IMPACT OF VARIOUS DEFECTS ON CARRIER MOBILITY IN ZnO THIN FILMS

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Abstract

In the present work, the impact of ionized impurity and dislocations defect over the carrier field mobility of ZnO thin films is discussed in details at the atomistic scale. The line dislocation and ionized impurities are included through scattering mechanisms. The TNL-EM^{TM} (electron mobility) simulator is used to track carrier transportation with various nonlinear scatterings over the three valleys on full band structure. The inbuilt solution of the Boltzmann transport equation (BTE) through Monte Carlo (MC) technique provides accurate prediction about the carrier transportation. The variation in carrier-occupancy densities at Γ-, U-valley, Γ_3- valleys conclude the causes of mobility degradation in the thin film sample. The negative differential mobility feature is also explained on the basis of carrier transitions in different valleys. The outcomes of simulation studies are given in terms of electron drift velocity under uniform electric field. The highest velocity of = 3908 m/s is found at an electric field at ~1 kV/m for the sample with an electron density of 1.4×10^{22} m^{-3}.

Numerical Technique

The carrier transportation on three valleys is described by solution of Boltzmann transport equation (BTE) coupled with various nonlinear scatterings through Monte Carlo (MC) technique inbuilt in TNL-EM^{TM} (electron mobility) simulator [1-2]. Under non-equilibrium conditions, the rate change of distribution function occurs due to external applied forces. The carrier transport process is initiated by assuming that all the carriers are at the equilibrium, the first free fight duration is chosen with a probability distribution determined by the scattering probabilities under the influence of external force. The electron–lattice, electron–electron and electron–defect coupling strengths are important physical quantities which dictate the interactions of the electron with lattice, with themselves and with extrinsic defects. These interactions are responsible for relaxing momentum and energy of the electrons, and are explained in terms of various scattering probabilities in the simulation algorithms. Scattering rates are strongly dependent on the electronic band structure [3]. Density of states in a particular valley at particular time plays important role in deciding the probability of scattering events which follow the energy

conservation principle (Fermi Golden rule). All physical quantities of interest, e.g. velocity, energy etc associated with each and every electron are mapped during the free fight of carriers. The free fight of carriers is interrupted by any one of the scattering processes and scattered electron goes into new k state which is randomly chosen as initial state for next free fight under repeated iterative scheme. The accuracy of simulated results depends on the precision in time scale for iteration [1-3].

Table 1: Material Parameters used in Monte Carlo simulation.

M - mass density v_s- Sound velocity, D_a -acoustic deformation potential, ε_s–static dielectric constant, ε_∞ - High Frequency dielectric constant, m_Γ - Effective mass at Γ valley, m_U- Effective mass at U, valley, $m_{\Gamma 3}$- Effective mass at Γ_3 valley, $U-\Gamma, \Gamma_3-\Gamma$ are valley separation, $\hbar\omega_{LO}$-Optical Phonon energies, $\hbar\omega_{ij}$-Intervalley Phonon Energies, D_{ij}-Intervalley Deformation Potentials, α- nonParabolicity factor

M (kg/m^3)	5534	**$\Gamma_3-\Gamma$(eV)**	0.7662	**Dislocation Density**		10^{20}	**α (eV^{-1})**	**Γ**	1.0281
v_s (m/s)	5368.4	**$U-\Gamma$ (eV)**	0.5232	**D_a (eV)**	**Γ**	6.3687		**U**	0.5212
ε_s	14.09	**$\hbar\omega_{LO}$ (meV)**	0.0325		**U**	7.398		**Γ3**	0.618
ε_∞	11.65	**D_{ij} (eV m^{-1})**	10^{10}		**Γ3**	7.304			
m_Γ	0.0418	**$\hbar\omega_{ij}$ (meV)**	0.02234	**eqiv. valleys**	**Γ**	1			
m_U	0.2236	**Doping (m^{-3})**	10^{22}		**U**	4			
m_{Γ_3}	0.6118	**Ionized Imp.**	10^{22}		**Γ3**	3			

Results & Discussion

This section concentrates on the results obtained regarding specific aspects of defects over the carrier field mobility. The results reported here provide valuable deeper insight. The whole simulation work is performed over the TNL-EM^{TM} simulator. The impact of various defects is observed in terms of scattering mechanisms during nonlinear carrier transport. The intrinsic fundamental scattering mechanisms (acoustic, intervalley and Coulomb) along with extrinsic scattering mechanisms (alloy disorder, ionized impurity and dislocation) are considered in present studied.

The variations of carrier-occupancy densities without and with extrinsic defect scatterings at Γ-, U-, Γ3- valleys are depicted in Fig. 1a, and 1b. It elaborates the carrier transition process with the ramping field. All the results are self explanatory. Initially total 20000 electrons were allocated at Γ-valley only, whereas no electrons were present at higher levels i.e. U-, and Γ_3- valleys under steady state conditions. The Boltzmann carrier population shown at the Γ-, U-, and Γ_3- valleys provides the exact information regarding the number of carriers contributing in the current conduction process at particular field strength. However, as the field strength increase from zero the electrons prompt to excite to higher energy U- or Γ_3- valleys and remain trapped there as

their effective masses are high in these valleys. The red curve depicts the Γ-valley (lowest energy valley) electron density which decreases with increase in field strength. The max electrons transfer to middle energy valley i.e. U-valley whereas few electrons transfer to Γ_3-valley i.e. height energy valley. Further increase in field strength prompts transfer electrons from U-valley to Γ_3-valley around 60kV/m. At 100kV/m field strength, only 1060 electrons out of 20000 electrons remain available for current conduction in the sample. The impact ionization process is ignored in current analysis, which is capable to accurately predict about the threshold voltage of the sample and breakdown event in the sample.

Fig. 2 shows the variation of carrier drift velocities when separate scattering mechanism is invoke to check the impact of various scattering mechanisms on the carrier drift velocities. It is clearly reflected from the curve that the drift velocity values are increases with the increase in electric field strength. Only intervalley scattering shows different characteristics, it increase upto 1 kV/m, then decrease afterward. It simply shows that more and more electrons are excited to higher valleys and velocity decreases. The analysis predicts more deep insight to predict microscopic electronic transportation behavior. Fig. 3 shows the overall carrier population density when all the scatterings taken simultaneously. It is clearly reflected from that the intervalley carrier transitions play significant role in extraction of carrier drift velocity.

The carrier field mobility in ZnO thin film is depicted in Fig.4. The field mobility increase with ramping of field from 0 to 1 kV/m, afterward it start decreasing upto almost 35kV/m, then become saturated. It is clear that after reaching a maximum value it donot increase with further increase in field values i.e. negative differential mobility effect which is simply dictated by intervalley carrier transition process. In present work impact ionization process is neglected which is responsible to increase the carrier densities i.e. the carrier mobility will be increase but as seen from Fig. 2, carrier-carrier Coulomb scattering will also increase with increase number of carriers due to impact ionization. Hence, the nature of mobility will remain same.

Conclusions

The maximum influence of ionized impurity and dislocation defect scatterings on ZnO thinfilm are observed during electrons transport under applied electric field and are found to be responsible for mobility reduction. The nonlinear mobility behavior is noticed for ZnO. The mobility results obtained in present work indicate that electron mobility can be increased by reducing the dominant scattering mechanisms. The impact of defects on mobility is dictating the

reduction of field mobility in 2-100 kV/m field strength. The electrons mobility data for other doping densities, considered also exhibit nonlinear behavior. The electron mobility simulated results of ZnO thin film have been compared with experimental results under appropriate conditions and good agreement has been found between them.

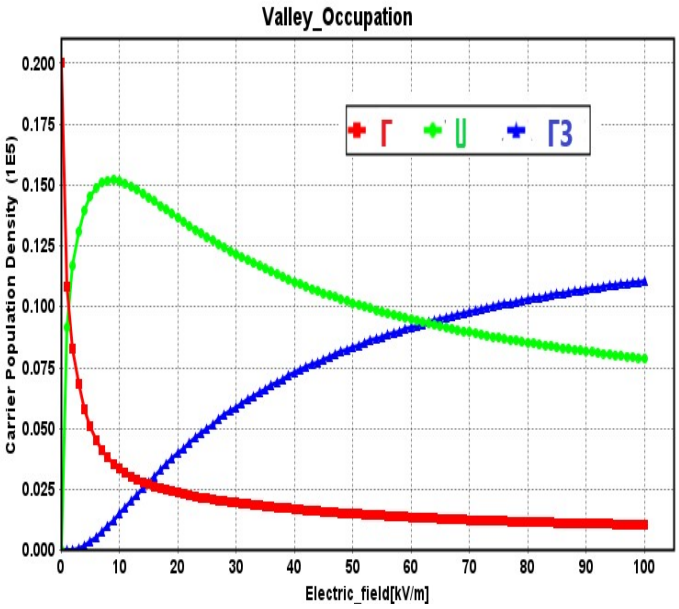

Fig. 1: Carrier Population Density

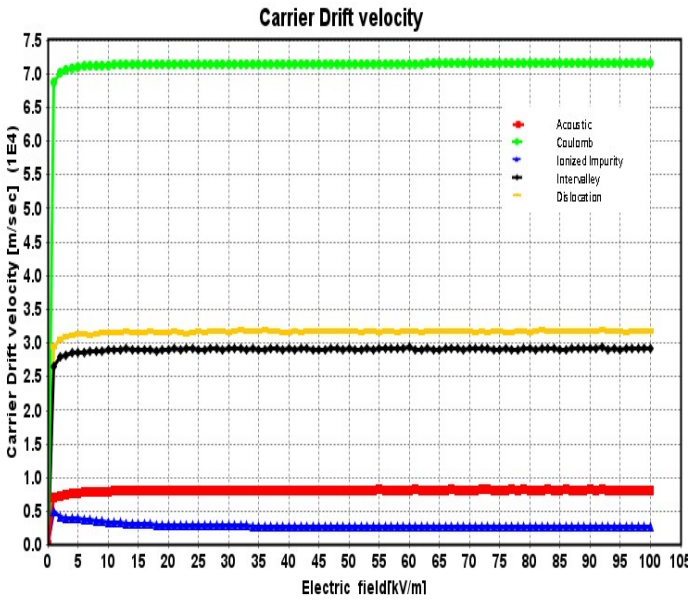

Fig.2: Carrier Drift velocities

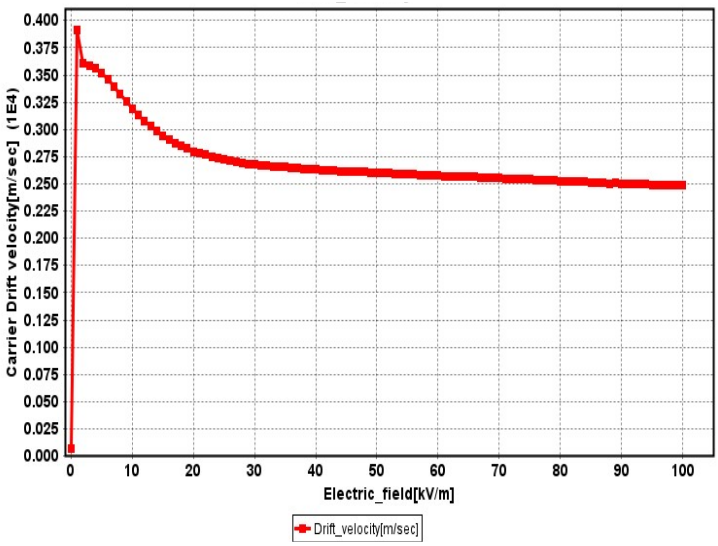

Fig.3 Drift velocity under all scattering mechanisms

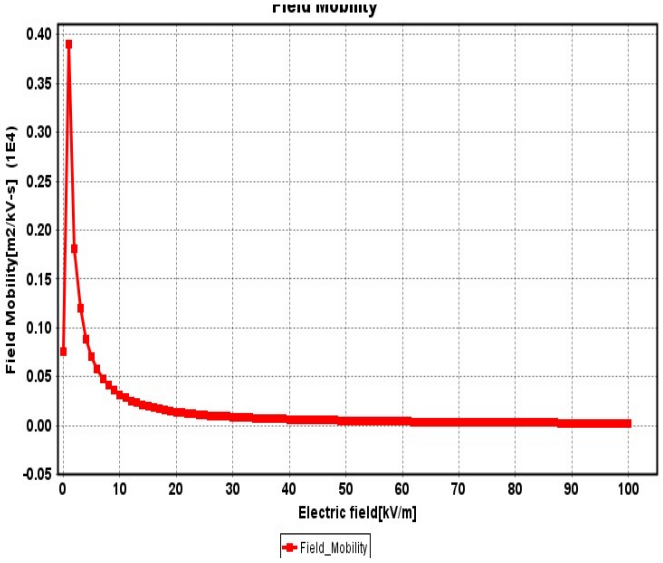

Fig.4 Carrier Field Mobility

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