CRYSTAL POLARITY DISCRIMINATION IN GaN NANOWIRES ON GRAPHENE

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In this work we report an *ab-initio* study of the preferred polarity for wurtzite GaN nanostructures on virtual graphene substrates. By means of the density functional theory analysis we show that N-polar nanostructures on graphene are energetically favorable in comparison to Ga-polar. These finding are in agreement with experimentally observed N-polarity of wurtzite GaN nanowires grown on graphene substrate. We believe that the revealed polarity preference is of importance for piezoelectric and optoelectronic device design.

The density functional theory (DFT) calculations were used to determine the most energetically preferable geometry of the GaN nanocluster on graphene. Such a clusters can represent the nucleus of GaN nanoisland or nanowire. To reproduce the hexagonal symmetry of the wurtzite structure at least ten gallium and ten nitrogen atoms should be considered. In addition sixty more carbon atoms form the monolayer graphene lattice.

This model system system allows eight possible geometric configurations of GaN nanocluster: four Ga-polar and four N-polar. DFT calculations were made in the plane-wave basis set for projector augmented-wave method implemented in GPAW package [1]. The calculations was carried out using the Perdew–Burke–Ernzerhof generalized gradient approximation for exchange-correlation functional, with the plane wave energy cutoff set to 450 eV and *k*-space sampling in 4×4×4 Monkhrost-Pack grid.

We observe that only two out of eight configurations are found to be stable during the energy optimization. The initially Ga-polar cluster changed the Ga-N dipole orientation during the optimization procedure. Meanwhile, the initially N-polar nanocluster only adjusted its shape while keeping the initial arrangement of the atomic planes and the Ga-N dipole orientation. Thus, both stable configurations evolve to N-polar geometry corresponding to minimal cluster energy.

To summarize, the presented DFT study have shown that N-polar GaN structures on graphene substrates are energetically preferable to Ga-polar ones. Among different possible configurations of Ga and N atoms in the cluster only the N-polar one is stable while the initially Ga-polar structure demonstrates the change of polarity during the *ab-initio* optimization. The DFT modeling results are consistent with the experimental observations of exclusive N-polarity of GaN nanowires grown on graphene layer on top of silicon substrate [2, 3].

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References

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