P:14 Charge corrections from exact electrostatics for metal-oxide interfaces

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Density functional theory (DFT) is a workhorse of electronic structure theory. When simulating charged defects, the use of periodic boundary conditions (PBC) ensures an accurate description of the host crystal's bandstructure, but negatively introduces fictitious interactions with image charges in neighbouring cells [1]. These interactions are large when the defect is in a high charge state, or when some dimensions of the simulation cell are small. This last case is especially severe when expensive hybrid functionals are utilised to study multiple interfaces. Several methods to correct for this interaction exist in the literature for the bulk case and are widely used to study charged defects [2-5]. Equivalent methods for surfaces and interfaces with varying dielectric profile are now starting to be developed [6].

We have been developing a new method that can be applied to this problem, by extending previous work based on charged molecular fragments in vacuum [7] to crystals Using the newly released electrostatics solver DL_MG, we have extended this method to interfaces and defect clusters. We have validated our electrostatic method for bulk problems, where it is important to well describe the internal response of the defect containing supercell. This behaviour is shown in Figure 1. We found a strong correspondence with the Lany-Zunger method for bulk crystals [4].

Now we have been applying the method to more complex interface systems, such as islands of MgO grown on a Ag substrate. This is shown in Figure 2. Such systems show very different behaviour, due to the metal substrate. When electrons or holes are transferred from the defect to the metal substrate, they occupy delocalised states and can lead to surface dipoles. The physics of this process is explored.

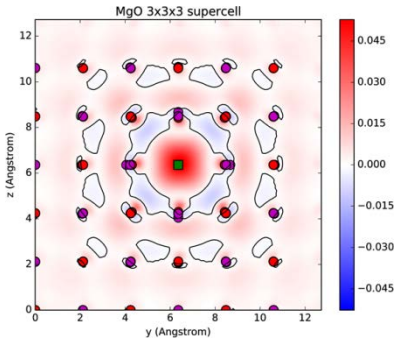

Figure 1 Internal polarisation response of a bulk supercell of MgO containing an F^{2+} centre, denoted by the green square. The clear bands of positive and negative polarisation show the ionic response of the host crystal to the charge of the defect complex, and act to reduce the defects interaction with it's own periodic images.

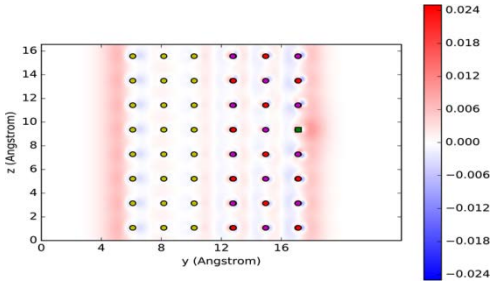

Figure 2 A similar plot for MgO (right three layers) grown on an Ag substrate (left three layers). An F^+ defect is present at the surface of the MgO film, denoted by a green square. Surface models show significantly greater movement of charge. In this case, there is a clear accumulation of positive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