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Monte Carlo Calculation for Transport Study and its Application to Device Design

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Recently, Monte Carlo simulation has been of much interest in microelectronics and has been intensively studied. Traditionally, Monte Carlo has been developed in the context of semiconductor physics, where electron transport is the principal concern [1]. With the reduction in device dimension, nonstationary effects such as velocity overshoot, have become important in device operation. Unfortunately, conventional device simulation based on the drift-diffusion equation can not handle these effects. Therefore, Monte Carlo calculation has been applied to the design of such devices. This paper describes recent developments in Monte Carlo simulation for transport study and its application to device design. Concerning transport study, it is shown that the carrier-carrier interaction including the screening and degeneracy effects becomes important with the increasing impurity doping. As an example for the application of the Monte Carlo simulation to device design, a transit time in HBTs is investigated.

Until now, transport studies using Monte Carlo simulation mainly focused on electron transport in n-type semiconductors with low or moderate doping densities and experimental data for carrier transport have been limited to these cases. Because small devices exhibit higher carrier concentrations, carrier transport under both high carrier and high electric field conditions has to be studied. With the advent in ultra-fast pulse lasers,carrier transport experiments, such as the time of flight method, can be performed with high resolution so that drift velocity and carrier temperature are obtained accurately [2]. Combining this experimental data with Monte Carlo calculation, scattering mechanisms in highly doped semiconductor can be clarified [3]-[5]. In Fig. 1, the measured drift velocity versus electric field is presented for three samples of Be-doped GaAs of which impurity concentrations are varied from 1.5×10^{17} to 1×10^{19}. This data is compared with calculated results. For moderately doped samples which correspond to samples A and B, the calculated results show good agreement with the experimental ones. In the calculation, the electron-hole interaction is taken into account in a similar

manner to the electron-electron scattering [6]. The screening effect is also considered introducing an appropriate screening length in the scattering potential. In Fig 1.(c), a chain-dotted curve shows the calculated result for a highly doped sample (sample C) using the same model as is used in the simulation of samples A and B. It can be seen that the calculated result is much smaller than the experimental one. In a highly doped semiconductor, many states have been occupied by carriers so that the scattering between electrons and holes is reduced due to Pauli's exclusion principle. Therefore, this effect should be considered for the highly doped case. The result in which the degeneracy effect is taken into consideration, assuming a constant hole temperature, is drawn in Fig. 1(c) by a broken line. Although the calculated result comes close to the experimental data at the low field, there remain some differences in high field region. With increasing electric fields, holes are heated so that their temperature increases slightly. From luminesence experiments, it can be determined that hole temperature varies from 300K to 500K. When the heating of holes is includes, the calculated result shows good agreement with the experimental one for a wide region in the electric field.

As was demonstrated above, Monte Carlo simulation is very useful for the investigation of carrier transport mechanisms in semiconductors. Another merit of Monte Carlo simulation is that it can handle nonstationary effects. To analyze these effect exactly, Monte Carlo simulation becomes indispensable. As an example of the Monte Carlo simulation to device design, we will show the effect of velocity overshoot on the device characteristics of HBTs. In this simulation, the accurate models described above were introduced. Fig. 2 (a) shows a schematic band diagram of the HBT modeled. The velocity overshoot effect in the HBT occurs in the collector region. An electron launched from the base edge runs into the depletion region with a velocity higher than its steady state value. Its velocity in the collector depends on the initial state of the electron when it reaches the collector and the electric field in the collector. The initial state of the electron at the collector is determined by its running history in the base region. Therefore, the structure of the base and collector of the device including its impurity profile, greatly affects the electron transit time. Fig. 2 (b) shows the transit time for an HBT versus various electric fields as calculated a Monte Carlo simulation of the collector region [7]. As for the initial states of the electrons, the results of a Monte Carlo simulation for the base region are used. As can be seen in the figure, there is an optimum value for the electric field for the collector length where the velocity overshoot effect is most pronounced. Although a constant electric field is assumed in the calculation, the transit time consistent with the local electric field can be obtained combining the Monte Carlo calculation with Poisson's equation.

In this paper, recent advances in Monte Carlo calculations for highly doped semiconductors and an application to device design were presented. With the reduction in device dimension, we cannot design any devices without a deep theoretical knowledge of their behaviour. Therefore, the Monte Carlo simulation will be increasingly needed. Device simulation using Monte Carlo method has not yet matured, and there remain many problems to be solved. For example, Monte Carlo calculation can not be applied to devices with complicated structure, because the number of carriers to be calculated is limited. In addition, it takes extensive computer resources so that the calculation cost is too expensive. To meet these problems, effective numerical algorithms and more advanced computers including parallel processors are required.

References

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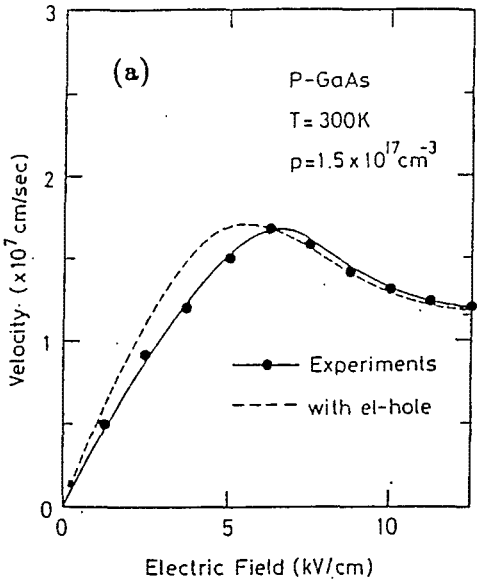
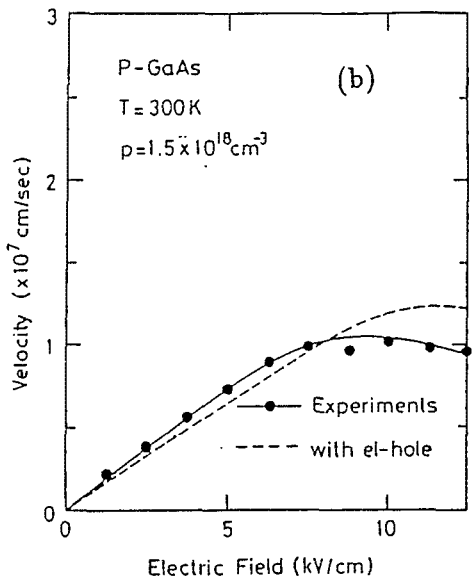




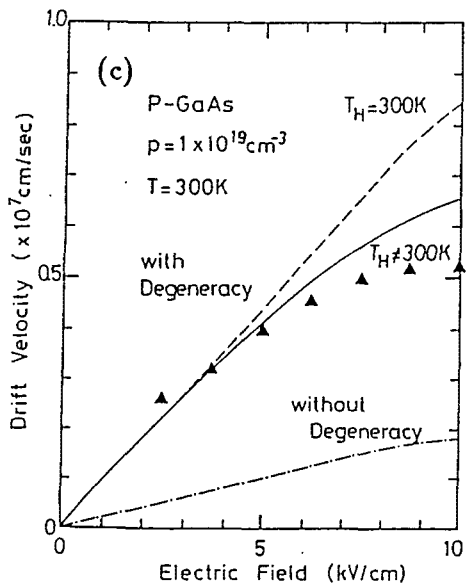
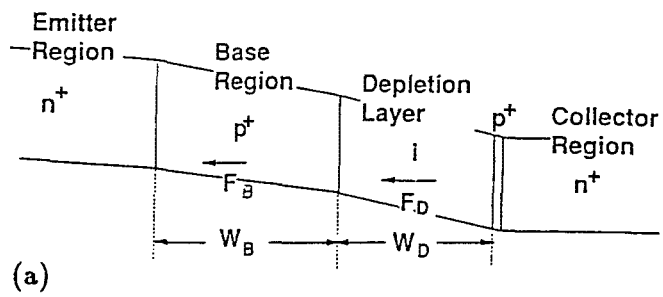


Fig. 1 Comparison between calculation and experiment in drift velocity (a) Sample A, (b) Sample B, and (c) Sample C.



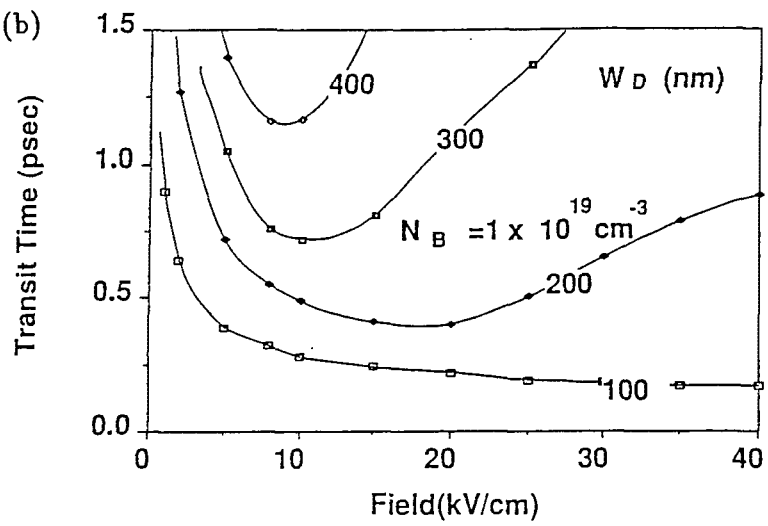


Fig 2 (a) Schematic band diagram of an HBT, (b) Transit time vs. F_D in HBT.