Structural, electronic and magnetic properties of Ti-doped polar and nonpolar GaN surfaces

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Abstract

Based on density functional theory, first-principles calculations were performed in order to study the titanium incorporation on polar and nonpolar GaN surfaces. The formation energy calculations indicate that Ti impurity atoms prefer to incorporate in surface layers (first and second) of GaN. It is also concluded that the incorporation of Ti atoms in Ga-substitutional sites are more energetically favorable compared with N-substitutional or interstitial sites on the polar and nonpolar GaN surfaces. For Ti-rich growth conditions, formation energy calculations show the formation of Ti_xN layers on the a and c GaN surfaces, which corroborates recent experimental observations. Results also display that the 3d-Ti states are the responsible for the metallization of the surface on the c and m planes, forming an intermetallic alloy (Ti_xN), which could be used as low-resistance ohmic contacts for GaN. In addition, the magnetic properties with Ti doping show magnetization of about 1.0 μ_B/Ti atom for the nonpolar GaN surfaces.

Keywords

Magnetic materials, Nitrides, Ohmic contacts, Semiconducting III-V materials.