

Comparison Of Electron Transport Properties In Inn At High Electric Field For Zincblende And Wurtzite Crystal Structure

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Abstract—Drift velocity and mobility of zincblende and wurtzite structure of InN has been calculated using a Monte Carlo technique. All dominated scattering processes have been included in our calculations. Our simulation is based on the three valley model. Our result show that InN has a electron field velocity of 3.6×10^5 m/s in break down electric field of 1.71×10^7 V/m for zincblende structure and has a electron field velocity of 2.8×10^5 m/s in break down electric field of 3.34×10^7 V/m for wurtzite structure.

Keywords—Drift Velocity; Mobility; Zincblende; Wurtzite; Electric Field.

I. INTRODUCTION

The small band gap of InN and higher electric pick drift velocity than other III-Nitride materials make InN a promising material for high-speed electron devices and also it could be suitable for optoelectric devices [1]. InN normally crystallized in the wurtzite (hexagonal) structure. The zincbelnde (cubic) form has been reported to occur in films containing both polytypes [2]. Compared wurtzite (WZ) InN much less is known on the properties of the zincblende (ZB) phase of InN. However, ZB InN layers have been grown and electronic structure of this material has been calculated [3,4]. Unfortunately, so far result on the carrier transport in this InN phase have been reported. This lack has motivated us to recalculate the band structure of ZB InN to perform low- and high-field transport simulation using the ensemble MC method [5,6]. The purpose of the present paper is to calculate electron drift velocity for various temperature and ionized-impurity concentrations. The formation itself applies only to central Γ valley conduction band and the two nearest valleys. The calculated band structure has been approximated by a nonparabolic three-valley model with the conduction band minima located at Γ, U and K points at wurtzite structure and Γ, X and L points at zincblende structure in the Brillouin zone. The valley have been approximated by

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(\varepsilon) = \varepsilon(1 + \alpha\varepsilon)$$

Where \hbar is the reduced plank constant, k is the wave vector, and ε is the electron energy relative to the bottom of the valleys [7].

II. SIMULATION METHOD

The ensemble Monte Carlo techniques have been used for well over 30 years as a numerical method to simulate nonequilibrium transport in semiconductor materials and devices and has been the subject of numerous books and reviews [8]. In order to calculate the electron drift velocity for large electric field, consideration of conduction band satellite valleys is necessary. A three-valley model for the conduction band is employed. we assume that all donors are ionized and that the free-electron concentration is equal to the dopant concentration. For each simulation, the motion of ten thousand electron particles are examined, the temperature being set to 300K, and the doping concentration being set to 10^{23} cm^{-3} . Electrons in bulk material in bulk material suffer intervalley scattering by polar optical, nonpolar optical and acoustic phonons scattering, intervalley phonons, and ionized impurity scattering. Electron transport is studied using the single Monte Carlo method.

The band structure and material parameters necessary for calculation the scattering probabilities used in present Monte Carlo simulation are given in table 1 [2].

Parameter	Wurtzite InN	Zincblende InN
Band gap (eV)	1.89	1.94
Electron effective mass (m^*)	0.11	0.07
Nonparaplicity (eV^{-1})	0.419	0.245
Low-Frequency dielectric Constant	15.3	12.45
High-Frequency dielectric Constant	8.4	8.4
Density (kgm^{-3})	6810	6970
Sound velocity (ms^{-1})	6240	5200
Acoustic Deformation Potential (eV)	7.1	7.1
Polar optical phonon energy (eV)	0.089	0.089

Table 1: Important parameters used in our calculations for WZ and ZB InN [2]

III. RESULTS AND DISCUSSION

Figure 1 show the electron drift velocity in both ZB and WZ InN calculated as a function of the applied electric field with and without dislocations for a crystal temperature of 300 K, assuming free electron and ionized impurity concentration of 10^{23} cm^{-3} . The difference in the calculated drift velocities between the two crystal phases is obvious.

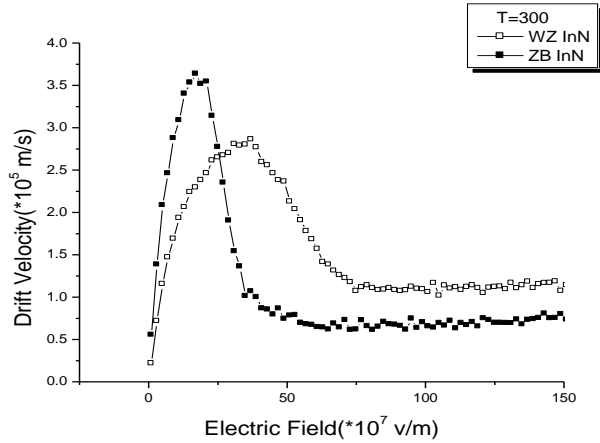
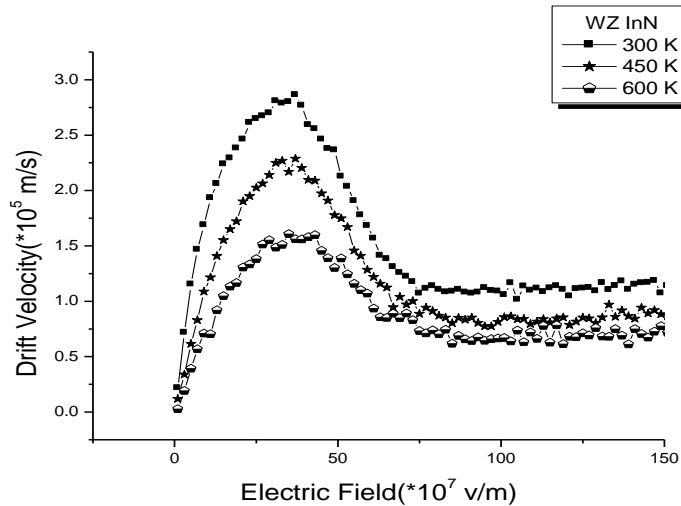


Figure 1. Electron drift velocity as a function of the applied electric field for ZB and WZ InN at 300 K.

In the case of ZB InN, the velocity increases with increasing electric field more rapidly owing to the lower effective mass in the central valley, the velocity increase in the case of WZ InN is relatively slower. Similar to the experimental result it is found that at a field of $3.33 \times 10^7 \text{ vm}^{-1}$ the pick velocity for WZ InN is about 80% lower in ZB InN ($2.8 \times 10^5 \text{ ms}^{-1}$ versus $3.6 \times 10^5 \text{ ms}^{-1}$).

Any further increase of electric field strength results in reduced drift velocity for both materials and a region of negative differential resistance are observed. It is due to the transfer of electrons from the central valley, where they have a larger effective mass, to the other valley, where they have a larger effective mass.



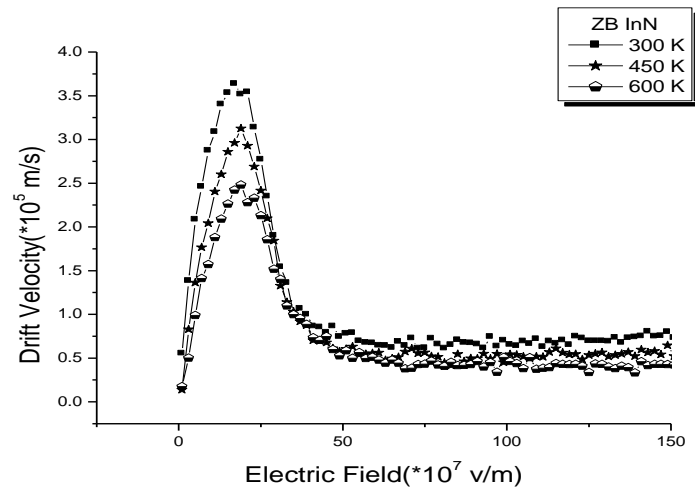
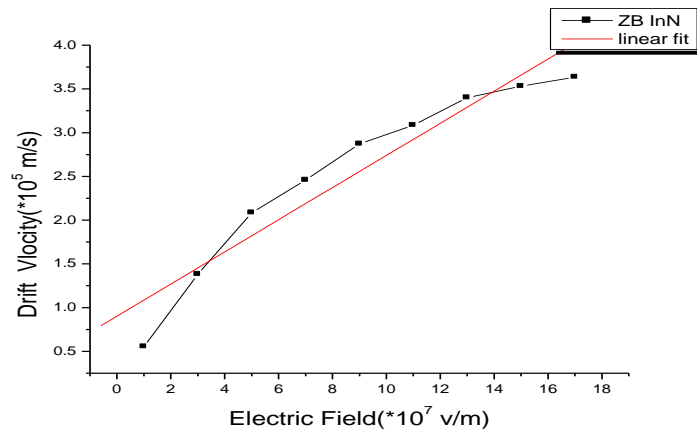


Figure 2. Calculated electron drift velocity as a function of electron field strength for temperature of 300, 450 and 600 K.

Figure 2 shows the calculated electron steady state drift velocity in bulk ZB and WZ InN as a function of applied electric field at various lattice temperature. The peak drift velocity decreases while the threshold field increases by same percent as the lattice temperature increase from 300 K to 600 K.

Next, we compare the mobility of two InN phases at low-field electrons. The low-field mobility has been calculated by the simple relation $\mu_0 = V_{drift} / E$ taken in the linear region of the simulated $V_{drift}(E)$ curves, where V_d is the electron drift velocity. In figure 3 the calculated low-field mobility μ for ZB and WZ InN is presented. Satellite valleys do not affect the low-field mobility calculation since no intervalley transfer occurs at low electric field in consequence, the low-field mobility is attributed solely to transport of Γ valley electrons.



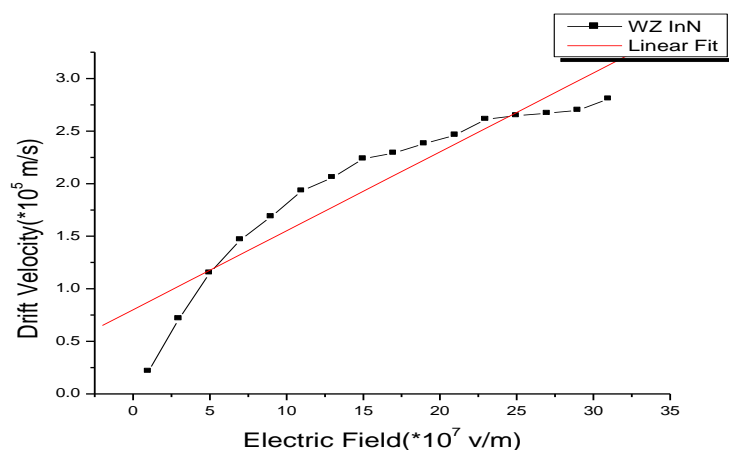


Figure 3. Mobility of two InN phases at low-field electrons.

The electron mobility at low electric field is about $0.183 \text{ m}^2/\text{Vs}$ for ZB InN compared to $0.075 \text{ m}^2/\text{Vs}$ for WZ InN.

IV. CONCLUSION(S)

Zinblende InN have higher electron pick drift velocity than wurtzite InN, because of its smaller effective mass. In both zinblende and wurtzite InN the electron pick drift velocity decrease while the lattice temperature increase from 300 K to 600 K. InN have higher mobility in zinblende structure than wurtzite structure, because its effective mass is small in ZB compared with WZ.

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