Atomistic modelling of dislocation cores in wurtzite GaN

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The atomic core structure of both prismatic and basal dislocations were modelled, in wurtzite GaN, by using different methods: elasticity theory (isotropic, anisotropic), empirical potentials (Modified Stillinger-Weber potential), ab-initio tight-binding (SCC-DFTB) and full ab-initio based DFT (Aimpro). While the elasticity theory and the empirical potentials were employed to investigate the long-range elastic effects introduced by the dislocations, the tight-binding and ab-initio methods were used to obtain realistic models of core structure and to investigate their eventual induced gap states.

In the case of prismatic dislocations, we have performed the first atomistic simulation of the $(\vec{a}+\vec{c})-$mixed dislocation core. For this dislocation two core configurations were found to be stable, one with a 5/7-atoms ring and the other with a complex double 5/6-atoms ring structure. While the core with a 5/7-atoms ring structure contains neither dangling nor wrong bonds, that with the complex double 5/6-atoms ring structure contain two rows of dangling bonds. Energetic calculations based on the Modified Stillinger-Weber potential and the SCC-DFTB methods suggest that the core with a 5/7-atoms ring structure is more energetically favourable.

In the basal plane, both perfect and partial dislocations have been investigated. The perfect $\vec{c}-$edge dislocation, which results from a 90° bending of a $\vec{c}-$screw threading dislocation during the ELO (Epitaxial Lateral Overgrowth), was found to present a multiplicity in core structure. The shuffle configuration with a 5/8/5-atoms ring structure and involving wrong bonds was found to be the most energetically favourable. All the core configurations were found to introduce empty states in the top half of the bandgap. In the ELO technique, close to the mask, the GaN layer is usually contaminated by Oxygen and Silicon atoms, we expect that the core of the $\vec{c}-$edge dislocation to be negatively charged.

Recent HRTEM (High Resolution Transmission Electron Microscopy) observations of GaN samples grown in the non-polar direction revealed the presence of Shockley partial dislocations. We performed an atomistic simulation of the 30° partial dislocation core. Our calculations show that glide configurations are energetically favoured over the shuffle ones. Moreover, in the glide set, configurations with double period reconstruction are lower in energy than those without reconstruction.