Hole Transport Characteristics in Pure and Doped GaSb

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The steady state hole transport properties of GaSb were investigated by the Ensemble Monte Carlo method (EMC). In our model we taken in to account heavy and light hole valence bands, and the following scattering mechanisms: inelastic acoustic phonon; polar optical phonon; nonpolar optical; ionized impurity. The theoretical calculations are compared with available experimental results for the GaSb hole mobility shown good agreement with temperatures from 90K up to 300K.

I Introduction

Among the III-V binary semiconductors, Gallium Antimonide (GaSb) has attracted considerable attention over the last several years. Many of its interesting properties are directly associated with its very low effective electron mass and high mobilities[1]. Consequently, it is an important candidate in high speed applications in transistors and other devices. The relatively low bandgap of GaSb lends itself well to mid/far range IR detectors and sources. From the device point of view, GaSb based structures have shown potentiality for applications in laser diodes with low threshold [2], photodetectors[5], superlattices with tailored optical and transport characteristics[6], heterojunctions [3] and resonant tunneling devices [4].

Undoped GaSb is always p-type, caused by the presence of an unusually large native acceptor background. Dutta *et. al.*[1] have shown that the conductivity arise from a doubly ionizable native defect. At higher temperatures the mobility depends basically on the concentration of native defects, which are related with the growth conditions. In this regime, significant contributions from acoustic, non-polar optical, and polar optical phonon scattering are observed, in agreement with the Monte Carlo simulation. The large negative resistance in n-GaSb are drastically affected by the increase of the density of defects, indicated by the decreasing of the carriers mobility.

From the theoretical point of view, a few work were reported in the literature related to p-GaSb transport properties. In a recent work[7], the results obtained for the hole mobility are in disagreement with the available experimental results[1]. The ionized impurity mechanism was not included in the calculations and it may seen that its play a important hole for the transport in p-GaSb.

In this work we investigate the steady state hole transport properties using Ensemble Monte Carlo method (EMC) in p-GaSb. The transport properties such as: hole drift velocity, average energy and mobility were studied and compared with available experimental results. Our results for the GaSb hole mobility shown good agreement with temperatures from 90K up to 300K.

II The model

The Ensemble Monte Carlo method is described elsewhere [8], so we focus our attention in the principal features of our model. In the case of the hole transport the analytic band structure is calculated from Warp model [8]. The nonparabolic valence bands were included and the warping parameters A, B, and C are fixed constant for GaSb. In despite, the others warping constants values can be found in the literature. Nintuze and co-workers[11] studied the influence of these parameters, on the hole transport properties. The velocities obtained, using three sets of parameters agree with experiment in the range of 12%-15%. For low fields, the agreement are closer to the experiment.

The scattering mechanisms included in our model are: inelastic acoustical phonon (deformation potential)[12]; polar optical phonon[10]; nonpolar optical process[13]; ionized impurity (Cowell-Weiskopft model)[14]. For acoustic interactions, we choose the inelastic model because the equipartition approximation $k_bT >> \hbar\omega_{ac}$ isn't more valid for low temperatures. Also, we included in our model the interband scattering. The Ensemble Monte Carlo was performed with 8000 particles.

The parameters used in our calculations are shown in table 1.

Table 1

Parameters	Values
heavy hole effective mass (300K)	0.22
light hole effective mass	0.05
$\|A\|$	11.80
$\|B\|$	8.06
$\|C\|$	11.71
Acoustic Deformation Potential (eV)	3.0
Optical Deformation Potential (eV/cm)	$0.6\text{x}10^9$
Density (g/cm^3)	5.613
phonon energy (meV)	32.90
optical phonon energy (meV)	32.90
Relative permittivity (high)	14.44
Relative permittivity (static)	15.69

In all calculations we took in consideration the effect of the temperature on the gap and effective mass. The effect of the temperature was not considered for the warping parameters.

III Results

In Fig. 1 we compare the experimental results[1] for the hole mobility temperature dependence with the results obtained by the EMC. Our results fit very well the experimental results down to 90K. The discrepancy for low temperature could be explained due to dependence of the valence band parameters with the temperature, not included in our model due to the absence of theoretical and experimental data reported in the literature. However, the results are in qualitative agreement with the experimental results.

In the Fig. 2, we show the drift velocity as a function of the electric field at 300K and 77K. For these data we can concluded that the ionized impurity scattering is more pronounced at 77K. However, when we observe the influence of the impurity concentration on the transport, the qualitative results remain the same for both temperatures. Also, is observed that at 300K the drift velocity is linear with the electric field (F) up to 8 kV/cm, so the relation for the hole drift velocity $v_h = \mu F$ is still valid in this range. This is a direct consequence that the dissipative effects still don't work up to 7 kV/cm. The similar effects has been found for GaAs [13] at room temperature. On the other hand, at 77K the GaSb shows a different behavior, the drift velocity remain liner up to 1.5 kV/cm at Ni = 0 and 3 kV/cm at Ni = $2.72\text{x}10^{17}$ cm^{-3}, but start later to show the sublinear behavior. This behavior can be explained due to the fact that the dominant part of the population of holes is scattered to emit optical phonons in an energy range which the emission sharply increasing with energy. On the other side, at 300K, the dominant part of the population of holes is shifted towards higher energies with respect to other case. The emission of optical phonons in this range of energy, is no more increasing but tends to saturate and for very high energies decrease[13].

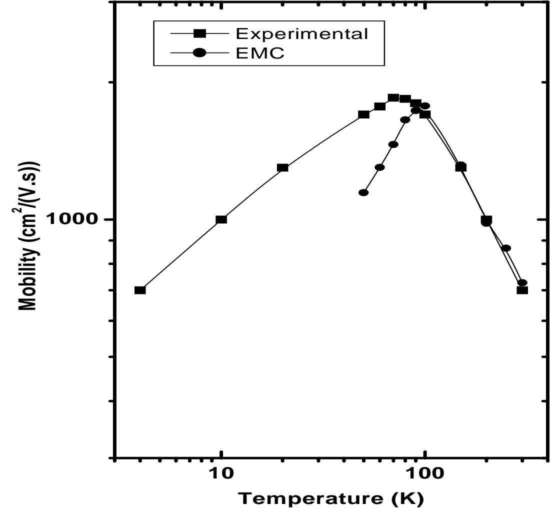

Figure 1. Dependence of the hole mobility with the temperature. We consider Ni = $2.72\text{x}10^{17}$ cm^{-3} for hole doping and a compensation of $5.2\text{x}10^{15}$ cm^{-3}.

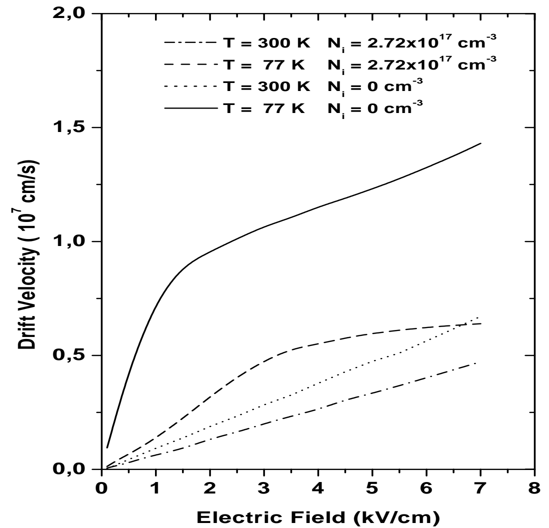

Figure 2. Hole drift velocity as a function of external electric field for two different temperatures and doping levels.

In the Fig. 3 we presented the ratio between the hole mean energy and its thermal energy as a function

of the applied electric field. The results shown that at 300K the system is more dependent of the thermal energy than at 77K. In this calculation, we observed that light holes start to heat up at fields for which heavy holes are still close to the thermal energy. It is interesting to note that at 77K a sharp transition from the thermal energy to the heated energy make the carriers unable to release for the lattice the increasing energy acquired by electric field [18].

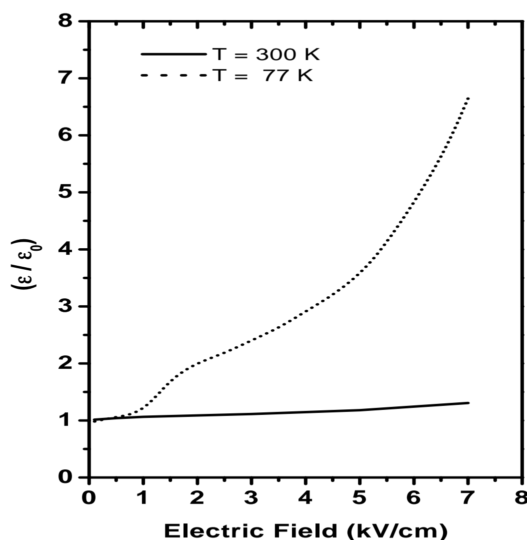

Figure 3. Ratio between the hole mean energy and the thermal energy as a function of the external electric field in pure p-GaSb.

IV Summary

From the presented study we shown results for the hole transport in GaSb. Our results for the temperature dependence of the mobility match with experimental results above 90K. The study realized by Damayanthi and co-workers[7] do not support the available experimental results. About this discrepancy, we speculate that there are two possible explanations: i) the effect of the band structure that make warp model unappropriated for low temperatures and low fields; ii) The parameters A, B and C slight change with temperature. We expected that a better understanding of the hole transport to this material can be improved when additional experimental results will be available for high fields and the influence of the temperature on valence band.

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