

Surface investigation of hexagonal non-collinear D0₁₉-Mn₃Ga thin film on GaN(0001) substrate

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In recent years, Mn₃Ga has garnered significant attention due to its exotic physical properties and potential applications in spintronic devices [1,2]. One of the most intriguing, yet less explored, phases is the hexagonal antiferromagnetic phase of Mn₃Ga (D0₁₉), which exhibits anomalous Hall effect and topological Hall effect in distinct temperature ranges [2]. In this presentation, we will delve into the growth and surface studies of a thin film of D0₁₉-Mn₃Ga on a Ga polar- GaN (0001) substrate.

The experiments are carried out in an ultra-high vacuum chamber equipped with a molecular beam epitaxy system and a room-temperature scanning tunneling microscope. Initially, the GaN epilayer is deposited on a GaN (0001) substrate at 700 °C under gallium-rich conditions, followed by the growth of D0₁₉-Mn₃Ga at 250 °C under manganese-rich conditions. Reflection high-energy electron diffraction is used during growth to monitor the sample, and the *in-plane* lattice constant is evaluated. Various *in-situ* techniques confirm that the grown sample exhibits epitaxial growth. Furthermore, scanning tunneling microscopy image shows the hexagonal atomic arrangements with an average *in-plane* atomic spacing of 5.37 ± 0.05 Å. However, the atomic spacing varies in the local region. The 1 x 1 surface structure of hexagonal D0₁₉-Mn₃Ga ($a = 5.40$ Å [2]) is shown in Fig. 1. Moreover, multiple flat terraces and steps with height of 2.20 Å are observed. The measured step height corresponds to the $c/2$ value of D0₁₉-Mn₃Ga ($c = 4.39$ Å [2]). The *ex-situ* X-ray diffraction clearly shows the Mn₃Ga 0002 peak, and the calculated *d*-spacing matched well with the step heights measured by scanning tunneling microscope. These measurements are consistent with the theoretically reported *c*-value of D0₁₉-Mn₃Ga. The concentration of manganese and gallium in the sample is confirmed to be 3.2:1.0 by Rutherford backscattering. Various *in-situ* and *ex-situ* measurements confirm the D0₁₉-Mn₃Ga growth. Further work is planned to investigate the non-collinear antiferromagnetism using spin polarized scanning tunneling microscope.

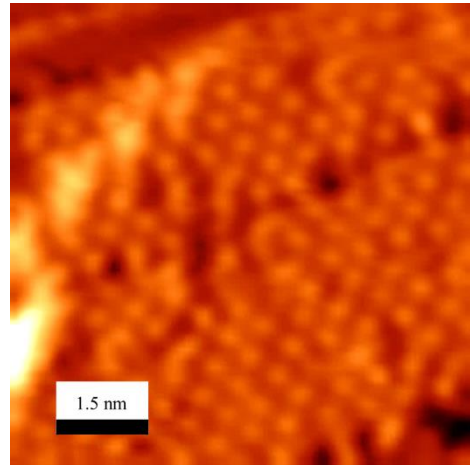


Figure 1: Atomic resolution STM image of D0₁₉-Mn₃Ga surface

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Supplementary information

The sample was grown using molecular beam epitaxy and monitored *in-situ* using reflection high energy electron diffraction (RHEED). The RHEED patterns of sample and substrate along both directions are shown in Fig. 1. The upper panel represents the GaN(0001) substrate just before the sample growth, while the lower panel represents the Mn₃Ga sample. The grown sample shows a 1 x 1 surface structure on directions. Based on the RHEED patterns, the *in-plane* lattice constant of sample is calculated, which agreed well with the model.

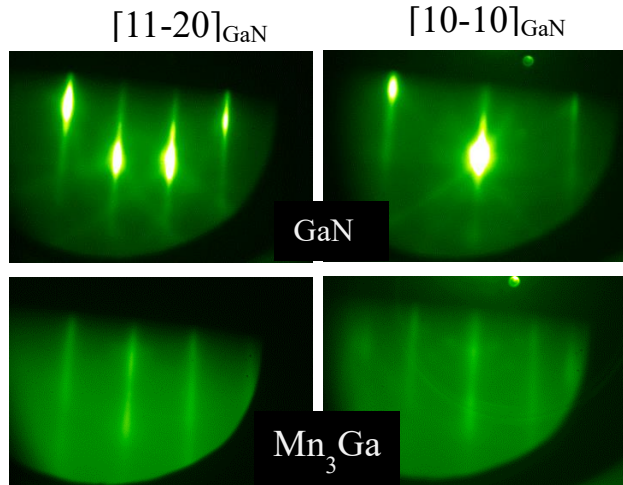


Figure 1: (a) RHEED pattern of GaN substrate (b) RHEED pattern of Mn₃Ga

The STM image in Fig. 2 displays the sample with multiple Mn₃Ga bilayers. The surface

appears atomically smooth, featuring multiple terraces and steps. The line profile along line AB gives the height of each step. From the line profile, we identified multiple steps each measuring 2.20 Å in height. The observed height corresponds to a single bilayer height of D0₁₉-Mn₃Ga, equivalent to the *c*/2 value. XRD measurements also exhibit a similar spacing. Both experimental findings align with the theoretical model.

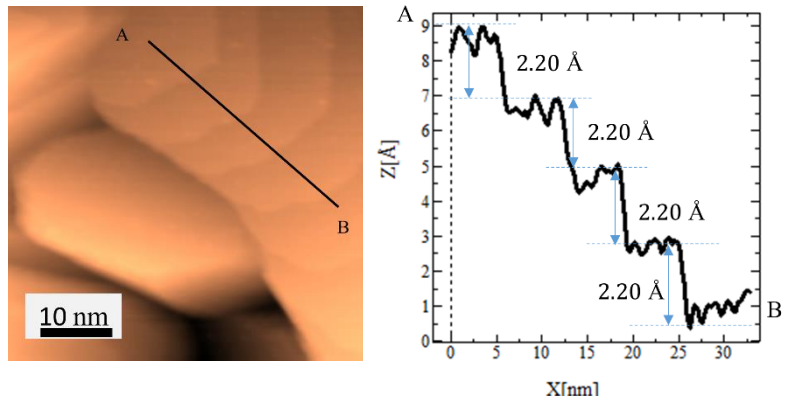


Figure 2: Multiple bi-layer stacking of Mn₃Ga surface.

The Atomic resolution STM image in Fig. 3 reveals mainly three distinct regions: a hexagonal region (HR), a rectangular region (LR), and a stripe region (SR). The HR region corresponds to the hexagonal D0₁₉-Mn₃Ga, exhibiting a 1 x 1 surface structure. The observed surface structure aligns well with the RHEED observation. The measured lattice spacing for this region is 5.37 ± 0.05 Å, consistent with the theoretically reported results. In the SR region, wide rows like structures are evident, as depicted in the figure. Meanwhile, the RR region shows the rectangular lattice with dimension of 6.65 ± 0.05 Å x 5.75 ± 0.05 Å. We are actively investigating the origin of such rectangular lattice within our D0₁₉-Mn₃Ga sample. Other interesting surface features will be discussed in the meeting.

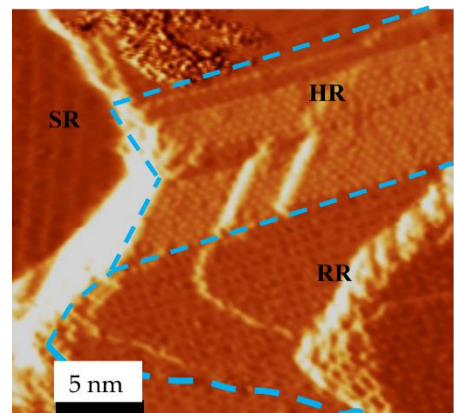


Figure 3: Atomic resolution STM image showing various surface features.