Hydrodynamic Device Modeling with Band Nonparabolicity*

J. CAI^a, H.L. CUI^a, E.H. LENZING^{a,b}, R. PASTORE^{a,b}, D.L. RHODES^b and B.S. PERLMAN^b

^a *Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030*

^b *U.S. Army Research Laboratory, Fort Monmouth, New Jersey 07703*

A semiconductor device model based on a set of quantum mechanically derived hydrodynamic balance equations are presented. This model takes full account of band nonparabolicity, in addition to its other useful features such as the explicit evaluation of momentum and energy relaxation rates, in the form of frictional force and energy loss rate, within the model, and inclusion of carrier-carrier interaction effects, such as dynamical screening. Numerical results of one-dimensional device simulations are presented and compared with parabolic approximations.

Recently, a semiconductor device model based on a set of quantum mechanically derived hydrodynamic balance equations was developed[1,2]. In this presentation we generalize these hydrodynamic equations to treat arbitrary electronic energy band structures[3,4]. Compared with the hydrodynamic balance equations for parabolic energy bands, the main difference is the introduction of a variable, ensemble-averaged, inverse effective mass tensor, which modifies the momentum balance equation directly and the other balance equations indirectly. As in the parabolic-band case, the momentum and energy relaxation rates are cast in the form of electric field dependent frictional force and energy transfer functions, with full account of electron-electron interaction effects, such as dynamical screening. These functions are calculated using the electronic dielectric function, which is normally treated within the random phase approximation. However, these calculations are now modified with the introduction of the ensemble-averaged inverse effective mass tensor to treat the arbitrary energy

band dependence on the crystal momentum. The device model is applied to a semiconductor with a Kane-type conduction band to demonstrate the usefulness of the new approach. Numerical simulations using this model is carried out for a submicron ballistic diode structure, using the Kane model conduction band, and the results are compared with those for the same device but under the parabolic-band approximation.

The new hydrodynamic balance equations express the following conservation laws : The conservation of charge-the equation of continuity,

$$\frac{\partial n(\vec{R})}{\partial t} + \frac{1}{q} \nabla_{\vec{R}} \cdot \vec{J}(\vec{R}) = 0, \quad (1)$$

the conservation of momentum-momentum/current balance equation,

$$\frac{\partial \vec{J}(\vec{R})}{\partial t} = -q \nabla_{\vec{R}} \cdot \vec{T}(\vec{R}) + q n(\vec{R}) \vec{K}(\vec{R}) \cdot [\vec{E}(\vec{R}) + \nabla_{\vec{R}} \phi_c(\vec{R})] + q \vec{A}(\vec{R}), \quad (2)$$

and the conservation of energy-energy balance equation,

* This work was supported by the U.S. Army Research Office.

$$\frac{\partial}{\partial t} H_e(\vec{R}) = \nabla_{\vec{R}} \cdot \vec{S}(\vec{R}) + \frac{\vec{J}}{q} \cdot [\vec{E}(\vec{R}) + \nabla_{\vec{R}} \phi_c(\vec{R})] + W(\vec{R}). \quad (3)$$

The various quantities appearing in the above equations are, the average electron density

$$n(\vec{R}) = \frac{2}{(2\pi)^3} \int d^3k f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})), \quad (4)$$

the average current density,

$$\vec{J}(\vec{R}) = q \frac{2}{(2\pi)^3} \int d^3k \nabla_{\vec{k}} \epsilon(\vec{k}) f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})), \quad (5)$$

the ensemble-averaged inverse effective mass tensor,

$$\tilde{K}(\vec{R}) = \frac{2n(\vec{R})}{(2\pi)^3} \int d^3k \nabla_{\vec{k}} \nabla_{\vec{k}} \epsilon(\vec{k}) f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})), \quad (6)$$

the average velocity-velocity tensor,

$$\tilde{T}(\vec{R}) = \frac{2}{(2\pi)^3} \int d^3k \nabla_{\vec{k}} \epsilon(\vec{k}) \nabla_{\vec{k}} \epsilon(\vec{k}) f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})), \quad (7)$$

the average electron energy,

$$w(\vec{R}) = \frac{2}{(2\pi)^3} \int d^3k \epsilon(\vec{k}) f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})), \quad (8)$$

and the average electron energy flux,

$$\vec{S}(\vec{R}) = \frac{2}{(2\pi)^3} \int d^3k \epsilon(\vec{k}) \nabla_{\vec{k}} \epsilon(\vec{k}) f(\epsilon(\vec{k} - \vec{p}_d(\vec{R})), T_e(\vec{R}), \mu(\vec{R})). \quad (9)$$

Here $\vec{p}_d$ is the center-of-mass momentum of the electron system (per particle), T_e is the electron temperature, μ is the chemical potential, $\epsilon(\vec{k})$ is the electron band energy, ϕ_c is the conduction band bottom, $\vec{E}$ is the total electric field, $f(\epsilon)$ is the Fermi-Dirac distribution function.

The frictional acceleration due to electron-impurity scattering, $\mathbf{A}_i$, the frictional acceleration due to electron-phonon interaction, $\mathbf{A}_p$, and the electron energy loss rate, W , for a nonparabolic energy band can be formulated as [3,4]

$$A_i(\vec{R}) = \frac{2\pi n_I}{(2\pi)^3} \int d^3k \sum_{\vec{q}} \left| g(\vec{k}, \vec{q}) u(\vec{q}) \right|^2 [\vec{v}(\vec{k} + \vec{q}) - \vec{v}(\vec{k})] \delta(\epsilon(\vec{k} + \vec{q}) - \epsilon(\vec{k})) \times \frac{[f(\epsilon(\vec{k} - \vec{p}_d), T_e, \mu) - f(\epsilon(\vec{k} + \vec{q} - \vec{p}_d), T_e, \mu)]}{\left| \epsilon(\vec{q}, \epsilon(\vec{k} - \vec{p}_d) - \epsilon(\vec{k} + \vec{q} - \vec{p}_d)) \right|^2}, \quad (10)$$

$$A_p(\vec{R}) = \frac{4\pi}{(2\pi)^3} \int d^3k \sum_{\vec{q}\lambda} \left| g(\vec{k}, \vec{q}) M(\vec{q}\lambda) \right|^2 [\vec{v}(\vec{k} + \vec{q}) - \vec{v}(\vec{k})] \delta(\epsilon(\vec{k} + \vec{q}) - \epsilon(\vec{k}) + \Omega_{\vec{q}\lambda}) \times \frac{[f(\epsilon(\vec{k} - \vec{p}_d), T_e, \mu) - f(\epsilon(\vec{k} + \vec{q} - \vec{p}_d), T_e, \mu)]}{\left| \epsilon(\vec{q}, \epsilon(\vec{k} - \vec{p}_d) - \epsilon(\vec{k} + \vec{q} - \vec{p}_d)) \right|^2} \times \left[n \left(\frac{\Omega_{\vec{q}\lambda}}{T} \right) - n \left(\frac{\epsilon(\vec{k} - \vec{p}_d) - \epsilon(\vec{k} + \vec{q} - \vec{p}_d)}{T_e} \right) \right], \quad (11)$$

$$W(\vec{R}) = \frac{4\pi}{(2\pi)^3} \int d^3k \sum_{\vec{q}\lambda} \left| g(\vec{k}, \vec{q}) M(\vec{q}\lambda) \right|^2 \Omega_{\vec{q}\lambda} \delta(\epsilon(\vec{k} + \vec{q}) - \epsilon(\vec{k}) + \Omega_{\vec{q}\lambda})$$

$$\times \frac{[f(\epsilon(\vec{k} - \vec{p}_d), T_e, \mu) - f(\epsilon(\vec{k} + \vec{q} - \vec{p}_d), T_e, \mu)]}{\left| \epsilon(\vec{q}, \epsilon(\vec{k} - \vec{p}_d) - \epsilon(\vec{k} + \vec{q} - \vec{p}_d)) \right|^2} \times \left[n \left(\frac{\Omega_{\vec{q}\lambda}}{T} \right) - n \left(\frac{\epsilon(\vec{k} - \vec{p}_d) - \epsilon(\vec{k} + \vec{q} - \vec{p}_d)}{T_e} \right) \right]. \quad (12)$$

Here, $\vec{v}(\vec{k}) = \nabla_{\vec{k}} \epsilon(\vec{k})$ the electron group velocity,

$u(\vec{q})$ is the Fourier transform of the impurity potential, n_i is the impurity concentration, $M(\vec{q}, \lambda)$ is the electron-phonon coupling matrix element for phonon of wavevector $\vec{q}$, branch index λ , and frequency $\Omega_{\vec{q}, \lambda}$. Also, $\epsilon(\vec{q}, \omega)$ the dielectric function of the electronic system, T is the lattice temperature, and $n(x) = (\exp x - 1)^{-1}$ is the Bose-Einstein distribution function. The expression for the function $g(\vec{k}, \vec{q})$ is given in Ref. [3].

An isotropic nonparabolic energy band model known as the Kane model, will be applied to simulate one-dimensional devices. If k denotes the distance of wavevector from the minimum of the valley, the Kane energy-momentum relation is given by

$$(1 + \alpha\epsilon)\epsilon = \frac{k^2}{2m}, \quad (13)$$

where the band structure is determined by the density-of-state effective mass m and the nonparabolicity factor α . The nonparabolic hydrodynamic balance equations can be discretized with the use of generalized Scharfetter-Gummel method[5] which was commonly used to provide a global convergent scheme for solving drift-diffusion model.

A simulation of novel one-dimensional ballistic diode with Kane energy band nonparabolicity has been carried out for lattice temperature $T = 300$ K, where the device size, doping profile and the material parameters are the same as those discussed in Ref. [2]. The nonparabolicity coefficient α is taken to be 0. and 0.5 /eV for a wide range of bias voltages (1-4V). Instead of an accurate integration of forces and energy loss rate for nonparabolic energy band, for this preliminary study we used those for parabolic energy band but replace the electron effective mass by the dynamic mass calculated using Eq.(6). Although this approximation is not necessary, it reduces the numerical task of calculating the three-dimensional integrals. Simu-

FIGURE 1 Electron drift velocity along the length of the device for different nonparabolicity parameter values $\alpha = 0$ /eV, (thick solid curves) and $\alpha = 0.5$ /eV, (thin solid curves). The 4 pairs of curves (from the bottom) correspond to bias voltages of 1V, 2V, 3V, and 4V

FIGURE 2 Electron temperature along the length of the device for different nonparabolicity parameter values $\alpha = 0$ /eV, (thick solid curves) and $\alpha = 0.5$ /eV, (thin solid curves). The 4 pairs of curves (from the bottom) correspond to bias voltages of 1V, 2V, 3V, and 4V

lation results are presented in the Figures, where we display the electron drift velocity and electron temperature, for various applied bias voltages and various nonparabolicity coefficients. The obvious difference between the parabolic case ($\alpha = 0$) and the nonparabolic case ($\alpha = 0.5$ /eV) appears at high voltages as expected.

References

- [1] X.L. Lei, J. Cai, and L.M. Xie, Phys. Rev. B **38**, 1529 (1988).
- [2] J. Cai and H.L. Cui, J. Appl. Phys., to appear, December 1, 1995.
- [3] X.L. Lei, Phys. Stat. Sol. (b) **170**, 519 (1992).
- [4] X.L. Lei, N.J. Horing, and H.L. Cui, Phys. Rev. Lett. **66**, 3277 (1991).
- [5] D.L. Scharfetter and H.K. Gummel, IEEE Trans. Electron Dev. **ED-16**, 64 (1969).

Biographies

Jian Cai is a graduate student in Department of Physics and Engineering Physics, Stevens Institute of Technology. His research interests include quantum transport theory, semiconductor device simulation, and computer software development.

H.L. Cui is an Associate Professor in the Department of Physics and Engineering Physics, Stevens Institute of Technology. His research interests include solid state theory, semiconductor device physics and semiconductor nanostructure physics. He is a member of IEEE and member of American Physical Society.