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Quantum Transport Simulation Based on Wigner Formula

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The superiority of nonequilibrium quantum transport simulation based on the Wigner Formula over a conventional Transfer Matrix Method is clarified for the first time. With a new contact model, the present simulation technique is applied to a double barrier Resonant Tunneling Diode and the influence of some perturbations on quantum interference effects is investigated systematically. In particular it predicts that both ohmic drop and electronic accumulation in quantum mechanical distribution in a cathode region cause a remarkable decrease in the peak to valley ratio in current voltage characteristics.

1. Introduction

With a view to designing novel quantum interference devices, it is important to establish a nonequilibrium quantum transport simulation technique. As compared with optical interference systems, the following proper elements make electronic ones more profound. Firstly, electrons are not in classical distribution but in quantum-mechanical distribution according to the biased potential profiles. Secondly, quantum interference effects can disappear by scattering processes. Thirdly, electrons belong to Fermion and can smear out the quantum interference effects at high temperature even if there are no scattering processes at all. The Wigner Formula is one of the most promising methods to analyze the physics and performance of these devices and has been studied intensively [1),2),3)]. Applying the simulation technique to a double barrier Resonant Tunneling Diode (RTD), the influence of these elements on the quantum interference effects is revealed and the significance of this formula dealing with nonequilibrium quantum mechanical distribution is made clear.

2. Modeling

The fundamental quantum transport equation is based on a quantum Boltzmann's equation and the models assumed in this study are described as follows.

1. The scattering processes are approximated by equilibrium relaxation.
2. The effective potential is approximated by the self-consistent Hartree model.
3. A new contact model adopting local chemical potential is proposed.

The concept of this contact model is that because the outside of an analyzed region are assumed to be the classical regions with charge neutrality and flat bands, the chemical potential is adjusted self-consistently to ensure carrier density continuity at the artificial boundaries. This chemical potential is defined as local chemical potential.

3. Systematic Analysis of Ip/Iv

The peak (Ip) to valley (Iv) ratio in current voltage characteristics is very important in the practical device applications. But from a physical point of view, a high Ip/Iv represents the striking evidence that the quantum interferences take place. Regardless of some perturbations as mentioned above, how the quantum interference effects appear is discussed.

3.1 Doping Concentration Dependence of Ip/Iv

The doping concentration dependence of Ip/Iv is shown in fig. 1. The result of the Wigner Formula (the solid line) has an optimum doping concentration. At a higher concentration, the decrease in Ip/Iv is due to an increase in the number of hot electrons as the Fermi level rises.

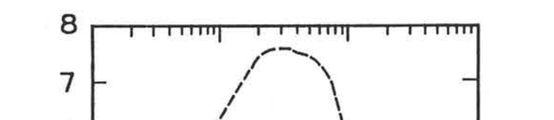
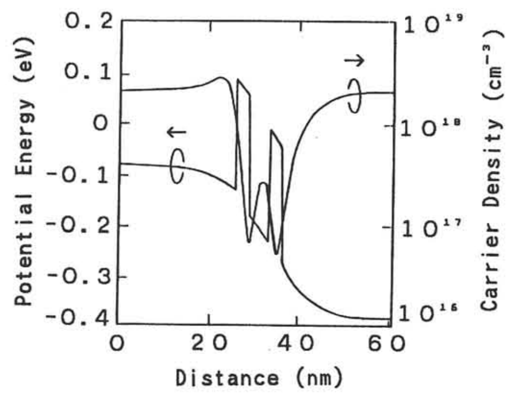


Fig. 1 Doping concentration dependence of Ip/Iv obtained from the Wigner Formula (the solid line) and the Transfer Matrix Method (the dotted line)

The decrease in screening effects at a lower concentration causes an ohmic drop in a cathode region. According to the biased potential profiles, electrons form an accumulation layer in quantum mechanical distribution.

The potential profiles and carrier densities on off-resonant states at high and low doping concentrations are shown in fig. 2. In the case of a lower concentration, the larger ohmic drop and electronic accumulation in the cathode region cause the increase in Iv relatively, therefore Ip/Iv decreases.

(a)



(b)

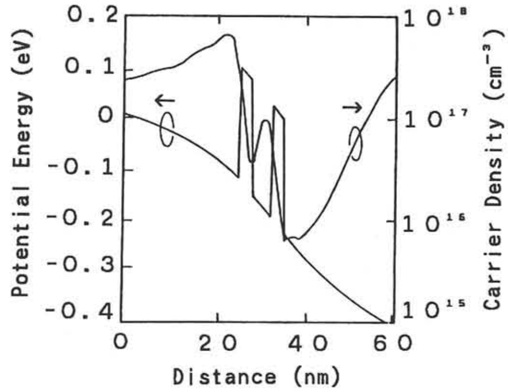


Fig. 2 Potential profiles and carrier densities on off-resonant states at (a) high and (b) low doping concentrations

The result of the Transfer Matrix Method (the dotted line), which is calculated using the results of potential profiles and the local chemical potential obtained by Wigner Formula, gives rise to remarkable deviations from that of the present formula. These results clearly reveal the significance of dealing with non-equilibrium quantum mechanical distribution in the n^+ layers.

3.2 Relaxation Time Dependence of Ip/Iv

The relaxation time dependence of normalized Ip, Iv and Ip/Iv are shown in fig. 3. As the relaxation time becomes shorter, Ip decreases and Iv increases, therefore, Ip/Iv decreases. This phenomenon is due to the broadening of the resonant peak of transmission probabilities. Note that if the relaxation time is longer than τ_e, where τ_e stands for the relaxation time of undoped GaAs at room temperature evaluated from mobility, there is little influence on Ip/Iv.

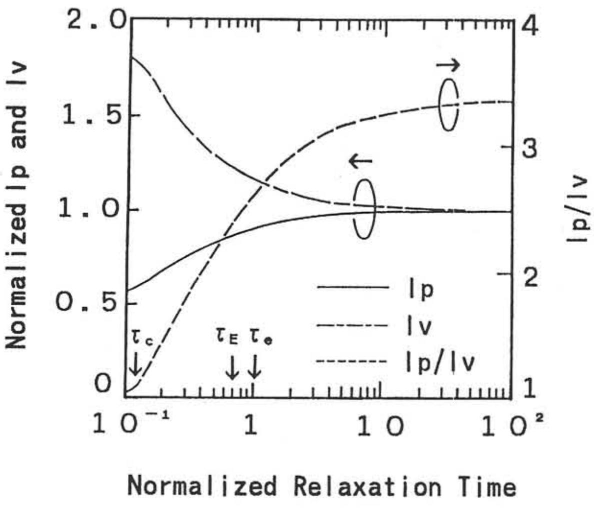


Fig. 3 Relaxation time dependence of normalized Ip, Iv, and Ip/Iv ($\tau_e \sim 0.3$ ps)

The limitation of the relaxation time to Ip/Iv is discussed. In fig. 3 two typical values τ_c and τ_E are shown, where τ_c stands for the time electrons with energies of the resonant level propagated through the double barriers, and τ_E represents the multiple reflection time between the double barriers, estimated from the linewidth of the resonant peak and the uncertainty principle. Ip/Iv decreases steeply from τ_E, and becomes nearly equal to unity at τ_c. It can be seen that the resonant phenomenon is not restricted by τ_c, but by τ_E in contrast with the usual quantum interference devices.

3.3 Temperature Dependence of Ip/Iv

The temperature dependence of Ip, Iv and Ip/Iv are shown in fig. 4. Because the temperature smearing effects are examined, the temperature dependence of scattering processes are neglected. As the temperature rises, Ip/Iv decreases due to the fact that hot electrons smear out the quantum interference effects.

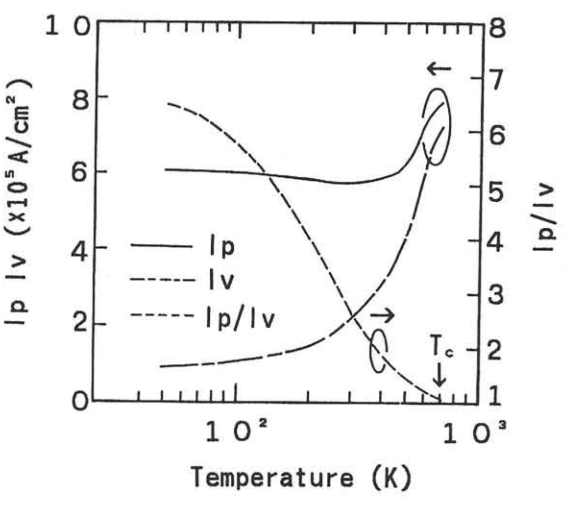


Fig. 4 Temperature dependence of Ip, Iv, and Ip/Iv (Relaxation time is assumed to be constant.)

The critical temperature represented by T_c, and shown in fig. 5, is estimated from the difference between the resonant and virtual levels of transmission probabilities at zero bias. Because the ohmic drop occurs in the cathode region, T_c is not always a good criterion for judgement of Ip/Iv. This indicates that conditions of the cathode region have a serious influence on device performance.

4. The Wigner Formula and Transfer Matrix Method

Theoretical analysis of RTD with heavily doping n^+ layers and without scattering between the double barriers is undertaken. Current voltage characteristics obtained from the present formula are compared with those from the Transfer Matrix Method. Results are shown in fig. 5.

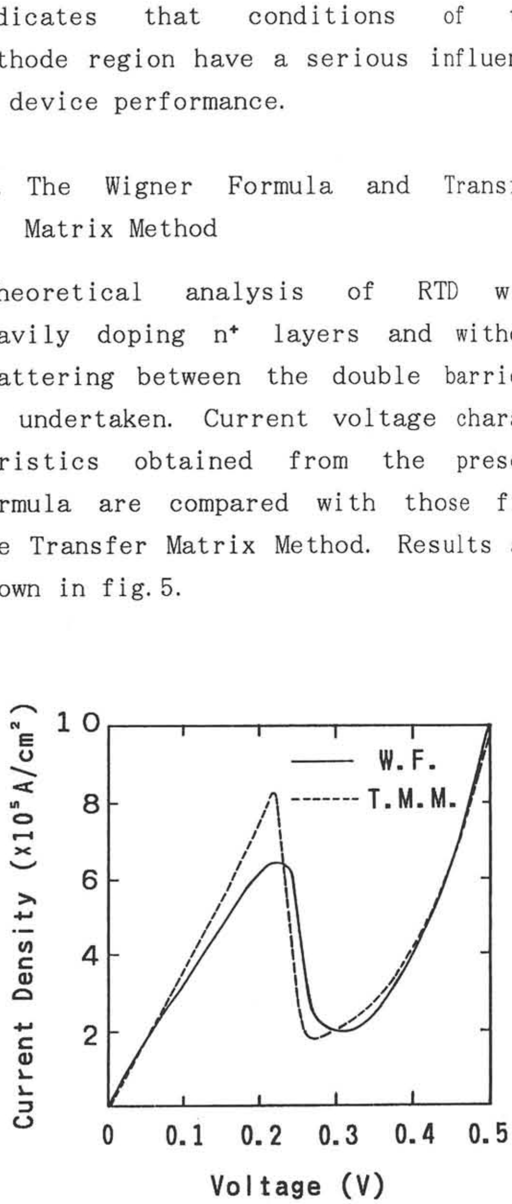


Fig. 5 Current voltage characteristics obtained from the Wigner Formula and the Transfer Matrix Method. RTD with the 2×10^{18} cm^{-3} doping concentration and without scattering between the double barriers is analyzed.

It can be seen that the two approaches show nearly the same results in this optimum condition. This is because strong scattering and screening effects in the cathode region maintain a flat band and electrons are in classical distribution in this region approximately.

5. Conclusion

Nonequilibrium quantum transport simulation technique based on the Wigner Formula have been investigated.

The usefulness of this formula is presented to research systematically the influence of some perturbations on the quantum interference effects.

Especially, if the ohmic drop and the electronic accumulation in quantum mechanical distribution in the cathode region occur, it predicts the remarkable influence on quantum interference effects in contrast with the conventional Transfer Matrix Method.

The importance of dealing with non-equilibrium quantum mechanical distribution can be understood.

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