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Study of Electron Transport in Semiconductor Materials

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Abstract

The Monte Carlo Simulation Technique is described and the technique has been applied to obtain the velocity-field characteristics of different compound semiconductors. The results agree with the available experimental data and with those obtained by Boltzmann Transport Equation analytically.

Keywords: *Monte carlo simulation, compound semiconductors, numerical technique, electron mobility*

INTRODUCTION

In recent times, the Monte Carlo simulation technique is being extensively used in various fields of science and engineering. In this technique, the motion of the carrier inside the semiconductor under the influence of an applied electric field is simulated in a computer through the use of random numbers. A single carrier is followed through a large number of two-step, free flight-collision interaction cycles until finally the time average of any of the estimators used to characterize the motion reaches a steady state that is not evolving any further with time. Under such a condition the ergodicity of the process can be invoked to describe the motion of the carrier ensemble from the study of the motion of the single carrier over a sufficiently long time. This ensures that both spatial and temporal stabilization of the energy distribution function of the carriers have been achieved and the computed time average of the estimator actually represents the true average value of the corresponding physical quantity.

This technique is applied for the calculation of electrical conductivity characteristics in some of the II-VI semiconductors. The analytical methods for obtaining the conduction properties in semiconductors involving the solution of the Boltzmann transport equation (BTE) under large applied electric field is beset with many complications. The Monte Carlo technique provides a better and more rigorous solution in such a situation. We have presented in this paper, the MC simulation technique for obtaining velocity-field characteristics in some II-VI compounds like ZnO, ZnS, CdS, CdSe and CdTe. We have applied the same method to obtain the mobility values in one emerging III-V compounds, InSb. The results obtained here, were compared with available results.

NUMERICAL SIMULATION TECHNIQUE

Monte Carlo simulation technique, regarded as one of the efficient numerical techniques, is being increasingly accepted due to the ease of programming and availability of fast processors. In this paper, we have discussed the Monte Carlo simulation technique as applicable to obtain the electron mobility values compound semiconductors. The crystal under investigation contains the lattice in thermal equilibrium with its ambient and the carriers.

Carrier Motion

The carrier is presumed to start with an initial wave vector k0. Under the influence of the external electric field, it accelerates and continues its motion in what is called free-flight. The duration of this free-flight is estimated by a (pseudo) random number r0 distributed uniformly between 0 and 1. The time at which a collision takes place is given by, $t_c = -(\ln r_0)/\Gamma$, Where Γ is the chosen Rees' parameter. Γ has been rendered constant over the energy range considered by including a self-scattering term such that the sum of all the real scattering rates plus the self-scattering rate remains constant over the entire energy range considered. It has been shown that the steady state value obtained by including self-scattering term is indeed the value corresponding to the real scatterings [1].

Trajectory of the Electron during Free Flight

Once t_c is determined, one may plot the trajectory of the electron from t_0 to t_c by

using the laws of Newtonian mechanics. Thus, $x = (\hbar/m^*) kx_0(t_c-t_0)$, $y = (\hbar/m^*) ky_0 (t_c-t_0)$, $z = (\hbar/m^*) [kz_0(t_c - t_0) + (eE/2\hbar) (tc - t_0)^2]$ where kx_0, ky_0, kz_0 are the x, y, z components of k_0, the value of k at $t = t_0$, and the polar axis z has been chosen as the direction of the applied electric field E.

Determination of the Type of Collision

Having determined the instant at which the free flight has terminated, we now have to determine the type of collision which has terminated the free flight. The various scattering rates, Si corresponding to the various scattering mechanisms for the carrier with wave vector *k* is obtained from Nag B R [2]. Next, another random number r1 is used to ascertain which one of the n scattering mechanisms including the self-scattering process has been operative. The detail of scattering process is available in our earlier work [3].

CALCULATION OF MOBILITY VALUES

The model for Monte Carlo simulation described earlier is implemented in C to calculate the electron mobility values of the II-VI compound semiconductors. The program incorporates a data table containing the various physical parameters of the materials [4].

Formulations for computation of different band properties, such as overlap integral, $\delta\gamma/\delta E$ are included in the program. Also included are scattering rate routines for various scattering processes. To run the simulation, the name of the material, the lattice temperature, the impurity concentration, the applied electric field and which of the scattering processes are to be considered (by default all the processes are assumed to be operative) and the Rees' parameter ɼ need be supplied. The simulation is found to converge between 50,000 and 100,000 real scatterings depending upon the applied electric field and the material considered. The simulation has been performed under fields ranging from $1kVcm^{-1}$ to $50kVcm^{-1}$ depending upon the particular semiconductor and lattice temperature. The calculated results agree within 5% to 10% of the available experimental data and with analytical calculations like the calculations based on a displaced Maxwellian distribution function. As an example we note that for cadmium telluride at 77K, the mobility obtained by Monte Carlo simulation is 2192.5 $cm^2V^{-1}s^{-1}$ while that obtained by

solving the Boltzmann equation using a displaced Maxwellian distribution function is 2122 $cm2V^{-1}s^{-1}$ at a field of $7kVcm^{-1}$ [4]. The experimental value of the mobility obtained at this field is 2143 $cm^2\ V^{-1}\ s^{-1}$ [5]. At a field of 8.5 $kVcm^{-1}$, the corresponding values are 2214.4, 2202.5 and 2330 $cm^2\ V^{-1}\ s^{-1}$, respectively. In the absence of known experimental data under identical conditions we cannot compare all of our results. Some existing theoretical results are, however, in good agreement with our present calculation. The variation of the electron mobility with the applied electric field for II-VI compound semiconductors like ZnO, ZnS, CdS, CdSe and CdTe has been plotted in the Figure 1 for impurity concentration of 1×10^{15} cm^{-3} in each. Curves such as presented in the Figure 1 are useful for device simulation where the field dependence of mobility is needed to study the behavior of devices under high field stress.

We have plotted in Figure 2 the values of the electron mobility in InSb, calculated by the Monte Carlo simulation technique, for different values of the applied electric field and impurity concentration. It is seen that the results obtained by Monte Carlo simulation technique agree quite satisfactorily with available theoretical

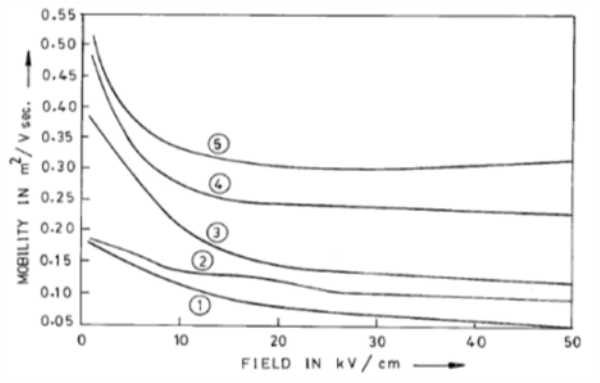

Fig. 1: *Variation of Electron Mobility with Applied Electric Field at 77K in (1) ZnO, (2) ZnS, (3) CdTe, (4) CdS, (5) CdSe for Impurity Scattering of* 1×10^{15} cm^{-3} *in Each.*

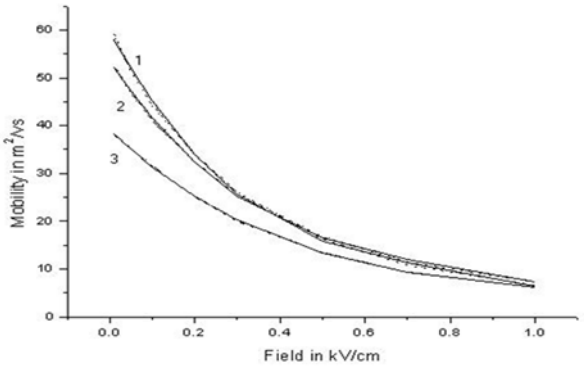

Fig. 2: *Variation of Electron Mobility with Applied Electric Field at 77 K for InSb at Different Ionized Impurity Concentrations (1)* $N_i = 0$, *(2)* $N_i = 1e^{14}$, *(3)* $N_i = 5e^{14}$.

and experimental data. A device modelling program requires the mobility values to be evaluated at a large number of

applied electric field. In such a case, the numerical technique can be put to use effectively without any loss of accuracy.

CONCLUSION

It can be concluded that the Monte Carlo Simulation technique can be effectively used to calculate the electron transport and hence the current conductivity required for any kind of electron devices. It can be also be used as a tool for device designers and also the material scientists.

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REFERENCES

1. Rees H D. Calculation of distribution function by exploiting stability of steady state. *Journal of Physics Chemistry Solids*. 1969; 30: 643p.
2. Nag B R. Electron transport in compound semiconductors. *Springer-Verlag, Berlin;* 1980.
3. Karthik R, Uma Sathyakam P, Mallick P S. Effect of dislocation scattering on electron mobility in GaN. *Natural Sciences*. 2011; 3: 812p.
4. Mukhopadhyay D, Bhattacharya D P. Electron transport in II-VI semiconductors. *Journal of Physics Chemistry Solids*. 1984; 45: 393p.
5. Canali C, Martini M, Ottaviani et al. Transport properties of CdTe. *Physics Review–B*. 1971; 4: 422p.