Inclusion of collision broadening in semiconductor electron-transport simulations

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(Received 21 May 1987)

The collision broadening of electronic states due to interactions with phonons is included in a semiclassical transport calculation for semiconductors. The quasiparticle spectral function is used in the transition rates of a Monte Carlo simulation to study the many-body effects of the interacting electron. The full semiconductor band structure is employed through an empirical nonlocal pseudopotential method and the scattering is calculated in the Fock approximation. We find a significant increase in the high-energy tails of the electronic distribution function when the broadening is included. Comparison is made with a similar calculation employing a simpler electronic model.

I. INTRODUCTION

The development of methods to calculate electronic transport properties of materials far away from equilibrium conditions is an unsolved problem in physics today. An understanding of the behavior of electrons in high electric fields is becoming increasingly important in semiconductor structures which approach angstrom sizes. Such effects as collision broadening, finite collision lifetimes, the intracollisional field effect, and extremely high electron scattering rates must be considered in studies of these nonequilibrium problems. For systems which are not highly perturbed from equilibrium and where such effects are of only limited importance, semiclassical calculations based on the Boltzmann equation prove to be very useful in predicting physical properties. Monte Carlo methods[1] in particular are very flexible and powerful for transport calculations in this semiclassical regime. Unfortunately, these methods fail in the high-field, high-scattering-rate environments which are of increasing interest in microstructured semiconductor devices.[2] In situations where the quantum-mechanical nature of the system becomes important, a technique which has the power to calculate electronic transport has not yet been found. Although a reasonably complete theoretic framework has been established,[3,4] quantum transport has, to this point, proven to be computationally intractable.

This paper will present results of a method which includes one particular quantum effect, collision broadening, into the semiclassical Monte Carlo method. Collision broadening is the spread of the electronic energy-momentum relation due to scattering. This quasiparticle nature of the electron is best described by the finite width of the spectral function[5] of an electron interacting with its environment. In a seminal paper, Chang *et al.*[6] explored the idea of including collision broadening into Monte Carlo calculations of electronic transport in semiconductors. Their approach was to include the broadening of the electronic states using the ideas developed by Barker[4] in his work on quantum transport and the intracollisional field effect. This paper by Chang has received much comment and has spurred further research into the problem.[7,8] Recently, Lugli *et al.*[7] included the broadening of the electronic states in a model Monte Carlo calculation using a more precise method which makes use of the many-body spectral function. Their work used a single parabolic band with no upper band edge and the Born approximation for the scattering.

In this paper we will apply the spectral-function collision-broadening technique to semiconductor transport calculations. This work will include the band structure of the semiconductor using a nonlocal pseudopotential method and calculate the scattering rates in the Fock approximation. Comparisons will be made with the work of Chang *et al.*[6] and Lugli *et al.*[7]

It should be emphasized that these calculations do not constitute a complete quantum transport method. This work incorporates only one of many quantum phenomena into a semiclassical transport calculation. A full quantum treatment is still a problem for the future. It is quite revealing, however, to study the effects of this single new mechanism. At high fields the broadening of the electronic states significantly changes the electronic distribution, particularly its high-energy tail. This will cause large changes in the calculated rates of any high-energy process, such as impact ionization or barrier emission. Therefore this work gives some indication of the importance of quantum effects in highly nonequilibrium situations.

II. MODEL

This work is based on the semiconductor model that was employed by Chang *et al.*[6] The full band structure of the bulk GaAs conduction band is calculated using an empirical nonlocal pseudopotential method.[9] The band structure is needed for a quantitative and even qualitative understanding of transport in semiconductors because of the large effect of the density of states on the scattering rates. Our model simplifies the electron dynamics by approximating the full electron scattering

from all the scattering mechanisms by an interaction with a single nonpolar optical-phonon mode with frequency ω_0. The coupling between the electrons and the phonons is chosen so that the cross section at an energy of 0.6 eV above the conduction-band edge is equal to the total cross of electrons scattering from all the scatterers in GaAs.[10]

The electronic scattering rate due to the phonons is calculated in the Fock[11] approximation by solving self-consistently the equation

$$\Sigma(\mathbf{k},E) = \int \frac{d^3k'}{(2\pi)^3} \frac{g^2(\mathbf{k}')}{E-\hbar\omega_0-\varepsilon(\mathbf{k}-\mathbf{k}')-\Sigma(\mathbf{k}-\mathbf{k}',E-\hbar\omega_0)} \quad (1)$$

for the electronic self-energy Σ. In Eq. (1), $g(\mathbf{k}')$ is the coupling between the electrons and the phonons, and $\varepsilon(\mathbf{k})$ is the dispersion relation for the electrons as given by the band-structure calculation. The use of Eq. (1) for the self-energy includes the approximation, used throughout this work, that phonon-absorption processes are negligible. At the temperature of 77 K which was used in our simulation, the phonon occupation coefficient for absorption is of the order 10^{-2} while the emission coefficient is of order 1. In the case of nonpolar optic phonons, $g(\mathbf{k})$ is well approximated by a constant. As pointed out by Chang *et al.*,[6] when the electron-phonon coupling is independent of the wave vector, the self-energy is a function of the electron energy alone, $\Sigma(\mathbf{k},E)=\Sigma(E)$. Figure 1 shows the self-energy as calculated self-consistently from Eq. (1) and the self-energy calculated by the Born approximation [where the Σ on the right-hand side of Eq. (1) is replaced by an imaginary infinitesimal $i\delta$]. In the Born approximation $\mathrm{Im}\Sigma(E)\sim\rho_0(E-\hbar\omega_0)$, where ρ_0 is the density of states. Thus we see from Fig. 1 that the first conduction band extends to approximately 4 eV. It is also evident that the Fock approximation results in considerably reduced

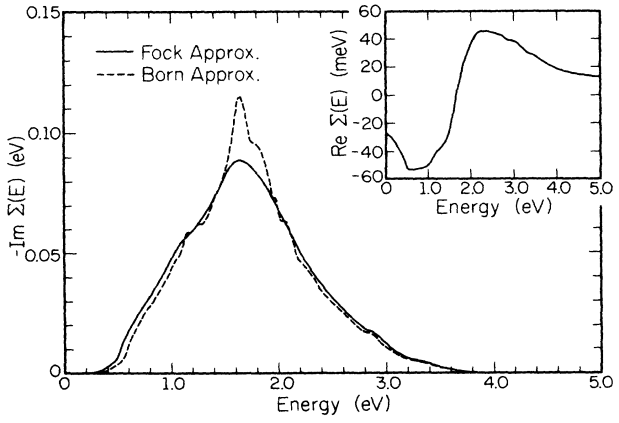

FIG. 1. Electron self-energy in the Fock approximation, $-\mathrm{Im}\Sigma(E)$ and $\mathrm{Re}\Sigma(E)$ (inset), plotted as a function of the electronic energy. Also shown is $-\mathrm{Im}\Sigma(E)$ calculated using the Born approximation (— — —).

scattering near the center of the band where the density of states is high. This approximation is therefore needed for a more accurate calculation of the scattering rates at high energies.

Collision broadening is introduced into Monte Carlo calculations by the inclusion of a distribution for the electronic energy after collisions. In the usual semiclassical transport calculations, the transitions of the electron state from before to after phonon collisions are given by the golden rule

$$W(\mathbf{k}_f,\mathbf{k}_i)\sim |V|^2\delta(\varepsilon(\mathbf{k}_f)-\varepsilon(\mathbf{k}_i)-\hbar\omega_0) , \quad (2)$$

where V is the effective electron-phonon potential. The final state is given exactly by the initial state and the phonon energy. As described in some detail by Reggiani *et al.*,[12] the quasiparticle nature of the interacting electron can be included by replacing the delta function in the golden rule by a spectral density K. K is a convolution over the initial- and final-state spectral functions,

$$K(\mathbf{k}_f,\mathbf{k}_i)=\int \frac{dE}{2\pi} A(\mathbf{k}_f,E-\hbar\omega_0)A(\mathbf{k}_i,E) . \quad (3)$$

The transition rate in this case is given by

$$W(\mathbf{k}_f,\mathbf{k}_i)\sim |V|^2 K(\mathbf{k}_f,\mathbf{k}_i) . \quad (4)$$

In Eq. (3), the spectral function for the interacting electron is calculated from the self-energy by

$$A(\mathbf{k},E)=\frac{-2\,\mathrm{Im}\Sigma(\mathbf{k},E)}{[E-\varepsilon(\mathbf{k})-\mathrm{Re}\Sigma(\mathbf{k},E)]^2+[\mathrm{Im}\Sigma(\mathbf{k},E)]^2} . \quad (5)$$

The final electron state after scattering from a phonon is given by the spectral density distribution $K(\mathbf{k}_f,\mathbf{k}_i)$, reflecting the spread in the quasiparticle energy. It is obvious that this method of including the broadening of the electronic states reduces to the golden rule when the bare electron spectral function $A(\mathbf{k},E)=2\pi\delta(E-\varepsilon(\mathbf{k}))$ is used in Eqs. (3) and (4).

To get some idea of the effect of the collision broadening, we need to look at the spectral density K. Since the self-energy is a function of the electron energy alone, K will be a function of only the initial and final electron energies, $K(\mathbf{k}_f,\mathbf{k}_i)=K(\varepsilon(\mathbf{k}_f),\varepsilon(\mathbf{k}_i))$. The quasiparticle energies E are integrated out in Eq. (3). In Fig. 2 the function $K(\varepsilon_f,\varepsilon_i)$ is plotted as a function of the final energy ε_f for three values of the initial energy, ε_i. We see that K has a width of up to 1 eV about its peak and is asymmetric, with an enhanced tail which extends into the region of the band where the density of states is large. This tail is due to the peak in the density of states near the band center. For ε_i below the peak in the density of states, this tail in K extends out for $\varepsilon_f>\varepsilon_i$, while for ε_i above the peak, this tail extends out for $\varepsilon_f<\varepsilon_i$. It will be shown below that the collision broadening spreads out the calculated electron distribution to both lower and higher energies, moves the peak in the distribution to lower energy, and gives a wide high-energy tail.

We also note that the integral $\int d\varepsilon_f K(\varepsilon_f,\varepsilon_i)=1$. This, of course, is needed for conservation of the electrons. This integral over K gives a check on the numerical calculation. Finally it should be pointed out that we

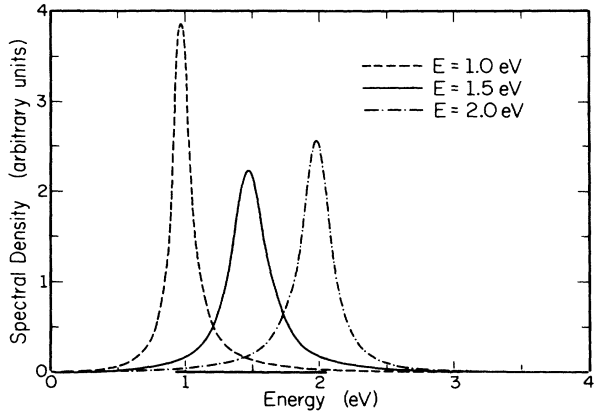

FIG. 2. Spectral density $K(\varepsilon_f,\varepsilon_i)$ plotted as a function of the final energy ε_f for $\varepsilon_i=1.0$ eV (— — —), $\varepsilon_i=1.5$ eV (——), and $\varepsilon_i=2.0$ eV (—·—·—·).

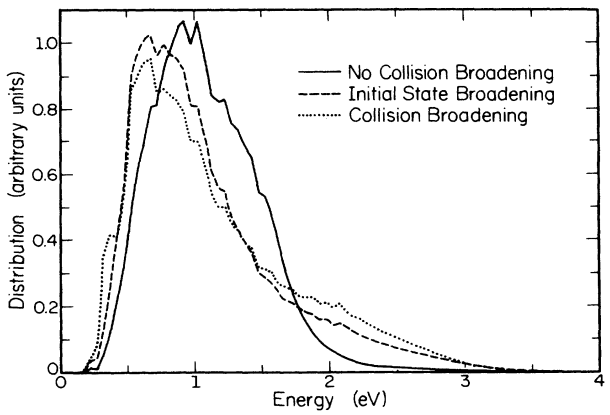

FIG. 3. Steady-state electronic distribution function plotted as a function of energy for golden-rule (nonbroadened) calculation (——), initial-state (Lorentzian) broadening (— — —), and full collision broadening (· · · ·).

have included the real part of $\Sigma(E)$ in the calculations, unlike Lugli *et al.*,[7] which gives the renormalization of the electronic band energies due to the phonons. This makes the model completely consistent with the quasiparticle picture of the electrons.

III. RESULTS AND DISCUSSION

Monte Carlo calculations of the electronic distribution function in a uniform electric field were performed using the model described above. The phonon energy was $\omega_0=29$ meV and the electron-phonon coupling was $g=0.2$ eV. The lattice temperature was set at 77 K for the calculation, and polar optical phonons and intervalley scattering were included for low electron energy loss and intervalley electronic motion, respectively. We also only considered emission of the nonpolar optical phonons, since, as mentioned above, absorption processes are smaller by a factor of 100. The simulations gave the steady-state distribution for the electrons and converged to the final result after about 50 000 scatterings.

Figure 3 shows the steady-state electron distribution for an external field of 500 kV/cm. Included in this figure are results of calculations using three different forms for the transition rate. The solid curve in Fig. 3 gives the result for a simulation using the golden-rule transition rate as given by Eq. (1). The dotted curve gives the electronic distribution with the full collision broadening as described above included. The dashed curve is a simulation using a Lorentzian approximation to the broadening similar to that used by Chang *et al.*[6] In this approximation the width of the state before the scattering, $\mathrm{Im}\Sigma(\varepsilon_i)$, has been used to broaden the transition rate. For this initial-state broadening, the spectral density distribution is

$$K(\varepsilon_f,\varepsilon_i)=\frac{1}{\pi}\frac{-2\,\mathrm{Im}\Sigma(\varepsilon_i)}{(\varepsilon_f-\varepsilon_i-\hbar\omega)^2+[\mathrm{Im}\Sigma(\varepsilon_i)]^2}\ . \tag{6}$$

This approximation simplifies the calculation of the spectral density $K(\varepsilon_f,\varepsilon_i)$ considerably while including an approximate broadening of the electronic states. This Lorentzian state broadening reproduces many of the features of the full broadening calculation. It should be possible to improve on this approximation by including the spread in both the initial and final states, as suggested by the work of Barker.[4]

It is easily seen from Fig. 3 that the collision broadening has a profound effect on the calculated electronic distribution. Although the average energies of all three models are equal within the accuracy of the calculation, the simulations which included broadening have a much larger spread in the electronic distribution with a maximum at a somewhat lower energy and a particularly pronounced enhancement in the high-energy tail. At the center of the band the electron population is enhanced by nearly a factor of 3. Even larger increases occur at high energies because the distributions with broadening included fall off more slowly at high energy than the golden-rule result. In fact we see that the broadened distributions have a very nonthermal (nonexponential) high-energy tail.

The high-energy electron-population enhancement due to broadening is exactly in the region of the band where processes such as impact ionization begin to occur. This significant change in the electronic distribution will have an equally large effect on the calculated rates of any high-energy effects. The accurate calculation of these processes would seem to require, therefore, the inclusion of the broadening of the electronic states.

Unlike our work, Lugli *et al.*[7] found a runaway phenomenon when the collision broadening was included. The average electron energy of their broadened distribution was significantly higher than that calculated using the golden rule. The inclusion of the precise band structure inhibits this runaway. The reason for this can be seen by considering the function K plotted in Fig. 2. High in the band the scattering probability is skewed towards lower energies due to the larger density of states there. For the strictly parabolic dispersion relation used by Lugli,[7] the density of states always increases. In our results, the electronic distribution is larger in both the

high- and low-energy regions than the golden-rule results, with little or no change in the average energy. There is no runaway when the band structure of the semiconductor is considered in the electronic model.

IV. CONCLUSION

In conclusion, we have calculated the electronic distribution of a semiconductor in large electric fields using Monte Carlo methods which take into account the quasiparticle nature of the interacting electrons. The spectral function is used to broaden the transition rates due to collisions with phonons. We find that the broadening has significant effects on the steady-state energy distribution of the electrons. The peak in the distribution occurs at a lower energy for simulations which include broadening than for simulations which do not, and the broadening causes a wide, nonthermal high-energy tail. This high-energy tail should have profound effects on the calculated rates of high-electron-energy processes such as impact ionization and emission over barriers. Unlike other authors, however, we do not find a runaway in the electronic energy. This appears to be due to the inclusion of the correct band structure in the simulation.

ACKNOWLEDGMENT

We wish to thank the Office of Naval Research, which support this work under Grant No. N00014-86-K-0253. B.A.M. was also supported by the Materials Research Laboratory at the University of Illinois under NSF Grant No. DMR86-12860.

[1]L. Reggiani and C. Jacoboni, Rev. Mod. Phys. **55**, 645 (1983).
[2]J. R. Barker and D. K. Ferry, Phys. Rev. Lett. **25**, 1779 (1979).
[3]L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962); L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys.—JETP **20**, 1018 (1965)]; W. Hansch and G. D. Mahan, Phys. Rev. B **28**, 1902 (1983).
[4]J. R. Barker, J. Phys. C **6**, 2663 (1973).
[5]G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).
[6]Yia-Chung Chang, D. Z.-Y. Ting, J. Y. Tang, and K. Hess, Appl. Phys. Lett. **42**, 76 (1983).
[7]Paolo Lugli, Lino Reggiani, and Carlo Jacoboni, Superlatt. Microstruct. **2**, 143 (1986).
[8]J. Lin and L. C. Chiu, Appl. Phys. Lett. **49**, 1802 (1986).
[9]M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141**, 789 (1966).
[10]H. Shichijo and K. Hess, Phys. Rev. B **33**, 4197 (1981).
[11]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
[12]Lino Reggiani, Paolo Lugli, and A. P. Jauho, Phys. Rev. B (to be published).