Abstract

GaN has a direct band gap of $\approx$ 3.4 eV and is therefore a suitable material for the production of blue and green light emitting diodes and lasers. GaN crystallises usually in the hexagonal (wurtzite) form. However, the production of high–quality material is difficult since the lack of suitable substrates causes a high density of extended defects and rough surfaces. So far, little is known about these defects and surfaces and their influence concerning the optical properties of the material. In this work we use local-density-functional methods to investigate the structures and electrical properties as well as the formation energies of surfaces and extended defects in hexagonal GaN. In particular, we explore pure dislocations and surfaces and the behaviour of oxygen at these structures.