High - Field and High - Temperature Transport in n-type 3C-SiC

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ABSTRACT

The physical model used in Monte Carlo simulation is developed considering the energy gap structures and the main scattering mechanisms in details. The static electron transport in the material 3C-SiC is analyzed by single particle Monte Carlo method at high field and high temperature .The results show the excellent high field and high temperature properties of the material. The scattering mechanisms at high temperature and high field are discussed by the analysis of the results. The calculations based on the ensemble Monte Carlo procedure reveal a velocity overshoot at different temperature

Keywords: Silicon Carbide, Monte Carlo, Velocity Overshoot , Electron Transport,

INTRODUCTION

Silicon carbide (SiC) with excellent physical and electrical properties have shown the attractive prospects for wide range applications to the various harsh condition and few other semiconductor materials and devices could be compared with, such as high temperature, high power, high frequency and/or radiation hardness. These favorable properties are a result of the wide band gap, its high conductivity, large saturated drift velocity, higher breakdown fields and material hardness. SiC is also being explored as a high resistivity material for device isolation, in possible non-volatile charge storage applications and as a blue-green luminescent emitter. Research of silicon carbide electronic materials and devices has made great progress in recent years [11].

Simulation of the SiC electronic transport properties have been carried out in the past [1,2] and yielded a number of important transport parameters. Numerical simulation of SiC devices have also carried out [12].It is the purpose of the present paper to describe in the detail our calculation of both high -field and high temperature transport properties of n-type 3C-SiC by Monte Carlo method. The field and temperature dependence of electron drift velocity and mobility, the momentum and energy relaxation times are obtained. The calculations reveal a velocity overshoot .We shall also compare our results with other theoretical and experimental data insofar as it is possible highlight the accuracy of the simulation results presented hers.

CALCULATIONAL MODEL

The Boltzmann transport equation can be solved using Monte Carlo method by following the transport history of one and more electrons (particles), subject to the action of external forces(such as applied field) in a statistical manner. Monte Carlo simulations require a detailed definition of the physical system in terms of the material parameters, the energy-band structure, scattering rates and lattice temperature.

It is found from experimental [4,5] and theoretical [6,7] studies that 3C-SiC is zinc blend type crystal with the band gap is 2.2eV and an indirect-gap semiconductor with the conductor band minima at boundary of the first Brillouin zone along the X directions, just as in silicon. It is assumed here that the electric field is oriented along <111> so that redistribution of carriers among equivalent valleys is unimportant and transfer to higher-lying subsidiary minima is negligible. That is to say, we assume a single equivalent isotropic valley instead of the full multiple-minima conduction band. The transverse and longitudinal effective electronic masses are taken to be 0.25 and 0.67 in keeping with the cyclotron resonance experimental data[5]. The band non-parabolicity is taken into account by the hyperpolic band model.

$$\frac{\hbar^2 k^2}{2m_C} = g(E) = E \cdot (1 + \alpha \cdot E) \quad (1)$$

Where the nonparabolicity factor $\alpha = 0.322\, eV^{-1}$ arises from repulsion from higher-lying conduction bands rather than from the valence band.

Scattering mechanisms considered here are Acoustic deformation potential scattering, polar-optical phonon scattering, two different equivalent-intervalley phonon scattering processes (first-order and zero-order interaction), ionized-impurity scattering and impact ionization. In high-temperature and high-field the acoustic deformation potential scattering is a elastic process, and the scattering probability used in Monte Carlo simulation should consider ellipsoidal and nonparabolic bands. The coupling constants of deformation potential scattering is 22eV. The effect of polar-optical phonon scattering is more

important in SiC than in Si and Diamond for which it has ionic semiconductor characteristic. The effective polar field is $1.08\times10^5\,V/cm$, which is the same as used in[1,2]. Electron intervalley scattering is also important in SiC for which is a semicondurctor whith many-valley band structure. The zero-order term is forbidden by the symmetry selection rules sometimes in SiC as in GaAs, so the first -order term must cosider [8]. For ionized-impurity scattering the Books-Herring formula is used with an ionzied impurity concentration of $5\times10^{16}\,cm^{-3}$. Impact ionization rates calculated using Ridley's approach with a 2.36eV energy threshold.

Two Monte Carlo methods to solve the Boltzmann transport equation: Single-particle Monte Carlo method and the ensemble Monte Carlo method are used to simulate the steady-state carrier transport under a static and uniform electric field and the carriers transport in an inhomogeneous field, the non-stationary behavior , respectively[9]. The adjustable method of electric field in the variable scheme has been improved in a self-consistent Monte Carlo method for analysis.

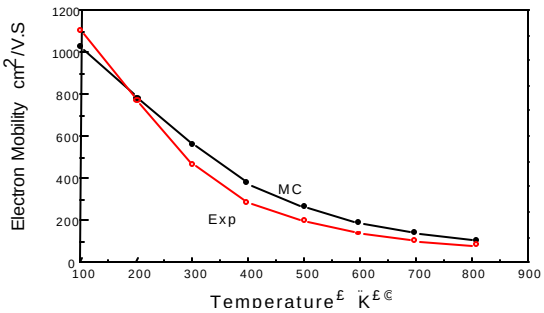

Fig.1 Electron Mobility Calculated for bulk 3C-SiC at various lattice temperatures.The experimental data come from [3]

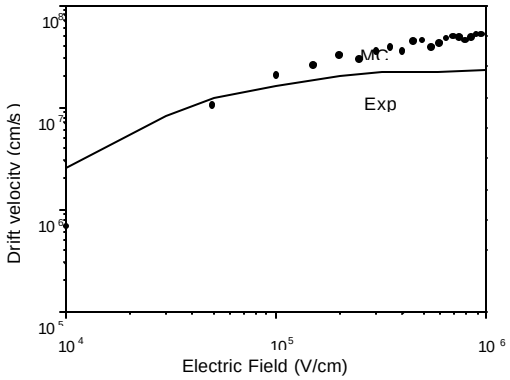

Fig.2 Drift velocity as a function of electric field strength for electron in 3C-SiC. Points refer to theoretical Monte Carlo calculations and curve to experiment[10]

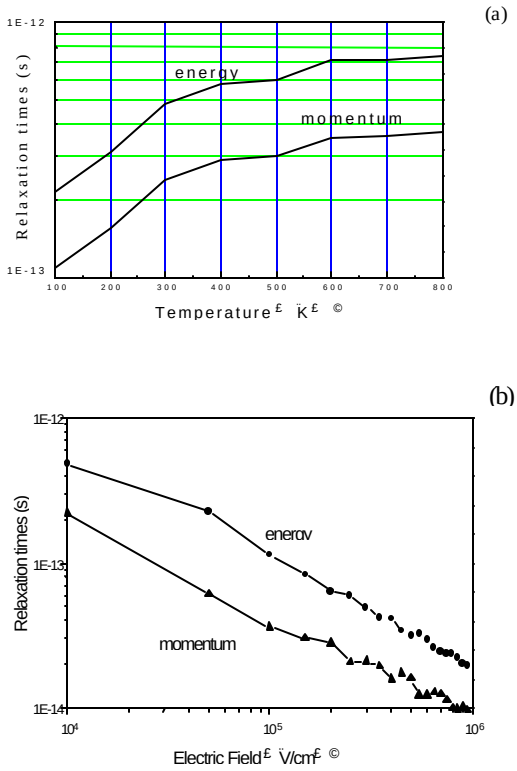

Fig.3 The momentum and energy relaxation times as functions of temperatures (a) and electric field (b)

RESULTS

The Monte Carlo simulation are used to obtain both the steady state and transient electron transport properties at various temperatures and d.c electric fields. Some results are shown in figure 1-5. Fig.1 shows the electron mobility vs. various lattice temperature. The calculated values agree well with a recent measurement data[3]. The difference between the simulation results and the experimental data in high temperature range is because non-polar optical phonon scattering is not taken into account and the selection of some material parameters may not exactly. Fig.2 shows the drift velocity as a function of electric field strength for electron in 3C-SiC at room temperature. Theoretical Monte Carlo calculations (Points) and experiment data (line) are fitted very well [10] . The velocity saturation occur for electric field beyond $2\times10^5\,V/cm$, It is found from the figure that the satured drift velocity in 3C-SiC is about $2\times10^7\,cm/s$. The different between experimental and simulation is the same reason above. The energy and momentum relaxation time of electron as a function of electric field and temperature are show in fig.3, respectively.

The transient electron transport in bulk 3C-SiC are performed by ensemble Monte Carlo simulation with

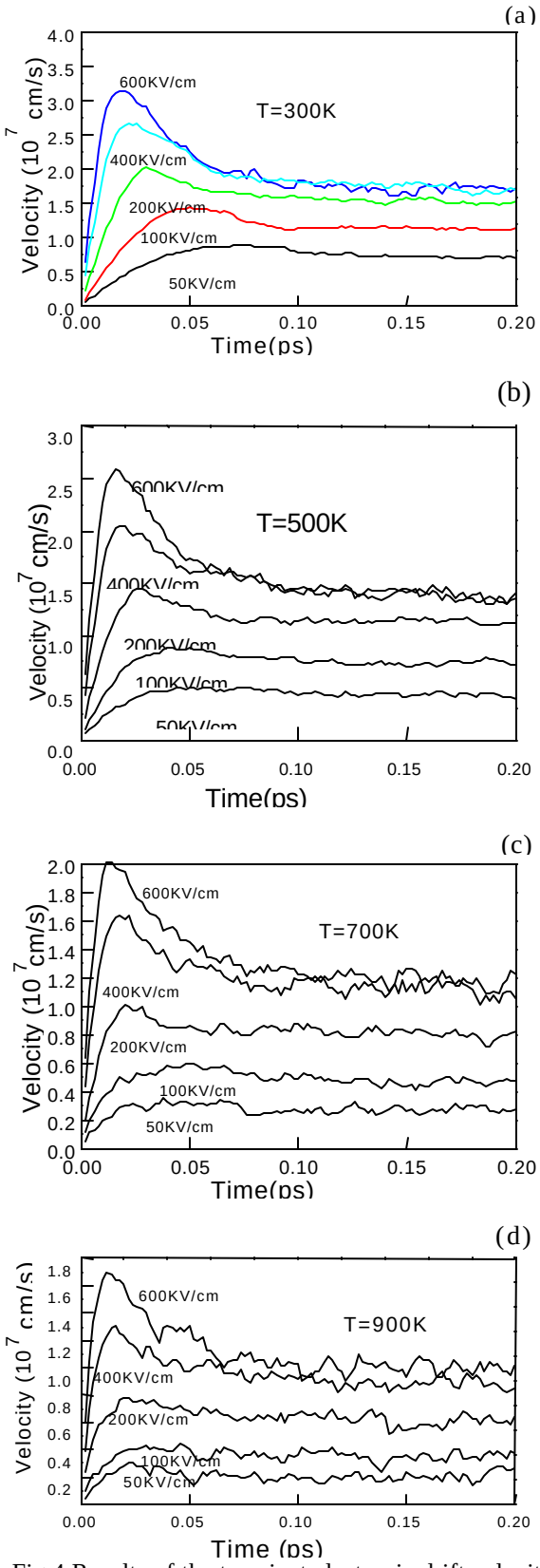

Fig.4 Results of the transient electronic drift velocity in bulk 3C-SiC obtained from Monte Carlo simulations for five different electric fields. (a)Data for 300K; (b)for 500K; (c)for 700K; and (d) for 900K

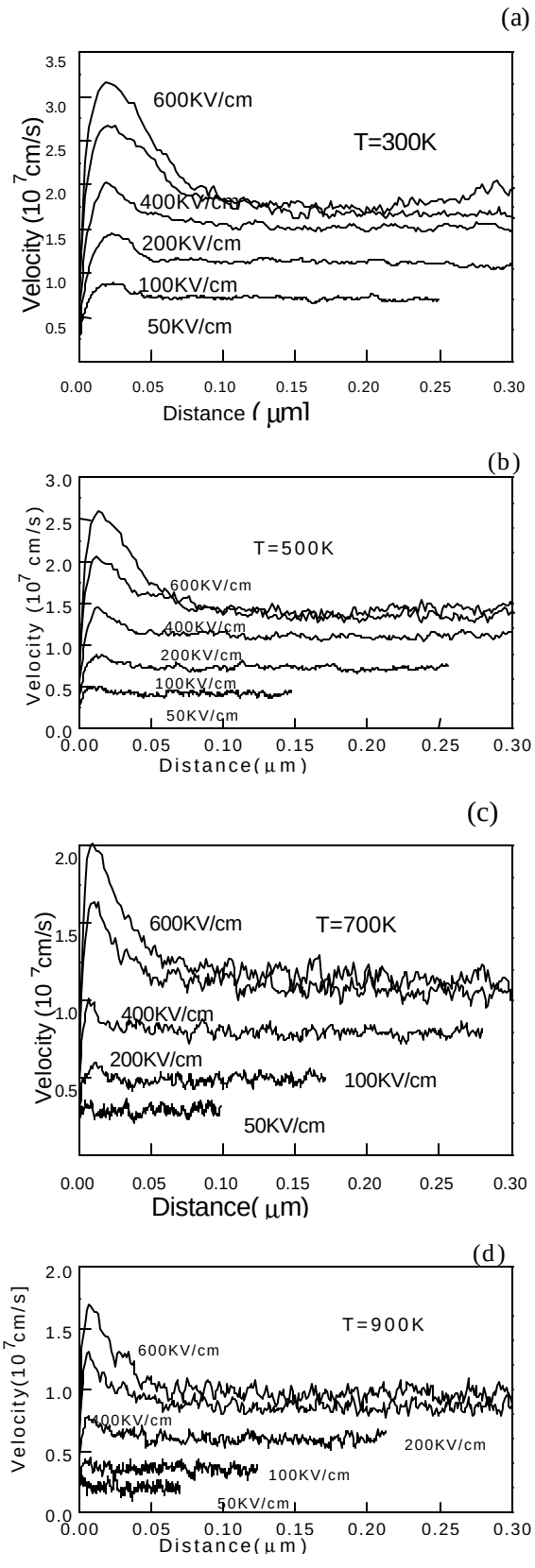

Fig. 5 Drift velocity overshoot as a function of distance in bulk 3C-SiC. (a)Data for 300K; (b)for 500K; (c)for 700K; and (d) for 900K

10000 particles. The overshoots at high fields are presented in fig.4 and fig.5 at 300K, 500K, 700K and 900K, respectively. The background doping concentration is assumed to be $10^{16} cm^{-3}$.The uniform electric field applied throughout the bulk semiconductor are 50,100,200,400 and 600 KV/cm at the given temperature. Figure.4 shows the time evolution of the mean drift velocity of electrons cold-injected at the position x=0 (call the cathode), and drifting in a region of uniform electric field. We note that the velocities exhibit large transient overshoots at high fields before the steady state values are reached. This is due to the disparity of the momentum and energy relaxation times as the function of electron energy. Transient overshoot is typically observed when the electric field applied is so high that electrons can reach the high-energy region, where the momentum relaxation time is smaller than the energy relaxation time. Somewhat later, energy relaxation becomes effective so that the distribution function spreads and drift velocity decreases. With increasing temperature however, the overshoot diminishes for two reasons, First, the higher temperature , the higher internal scattering. The optical phonon interactions begin to dominate, and swamp out all elastic scattering contributions of the acoustic phonons. In addition, the effectiveness of elastic ionized impurity scattering also diminishes with temperature. Second, at the higher temperature, the energy of electrons injected from cathode are much higher, and can easily exceed the typical LO phonon quanta, this contributes towards increasing the average energy relation with the devices.

Fig.5 shows the drift velocity as a function of distance from the source, and this case is more relevant to the discussion of electron transport in submicron semiconductor devices. The distance over which the drift velocity overshoots the saturation value in 3C-SiC is less than $0.1mm$, the speed performance of 3C-SiC devices with dimensions larger than $0.1mm$ may not be affected by the overshoot phenomenon.

CONCLUSION

The field and temperature dependence of electron drift velocity and mobility, the momentum and energy relaxation times of bulk 3C-SiC are obtained from Montr Carlo simulation. The results show the excellent high-field and high-temperature properties of the material. The scattering mechanisms at high-temperature and high-field are discussed by the analysis of the results. The calculations based on the enhance Monte Carlo procedure reveal a velocity overshoot at different temperature . However, it occurs at the higher electric field and may have less affect on the submiciron SiC devices than currently semiconductor devices.

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