Research Journal of Applied Sciences 6 (3): 213-217, 2011
ISSN: 1815-932X

Calculation of High Field Electron Transport Properties in GaSb and GaAS Using a Monte Carlo Method

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Abstract: Electron transport properties in GaSb and GaAs are calculated for different temperature, doping dependencies at high electric field applications. The calculations are performed using a three valleys ensemble Monte Carlo model that includes numerical formulations of the phonon scattering rates and ionized impurity scattering rates. For two materials, it is found that electron velocity overshoot only occurs when the electric field in increased to a value above a certain critical field. This critical field is strongly dependent on the material parameters. Results from the two materials are finally compared. The agreement with the available experimental data is found to be satisfactory.

Key words: Monte Carlo method, ionized impurity scattering, overshoot velocity, materials, numerical formulations, Iran

INTRODUCTION

GaSb and GaAs semiconductors are becoming of increasing importance in many emerging optoelectronic and electronic device applications. Among these applications are ultraviolet photodetectors, blue and UV light emitters and high frequency, high power electronic devices. As an aid to the device-related work, the transport coefficients of the materials need careful investigation. Transport properties of electrons in GaSb and GaN semiconductors can be conveniently derived by direct solution of the Boltzmann equation (Chattopadhyay and Queisser, 1981). Previous applications of this technique were directed toward calculations of drift mobility in ideally pure semiconductors. There is also considerable interest in accurate descriptions of impure crystals, from both the experimental and the theoretical points of view. In the former case, for example, one may take advantage of the sensitivity of mobility to ionized impurities in analyses of impurity content. In the latter case, highly doped materials allow one to probe regions of the conduction band in the neighborhood of the Fermi level, well above the band edge. Obviously, accurate calculations in conjunction with experimental data are helpful in exposing weaknesses of the theoretical model, particularly with regard to electron scattering by ionized impurities at low temperatures (Gonze *et al*., 2002). The purpose of the present paper is to calculate electron drift velocity for various temperatures and ionized-impurity concentrations. The formulation itself applies only to the central Γ valley conduction band and the two nearest valleys. We have also consider band nonparabolicity, admixture of p-type valence-band wave functions, degeneracy of the electron distribution to any arbitrary degree and the screening effects of free carriers on the scattering probabilities (Kohn and Sham, 1965). All the relevant scattering mechanisms in cluding the two-mode nature of the polar optic phonon scattering, are taken into account (Hohenberg and Kohn, 1964). In this communication, we present Monte Carlo calculations of steady-state electron transport conditions in GaSb and GaAs (Di and Brennan, 1991). We demonstrate the effect of injection energy and electric field on the electron transport properties.

MATERIALS AND METHODS

Model details: In order to calculate the electron drift velocity for large electric fields, consideration of conduction band satellite valleys is necessary. The first-principles band structure of zincblende GaSb and GaAs predicts a direct band gap located at the Γ point and lowest energy conduction band satellite valleys at the X point and at the L point. In the Monte Carlo simulation, the Γ valley, the three equivalent X valleys, the four equivalent L valleys are represented by ellipsoidal, nonparabolic dispersion relationships of the following form (Look *et al*., 1998):

$$E(k)[1+\alpha_i E(k)] = \frac{\hbar^2 k^2}{2m^*} \quad (1)$$

Where:
m^* = The effective mass at the band edge
α_i = The non-parabolicity coefficient of the i th valley

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Table 1: Important parameters used in the calculations for GaSb, GaAs (Makino *et al*., 2001)

Parameters	GaSb	GaAs
Band-gap (eV)	0.726	1.420
Electron effective mass (m^*)	0.041	0.063
Nonparabolicity (eV^{-1})	0.500	0.610
Static relative permitivity (ε_0)	15.700	12.500
Optical relative permitivity (ε_∞)	14.400	8.700
Density (k gm^{-3})	5610.000	5370.000
Sound velocity (m sec^{-1})	6070.000	5500.000
Deformation potential (eV)	8.900	8.800
Piezoelectric constant (C m^{-2})	0.080	0.050
Optical phonon energy (eV)	0.029	0.020

The band structure and material parameters necessary for calculating the scattering probabilities used in the present Monte Carlo simulation are shown in Table 1. Scattering mechanisms included in the simulation are acoustic deformation potential scattering (treated either as an elastic process or as an inelastic process) and pizoelectric scattering (which is found to be negligible in the temperature range). Furthermore, longitudinal optical phonon scattering, nonequivalent and where applicable, equivalent intervalley scattering events are taken into account among all valley types with the transfers assumed to be governed by the same deformation potential fields and the same phonon frequencies. Degeneracy effects are expected to be negligible over almost all of the temperature and electron concentration ranges of interest here and hence are not considered in the calculation. In the model at the start of each simulation, ten thousand electron particles are distributed in momentum space according to a Maxwell-Boltzmann distribution function. These particles are propagated classically between collisions according to their velocity, effective mass and the prevailing field. The selection of the propagation time, scattering mechanism and other related quantities is achieved by generating random numbers and using this numbers to select for example, a scattering mechanism.

In the case of the ellipsoidal, non-parabolic conduction valley model, the usual Herring-Vogt transformation matrices are used to map carrier momenta into spherical valleys when particles are drifted or scattered. Steady-state results of high field transport studies have been obtained for lattice temperatures up to 600 K in order to gain some insight into the hot carrier transport and the energy distribution function that would be generated in the gate-drain region of a power field effect transistor.

RESULTS AND DISCUSSION

Electron drift velocity as a function of electric field is important in determining the performance of high-speed and microwave semiconductor devices. Here we show the

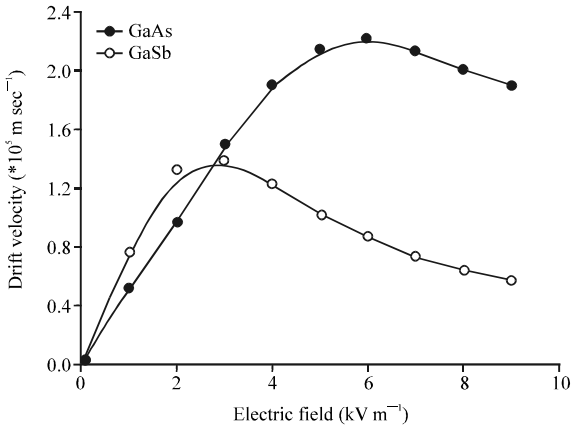

Fig. 1: Calculated steady-state electron drift velocity in bulk zincblende GaSb and GaAs using non-parabolic band models

results of temperature dependence of the steady-state velocity-field characteristics and valley occupancy in bulk GaSb and GaAs materials.

Figure 1 shows the simulated velocity-field characteristics at 300 K with a background doping concentration of 10^{17} cm^{-3} and with the electric field applied along one of the cubic axes.

Similar to the experimental results the simulations suggest that the peak drift velocity for zincblende GaAs is ~2.2×10^5 m sec^{-1} while that for GaSb is about 1.2×10^5 m sec^{-1}. At higher electric fields in tervalley optical phonon emission dominates causing the drift velocity to saturate at around 0.7×10^5 m sec^{-1} for GaSb and 1.7×10^5 m sec^{-1} for GaAs. The calculated high field electron drift velocity apparent from Fig. 1 is fractionally lower than those that have been simulated by experimental works which assumed an effective mass in the upper valleys equal to the free electron mass. The threshold field for the onset of significant scattering into satellite conduction band valleys is a function of the intervalley separation and the density of electronic states in the satellite valleys.

The importance of electron intervalley transfer at high electric fields can be clearly shown in Fig. 2. In this figure the fractional valley occupancies for different materials is plotted. It is obvious that the inclusion of satellite valleys in the simulations is important. Significant electron transfer to the upper valleys only begins to occur when the field strength is very close to the threshold value. At the threshold field the electron valley occupancies at room temperature for Γ, L and X are about 85, 13 and 2%, respectively.

Figure 3 shows the calculated electron drift velocity as a function of electric field strength for temperatures of 300, 450 and 600 K.

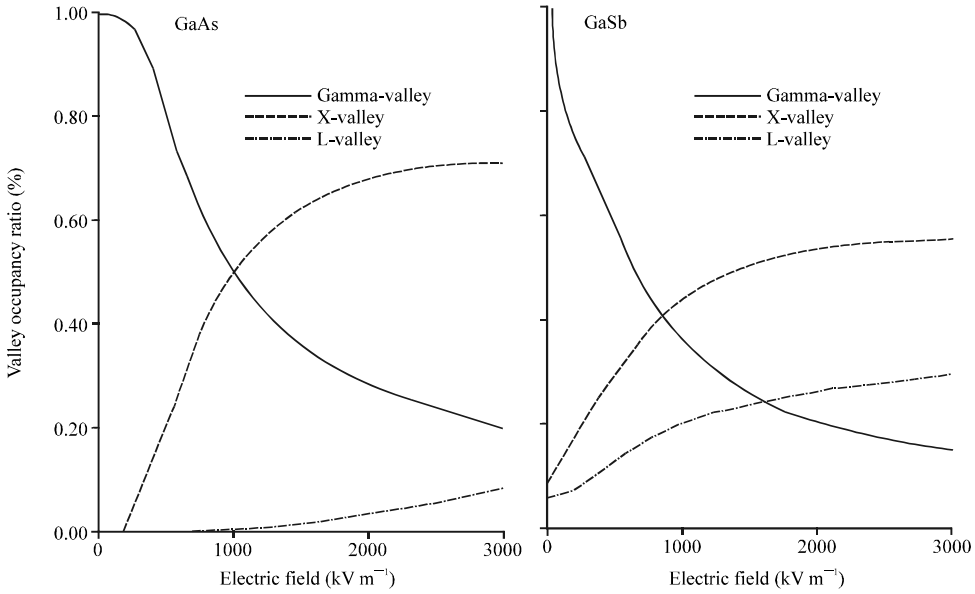

Fig. 2: Fractional occupation of the central and satellite valleys in GaSb and GaAs as a function of applied electric field using the non-parabolic band model

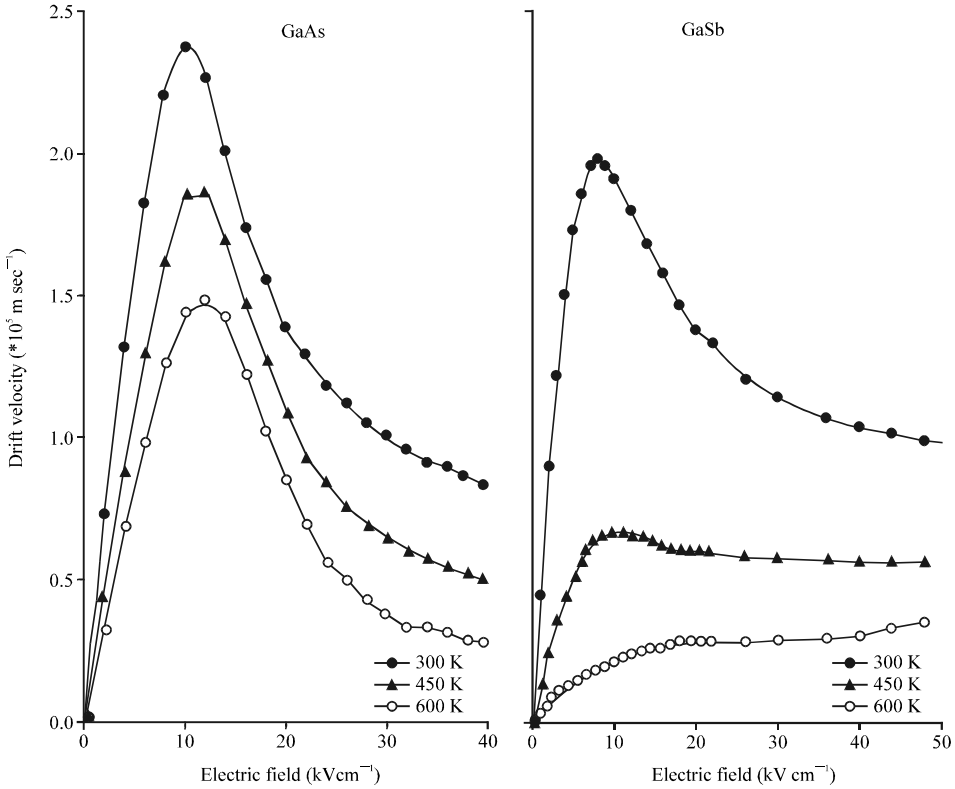

Fig. 3: Calculated electron steady-state drift velocity in bulk GaAs and GaSb as a function of applied electric field at various lattice temperatures and assuming a donor concentration of 10^{17} cm^{-3}. The peak drift velocity decreases while the threshold field increases by same percent as the lattice temperature increases from 300-600 K

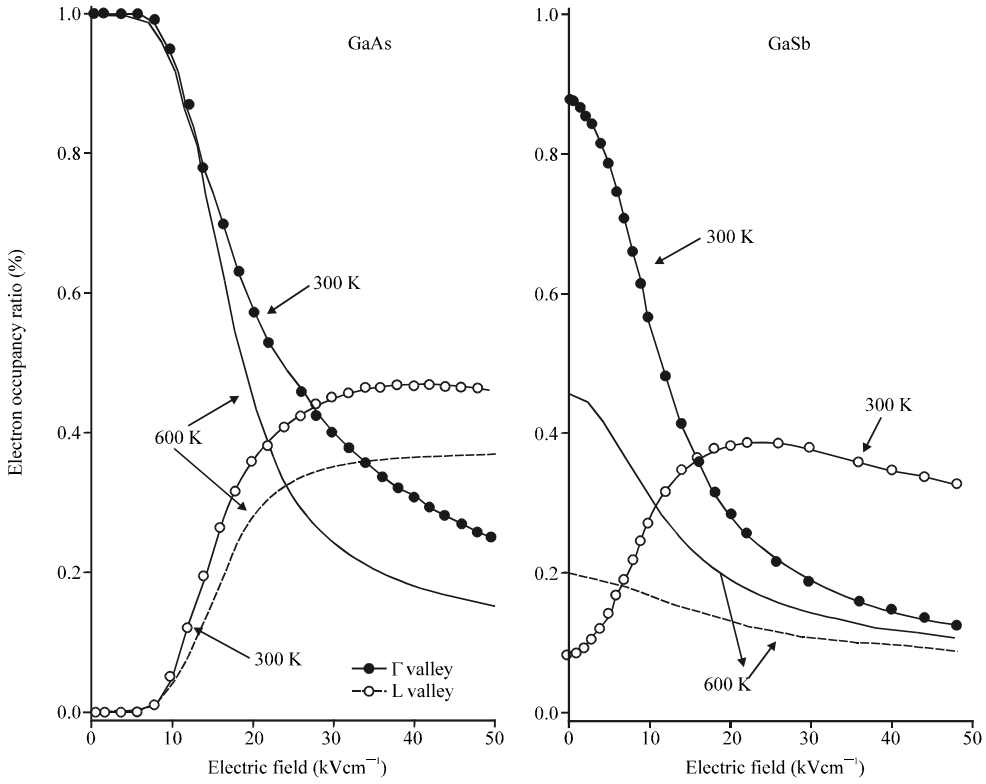

Fig. 4: Temperature dependence of the valley occupancy in the Γ and L valleys of GaAs and GaSb materials as a function of applied electric field

The decrease in drift mobility with temperature at low fields is due to increased intravalley polar optical phonon scattering whereas the decrease in velocity at higher fields is due to increased intra and intervalley scattering. It can be seen from the figure that the peak velocity also decreases and moves to higher electric field as the temperature is increased. This is due to the general increase of total scattering rate with temperature which suppresses the electron energy and reduces the population of the satellite valleys. This latter effect is apparent from the fact that the electron population in the central Γ-valley increases with temperature as shown in Fig. 2.

Figure 4 shows how the electron occupancy ratios changes with temperature for electrons in the most populated Γ and L valleys. There are significant statistical fluctuations in the results for the electrons in the L valleys for fields around 500 k Vm^{-1} which are caused by the relatively small number of electron particles occupying the valleys just above the threshold for intervalley transfer. Nevertheless it can be seen that the number of electrons decreases as the temperature increases for both valleys. Comparison of the temperature dependence of the valleys occupancy in GaAs and GaSb materials show that the change in peak velocity of GaAs from 300-600 K is a reduction of about 45% whereas for GaSb it is about 25%. The reason can be explained in terms of the energy band structure. In particular, the different electron effective mass within the central valley. This is important because electrons which are near a valley minimum have small kinetic energies and are therefore, strongly scattered. It is apparent that intervalley transfer is substantially larger in InAs over the range of applied electric fields shown due to the combined effect of a lower Γ effective mass, lower satellite valley separation energy and slightly lower phonon scattering rate within the Γ valley.

Therefore, the electron velocity in GaAs is less sensitive to temperature than in GaSb so GaAs devices are expected be more tolerant to self-heating and high ambient temperature.

Figure 5 shows how the velocity-field characteristic of GaAs and GaSb materials change with impurity concentration at 300 K. It is clear that with increasing donor concentration, there are reduction in the average peak drift velocity and the threshold field because of

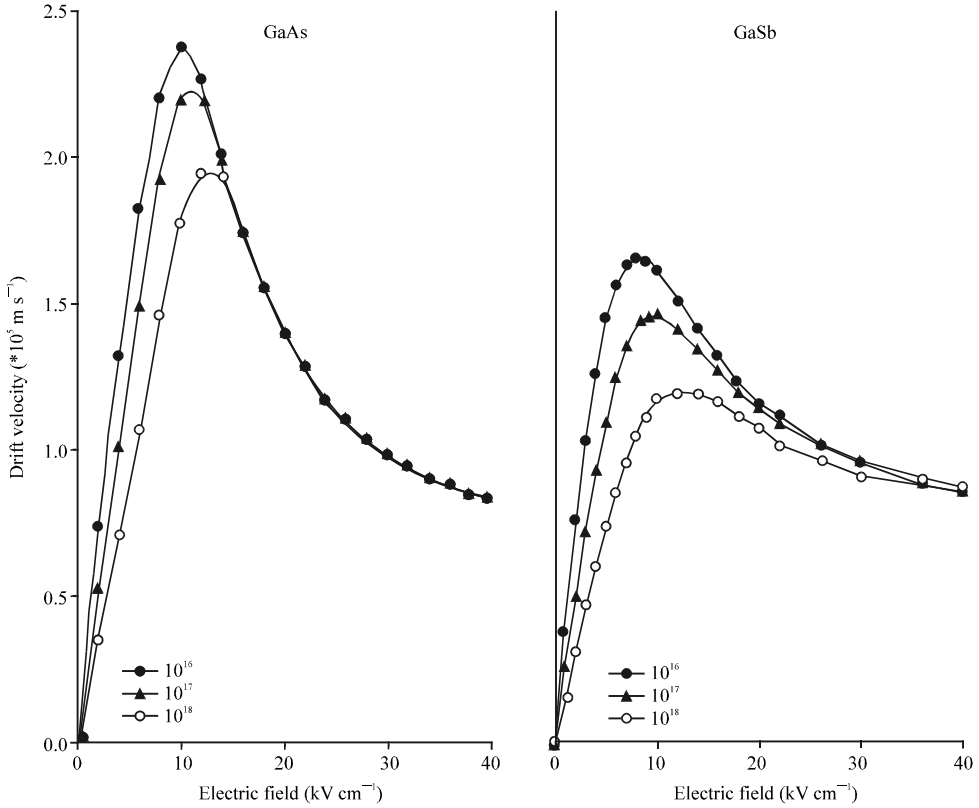

Fig. 5: Calculated electron steady-state drift velocity in bulk GaAs and GaSb as a function of applied electric field at various donor concentration up to 10^{18} cm^{-3} at room temperature

increasing scattering rate events. The results show the trend expected from increased ionized impurity scattering is in good general agreement with recent calculations by other workers.

CONCLUSION

Electron transport at different temperatures in bulk zincblende GaAs and GaSb have been simulated using an ensemble Monte Carlo simulation. Using valley models to describe the electronic bandstructure, calculated velocity-field characteristics show that the intervalley transitions in high electric fields play an important role in these materials.

The intervalley transitions lead to a large negative differential conductance. Saturation drift velocities of about 1.2×10^5 m sec^{-1} match recent measurements on low-doped bulk samples.

The researchers have also demonstrated that low temperature sensitivity of the electron transport properties of GaAs and is attractive for high-temperature and high-power electronic applications.

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