Scanning Tunneling Microscopy and First-Principles Theoretical Study of Manganese-induced Stripe Phase Superstructures on GaN(0001)

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The formation of magnetic nanostructures on semiconductor surfaces is a topic of considerable fundamental as well as technological interest. Gallium nitride is a next-generation semiconductor material with a bright future in optoelectronics; yet this material will also be of great interest for spintronics if it is possible to combine spin functionality with its amazing electronic properties. For this reason, we have explored the epitaxial growth of Mn on the pseudo-1x1 surface of gallium polar GaN(0001). At the appropriate deposition temperature near 250 °C, we find that Mn incorporates into the surface at sub-monolayer coverages first in narrow stripe phases having a Mn zig-zag $4\times\sqrt{3}$ structure oriented along $[10\bar{1}0]$ surrounded by a sea of pseudo-1x1; while at higher coverage (but still less than 1 ML), the surface shows wider Mn stripe phases having $\sqrt{3}\times\sqrt{3}$ - R30° type structure. We explore both the narrow and wide stripe superstructures using a combination of scanning tunneling microscopy and first principles theory. Various models are considered for the wide stripe phases having $\sqrt{3}\times\sqrt{3}$ - R30° structure, including both adatom and substitutional models. Surprisingly, first principles theory using LDA/GGA + U finds that the lowest energy structural model is instead a rotated, in-plane structure. Such a novel structure has not previously been reported for Mn/GaN. The calculated spin-polarized local density of states is best fit to the experimental data using U = 6 eV, resulting in a dip and strong spin polarization near the Fermi level. Theory also finds a similar in-plane type model for the narrow $4\times\sqrt{3}$ stripe structure; results are compared with the STM data, and in this case an antiferromagnetic ground state is calculated, consistent with STM images showing an asymmetry between the two Mn atoms of the Mn zig-zag chain.