Kagome Antiferromagnetic Mn_3GaN grown on MgO(001) using Molecular Beam Epitaxy

A. Abbas,[1] A. Shreshtha[1], S. Upadhyay[1], T. Erickson[1], K. Sun[2], David C. Ingram[1], and A. R. Smith[1]

[1] Nanoscale and Quantum Phenomena Institute, Department of Physics and Astronomy, Ohio University, Athens, OH 45701

[2] Department of Materials Science and Engineering, The University of Michigan, Ann Arbor, Michigan 48109.

Antiperovskite materials are intermetallic compounds with perovskite crystal structure (space group Pm3m) but with anion and cation positions interchanged in the unit cell [1]. Similar to oxide-perovskite structure, antiperovskite materials have a variety of physical properties including antiferromagnetism, superconductivity and giant magnetoresistance [2]. There have been very few studies of antiperovskite structure Mn_3GaN in general although it was seen in molecular beam epitaxial growth as a second-phase precipitate when growing MnGaN [3]. Here we discuss the molecular beam epitaxial growth and surface study of Mn_3GaN. In our work, Mn_3GaN is deposited at 250 ± 10 °C onto magnesium oxide (001) substrates with a Mn: Ga: N flux ratio of 3:1:1. The sample surface is continuously monitored throughout the growth using reflection high energy electron diffraction. During the growth, the RHEED pattern was observed to be highly streaky, indicating an atomically smooth surface. The calculated *in-plane* lattice constant based on RHEED is 3.89 ± 0.06 Å. This value is close to the theoretical lattice constant *a* of Mn_3GaN (3.898 Å) [3]. X-ray diffraction confirms the majority 002 peak, and the value calculated is 3.84 ± 0.06 Å which also agrees well with the theoretical value (3.898 Å) [3] and with the experimental reported *c* value (3.881 Å) [2]. Since we did not observe significant second-phase peaks, the phase purity of the sample is quite high. Furthermore, cross-sectional STEM was done to understand the interface and the surface of the film. The plan is to also present *in-situ* scanning tunneling microscopy results for the surfaces of these MBE-grown Mn_3GaN layers.

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Supplementary Information

Figure 1(a)&(b) left and right panel shows the MgO RHEED patterns along [100] and [110] directions before growth. The half order streaks were initially non observable but later became visible as seen in Fig. 1(c). Streaky patterns show that the grown film is flat and epitaxial.

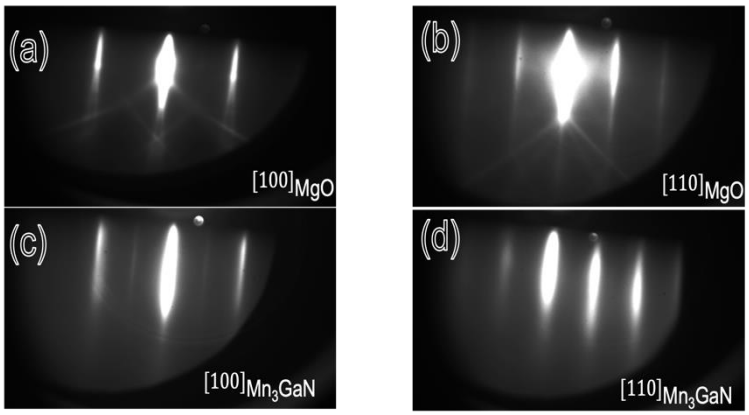

Figure 1. RHEED pattern evolution of Mn_3GaN growth. (a),(b) Representative images showing $[100]_{MgO}$ and $[110]_{MgO}$ azimuths before growth at 250 °C; (c), (d) after 25 minutes of growth showing strong 1st-order streaks and weak 2nd-order streaks along $[100]_{Mn_3GaN}$.

Figure 2 shows the lattice imaging of the Mn_3GaN film. Here we see a clear cubic lattice corresponding to *a*-plane and matching an *a*-plane model. HAADF stem image further confirms the epitaxially smooth and flat surface(bright colored layer).

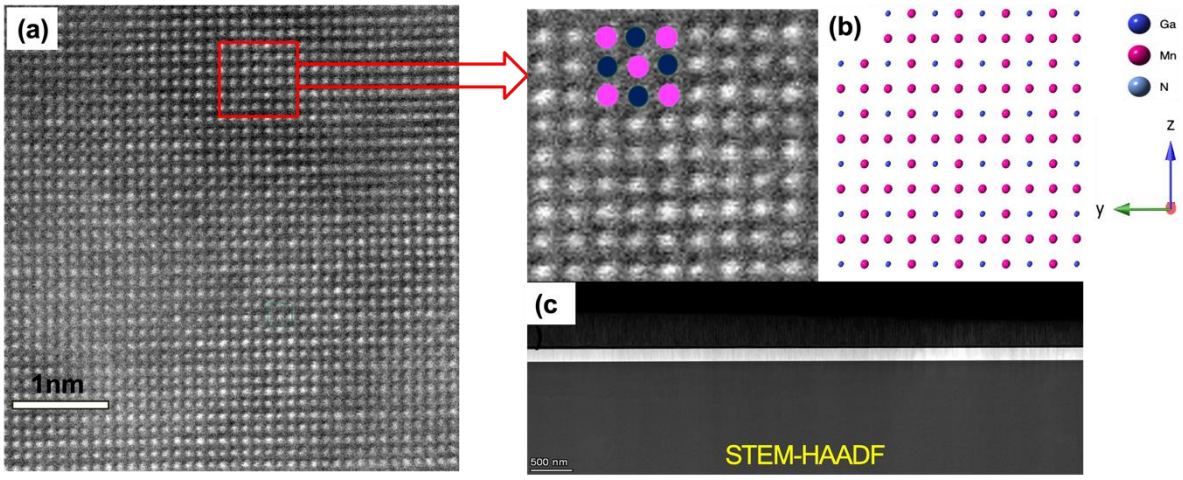

Figure 2. (a) HAADF image of Mn_3GaN Lattice confirming cubic structure. ;(b) STEM model corresponding to the lattice image matching with Mg (purple) and Ga (blue) atoms; (c) Low magnification HAADF-STEM image of the Mn_3GaN film on MgO (001)