The equations were discretized by using the methods in references [8] and [9]. For the exponential terms in the discretization equation with factors composed of powers of the temperature we have made the assumption that the position dependent temperature can be replaced by the average nodal temperature.

3. Results

Figures 2 through 5 show the results of applying the model to ballistic diodes of both Si and GaAs. Figure 2 shows the current for a Si ballistic diode using the non-parabolic formulations is lower than the parabolic case, Figure 3 shows that the energy is also lower at a 1 volt bias. Figures 4 and 5 show the same trends for the GaAs ballistic diodes. One should note that at low biases the power law formulation predicts lower current than the α formulation until a certain bias voltage. At low bias, the devices are close to equilibrium and the carriers are relatively cold. Consequently, the system responds as in the drift-diffusion case resulting in a greater current for the α case than the power law case. At higher biases, the effects of carrier heating are more important, and the situation reverses, since the full hydrodynamic results dominate the 'effective' mobility.

4. References

[1] R. A. Stewart and J. N. Churchill, "A fully nonparabolic hydrodynamic model for describing hot electron transport in GaAs," Solid State Elec., Vol 33, #7, pp. 819, 1990.

[2] R. Thoma, A. Emunds, B. Meinerzhagen, H.-J. Peifer, and W. L. Engl, "Hydrodynamic equations for semiconductors with nonparabolic band structure," IEEE Trans Elec. Dev., Vol. 38, #6, pp. 1343, 1991.

[3] T. J. Bordelon, X.-L. Wang, C. M. Maziar, and A. F. Tasch, "Accounting for band structure effects in the hydrodynamic model: a first-order approach for silicon device simulation," Solid State Elec., Vol. 35, #2, pp. 131, 1992.

[4] D. Chen, E. C. Kan, U. Ravaioli, C.-W. Shu, and R. W. Dutton, "An improved energy transport model including nonparabolicity and non-maxwellian distribution

effects," IEEE Elec. Dev. Letts., Vol. 13, #1, pp. 26, 1992.

[5] E. O. Kane, "Band structure of indium antimonide," J. Phys. Chem. Solids, Vol. 1, pp. 249, 1957.

[6] D. Cassi and B. Riccò, "An analytical model of the energy distribution of hot electrons," IEEE Trans Elec. Dev., Vol. 37, #6, pp. 1514, 1990.

[7] A. W. Smith and K. F. Brennan, "Non-parabolic hydrodynamic formulations for the simulation of inhomogeneous semiconductor devices," submitted for publication in Solid State Electronics

[8] A. W. Smith, "Light confinement and hydrodynamic modelling of semiconductor structures using volumetric methods," Ph.D. Dissertation, Georgia Institute of Technology, 1992.

[9] A. W. Smith and A. Rohatgi, "Non-isothermal extension of the Scharfetter-Gummel technique for hot carrier transport in heterostructure simulations," IEEE Trans. CADICS, Vol. 12, #10, pp.1515, 1993.

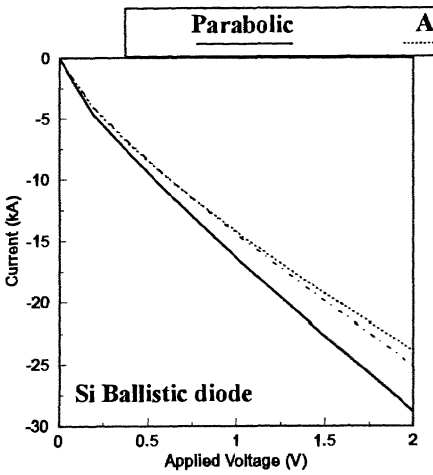

Figure 2. Current vs voltage

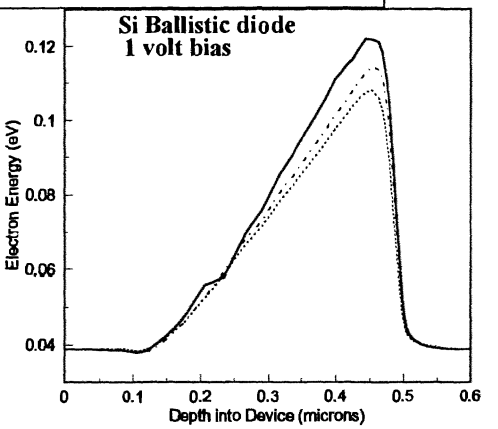

Figure 3. Electron energy

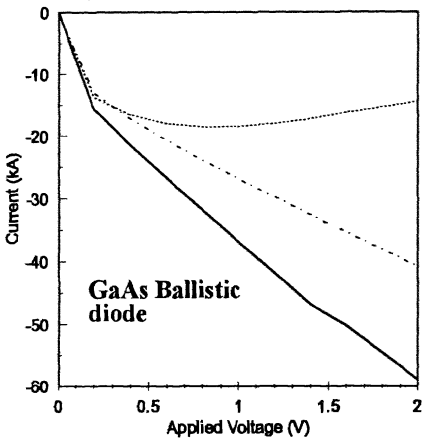

Figure 4. Current vs voltage

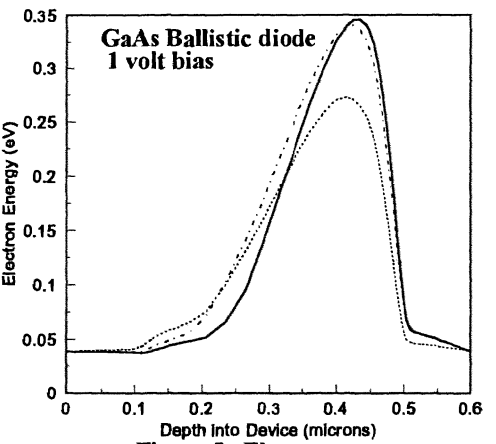

Figure 5. Electron energy