Structural phase transition in Mn-doped Gallium Nitride explored by first principles calculations

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Manganese atoms deposited onto the N-polar face of wurtzite gallium nitride [GaN $(000\bar{1})$] results in two unique surface reconstructions, depending on the deposition temperature. At low temperature, a metastable 3×3 structure forms, which upon mild annealing converts to a more stable $\sqrt{3}\times\sqrt{3}-R30^{\circ}$ structure through an irreversible phase transition. Using ab initio techniques, we study the energetics of this system proposing models in consonance with the experimental findings. Our results are compared with Scanning tunneling microscopy (STM) images along with reflection high energy electron diffraction data. We find that the lowest energy model for the 3×3 structure consists of trimers of Mn atoms bonded to the Ga adlayer but not with N atoms, while the most stable energy model for the $\sqrt{3}\times\sqrt{3}-R30^{\circ}$ structure involves Mn atoms substituting for Ga within the Ga adlayer and thus bonding with N atoms. Tersoff-Hammann simulations of the resulting lowest-energy structural models are found to be in excellent agreement with the experimental STM images.