Influence of native point defects on the stability of GaN tilt grain boundary using a Self-Consistent Charge Density Functional Tight-Binding (SCC-DFTB) approach

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Abstract

The evolution of the development of the III-V nitride semiconductors has been remarkable and industrial devices, light emitting diodes in the blue region and laser diodes, were commercialised. Dislocations are the main extended defects in the layers of gallium nitride and related compounds heteroepitaxially grown on various substrates. They may interfere in the electronic properties of the semiconductor and change the optical properties of the devices by the introduction of levels in the band gap. Another origin for these levels could be impurities or their segregation at the grain boundary. In order to explore the extended defects that are responsible of these levels, several atomistic models may be considered. However, confusion can result from comparisons of theoretical modelling studies which do not include impurities or native point defects effects with experimental studies on grain boundary which naturally contain these defects. Then, grain boundary energy differences among various structures may be minimized by impurities or native point defects.

This work presents the investigation of relative stability and electronic properties of native point defects in a wurtzite GaN tilt grain boundary. Molecular static atomistic simulations using a Self-Consistent Charge Density Functional Tight-Binding approach was applied for this study. We found that the structure of the $\Sigma=19$ tilt boundary characterized by a mixture of 6- and 8-atom rings in interaction with Ga or N interstitial transform to a structure formed by a mixture of 6-atom ring and by a new 5/7-atom ring involving dangling bonds. The calculations showed that the Ga interstitial interface is more stable structure energetically than the perfect and vacancy interfaces.