

Substrate-strain-controlled molecular beam epitaxial growth and scanning tunneling microscopy of antiperovskite Mn_3GaN

**A. Abbas¹, J. C. M. Hernandez², A. Shrestha¹, D. Russell³, F.-Y. Yang³,
K. Sun⁴, and A. R. Smith¹**

¹*Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, OH 45701 USA*

²*Popular Autonoma del Estado de Puebla, Puebla 72410, Mexico*

³*Department of Physics, The Ohio State University, Columbus, Ohio 43210*

⁴*Department of Mat Sci & Engin., University of Michigan, Ann Arbor, MI 48109*

This study investigates the epitaxial growth, structural characterization, and theoretical modeling of thin-film antiperovskite Mn_3GaN , a chiral antiferromagnetic material with a kagome spin lattice grown on MgO (001) substrates via nitrogen plasma-assisted molecular beam epitaxy (MBE). The resulting films exhibit a homogeneous composition with atomically smooth surfaces and sharp interfaces, characterized by minimal *in-plane* tensile strain and *out-of-plane* compressive strain. First-principles calculations are employed to determine the energetically favorable configurations of both the MGN surface and the MGN / MgO heterostructure, and STM images reveal an atomically smooth surface with atomic-height steps [1].

The results show that the MnGa layer along the (001) direction is energetically favorable [1]. This layer is ferromagnetic *in-plane*, whereas in the (111) plane, all Mn_3Ga layers have chiral antiferromagnetic spin structure, making these very interesting from the spin perspective. In principle, this spin structure is accessible via spin-polarized STM which is currently our aim. Furthermore, measurements at low temperatures can be accomplished using our new variable-temperature STM system which enables better tip stability and lower noise. Since the Neel temperature of Mn_3GaN is 298 K, by investigating this system using spin-polarized STM tips at cryogenic temperatures, it is possible to resolve the temperature-dependent spin structure, and even the Neel transition.

This research has been supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award No. DE-FG02-06ER46317 (MBE, RHEED, STM) and under award No. DE-SC0001304 (XRD, SQUID).

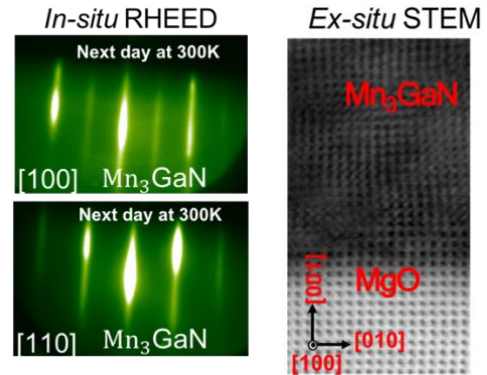


Fig. 1 (a) In-situ RHEED images of Mn_3GaN (001) surface after MBE growth. Half-order streak is related to the antiperovskite structure; (b) bright-field TEM image of $\text{Mn}_3\text{GaN}/\text{MgO}$ interface.

[1] A. Abbas, J. C. M. Hernandez, A. Shrestha, D. Russell, T. Erickson, F.-Y. Yang, K. Sun, and A. R. Smith, *Surfaces and Interfaces*, **64**, 10620, 2025.

[2] G. Gurung, D. F. Shao, T. R. Paudel, and E. Y. Tsymbal, *Physical Review Materials*, **3**(4), 044409, 2019.