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Formation of two-dimensional SiN_x layers on GaN nonpolar surfaces

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Abstract

Density functional theory calculations were performed to study the adsorption and incorporation of silicon atoms over GaN $(11\overline{2}0)$ and GaN$(10\overline{1}0)$ aiming to gain insight into epitaxial growth of two-dimensional layers of silicon nitride (SiN_x) on the GaN nonpolar surfaces. Results show that the adsorption of silicon atoms on the bridge sites is energetically more favored as compared with other possible adsorption sites. Formation energy calculations indicate that the silicon impurity atoms prefer to incorporate in second or deeper GaN surface layers. However, it is concluded that the incorporation of Si atoms in the Ga-substitutional site is energetically more favorable compared with the N-substitution and Si-adsorption on the top layers. At full coverage, calculations show the formation of two-dimensional SiN_x layers on the GaN nonpolar surfaces over the entire range of Ga chemical potentials, in agreement with experimental observations. In addition, the electronic structure of the GaN nonpolar surfaces with Si doping were analyzed and compared with those of undoped surfaces.

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