Computational study of Mn-doped GaN polar and non-polar surfaces

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Abstract

First-principles calculations were carried out in order to study the magnetic, electronic and structural properties of the Mn-doped polar GaN(0 0 0 1) and non-polar GaN(101¯0) and GaN(112¯0) surfaces, with the aim of refining the growth of thin films of this material. The results indicate that the surfaces present magnetization of approximately 4.0 μβ/Mn atom, in agreement with the recently reported theoretical and experimental results. Calculations of surface formation energy indicate that Mn atoms are incorporated into top surface layers (first and second) of GaN, being the MnGa incorporation in the polar surface more energetically favourable than in the nonpolar surfaces. In addition, it was observed that the magnetic coupling between the Mn impurities depends on the surface orientation, which could be useful for the design of magnetic nanodevices.

Keywords

First-principles, GaN surfaces, Magnetic materials, Mn-doped GaN, Surface magnetism