Figure 2 A similar plot for MgO (right three layers) grown on an Ag substrate (left three layers). An F^+ defect is present at the surface of the MgO film, denoted by a green square. Surface models show significantly greater movement of charge. In this case, there is a clear accumulation of positive charge on the surfaces of the interface model.

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P:15 Monte Carlo simulations of electron transport in bulk GaN

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Gallium Nitride (GaN) based transistors have become increasingly attractive for radio frequency (RF) and power applications due to their excellent material properties [1]. This has led to benefits in circuit performance and a reduction in both the size and the cost of RF and power electronic circuits. Although the desire for GaN based transistors, for example, the High Electron Mobility Transistors (HEMTs) has increased over the years, some reliability issues such as current collapse and the DC/RF dispersion persist. A physical understanding of the cause for these issues is difficult to obtain through experimental observations only. Consequently, the need for a physical based modelling is urgently needed. Physically based simulations are usually differentiated by their levels of accuracy and computational cost even other criteria might also play a role.

In this work, we have used the Monte Carlo (MC) transport model to study the effects of material parameters (which are not well known in the GaN) on electron transport in a bulk GaN. Additionally, we have studied the effects of impurity scattering on electron mobility. By assuming that the transport properties in the bulk GaN at high electron concentrations are similar to that of the two-dimensional electron gas (2DEG) [2], we expect that the data we obtain can easily be used to accurately predict the DC and RF performance of GaN based HEMTs.

The band structure of GaB we have considered comprises of a four-valley model of the conduction band namely the Γ_1, U, Γ_3 and K valleys as shown in Fig. 1. In the models, we have assumed a anisotropic non-parabolic approximation of the band structure. In general, we thus consider GaN in wurtzite phase using parameters reported in Ref. [3] with the addition of the K valley. Fig. 2 compares the variation of drift velocity with the applied electric field. Our result are in a good agreement with experimental data [4] and other MC simulations [4, 5]. Furthermore, we have varied the dislocation density in order to study the effect of a dislocation scattering on the electron drift velocity. We report in Fig. 2 that increasing the dislocation density by an order of magnitude reduces the saturation velocity by half although the peak drift velocity appears to be unaffected. Fig. 3 shows the gradual reduction in mobility, from a steady mobility of approximately 600 $cm^2V^{-1}s^{-1}$ to almost zero when the ionised impurity concentration exceeds 10^{17} cm^{-3}. The mobility is observed to be approximately constant when the neutral impurity concentration is varied, fluctuating about an average value approximately of 620 $cm^2V^{-1}s^{-1}$ (see Fig. 4) which agrees quite well with experimental measurements [2].

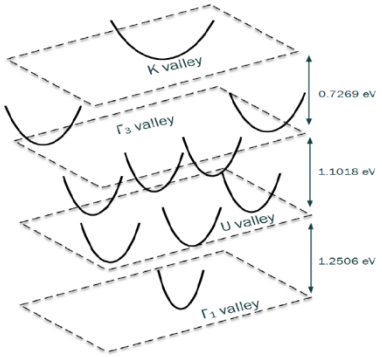

Figure 1: Band structure of Gallium Nitride indicating the four valleys that have been considered in our simulations.

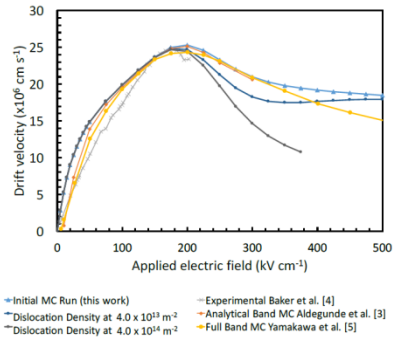

Figure 2: Electron drift velocity as a function of applied electric field in bulk GaN where the dislocation density has been increased by an order of magnitude comparing data from an ensemble Monte Carlo simulations to both experimental data [4] and other Monte Carlo simulations [3, 5].

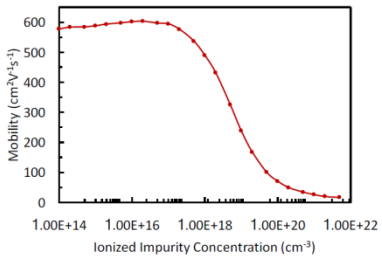

Figure 3: Electron mobility as a function of ionized impurity concentration in bulk GaN obtained from our ensemble Monte Carlo simulations.

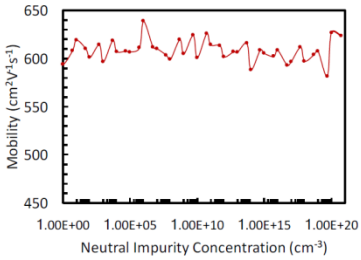

Figure 4: Electron mobility as a function of neutral impurity concentration obtained from our ensemble Monte Carlo simulations showing variations of the runs since the neutral impurity scattering has negligible effect on the mobility.

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