Interface Formation of Scandium Nitride on GaN(0001) Surface: A First-Principle Study

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Self-consistent periodic density functional theory calculations are used to investigate the role of scandium (Sc) impurity atoms during GaN growth. Adsorption and diffusion of Sc on GaN(0001)-2×2 surface is examined and it is shown that Sc atoms preferentially adsorb at the T_4 sites at low and high coverages (from 1/4 up to 1 monolayer). It is also found that N atom is relatively immobile compared to Ga as well as Sc atoms on the GaN(0001) surface. In addition, calculating the relative surface energy of several configurations and various Sc concentrations, we constructed a phase diagram showing the energetically most stable surfaces as a function of the Ga chemical potential. Based on these results, we found that incorporation of Sc adatoms in the Ga-substitutional site is energetically more favorable compared with the adsorption on the top layers. This effect leads to the formation of an interfacial crystalline ScN layer on the GaN(0001) surface, which can offer a good interfacial combination between Sc and GaN substrate. Our calculations show that the scandium incorporation is most favorable under a nitrogen environment, in agreement with experimental results [1].

This work is funded by the Division de Investigación, Desarrollo e Innovación, Universidad del Norte, Barranquilla, Colombia.

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