Molecular beam epitaxial growth and scanning tunneling microscopy studies of Weyl semimetals Mn_3Ga and Mn_3Sn on hexagonal wurtzite GaN substrates

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Weyl semimetal systems including Mn_3Ga and Mn_3Sn are known for their fascinating electronic and magnetic properties and effects including anomalous Hall effect, topological Hall effect, giant piezo spintronic effect, large exchange bias, full electronic switching, and more [1, 2, 3, 4, 5, 6] Both Mn_3Ga and Mn_3Sn are non-collinear antiferromagnetic having the Kagome inverse triangular spin structure. We utilize a combination of molecular beam epitaxial growth and *in-situ* scanning tunneling microscopy to investigate high-quality, mirror-like surfaces of these materials and to study the structural, electronic, and magnetic properties of the surfaces using ultimately spin-polarized STM and tunneling spectroscopy.

In the case of Mn_3Ga, we have successfully performed MBE growth on *c*-plane wurtzite GaN and carried out room-temperature STM investigations of the surface, finding smooth spiral growth mounds and a spattering of pinholes on the surface (see Fig. 1). The surface step edges indicate that the structure is hexagonal given the 120° step angles. Atomic resolution images reveal the hexagonal structure with lattice constant $a = 5.60 +/- 0.10$ Å (reported $a = 5.4037$ Å [4]).

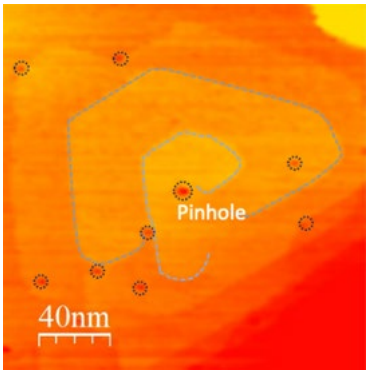

Figure 1 200 nm × 200 nm STM topographic image of Mn_3Ga showing spiral growth on the surface with several pinholes (Vs = -0.2 V, It = 90 pA).

In the case of Mn_3Sn, we grew extremely high-quality films on *c*-plane wurtzite *GaN* grown on sapphire (0001). Reflection high energy electron diffraction and x-ray diffraction were used to determine the *in-plane* and *out-of-plane* lattice constants, respectively. The final determined values were $a = 5.670$ Å, $c = 4.526$ Å which are in excellent agreement with ideal expected values (differences from expected are +0.0833% for *a* and -0.1104% for *c,* respectively). Preliminary STM results show an atomically smooth surface.

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Supplementary Information:

Mn_3Ga case

STM images of the Mn_3Ga on GaN substrate are shown in Fig. 2. We can see that the sample surface exhibits a spiral growth step morphology, with step heights of $c/2$ (c = 4.357 Å [H. Kurt, …, and J. Coey, Appl. Phys. Lett. 101 (2012)]), at least in some regions of the sample surface. Further, we observe an array of pinholes with ~5 nm diameters. These pinholes appear be either one or two atomic layers deep, as seen in Fig. 11(e). The cause of these features is uncertain, but they may be caused by some type of defects. We can also see at the inset of Fig. 11(b) the atomic resolution image of the surface which shows a hexagonal-like structure. Preliminary *dI/dV* measurements suggest a peak of state density near or above the Fermi level.

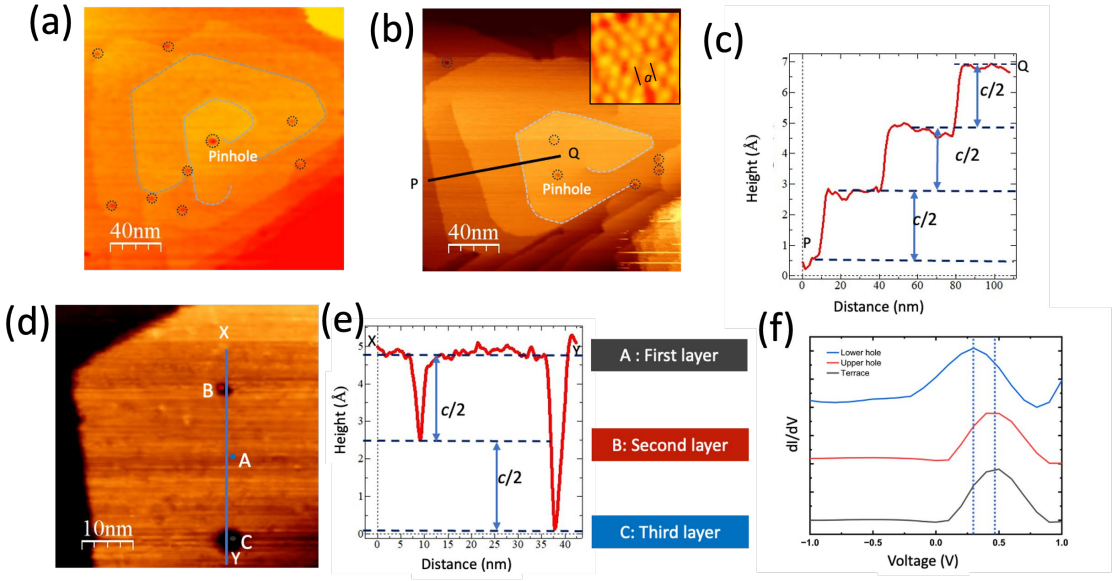

Fig. 2 200 nm × 200 nm STM topographic image showing spiral growth on the surface with several pinholes in a) region 1 (Vs = -0.2 V, It = 90 pA) and b) region 2 (Vs = 2 V, It = 90 pA), and inset shows an atomic resolution image with Vs = 1 V, It = 183 pA; c) line profile along line PQ showing the step height of terraces in (b); d) zoom-in view of top terrace of (b); e) line profile along line XY in (d) showing the size and depth of the pinholes; f) dI/dV spectra taken (in d) at: top terrace (A), upper pinhole (B), and lower pinhole (C).

The *out-of-plane* crystal structure is clear as seen by XRD, where we see a strong Mn_3Ga 0002 peak along with the GaN 0002 and Al_2O_3 0006 peaks. This suggests a highly crystalline sample.

Mn_3Sn case

The azimuthal RHEED scan map seen in Fig. 3 shows that the crystalline quality is good along all the available *in-plane* directions across the surface. The patterns alternate between the two crystalline azimuths, and all patterns are smooth and streaky. This indicates that the film is highly crystalline.

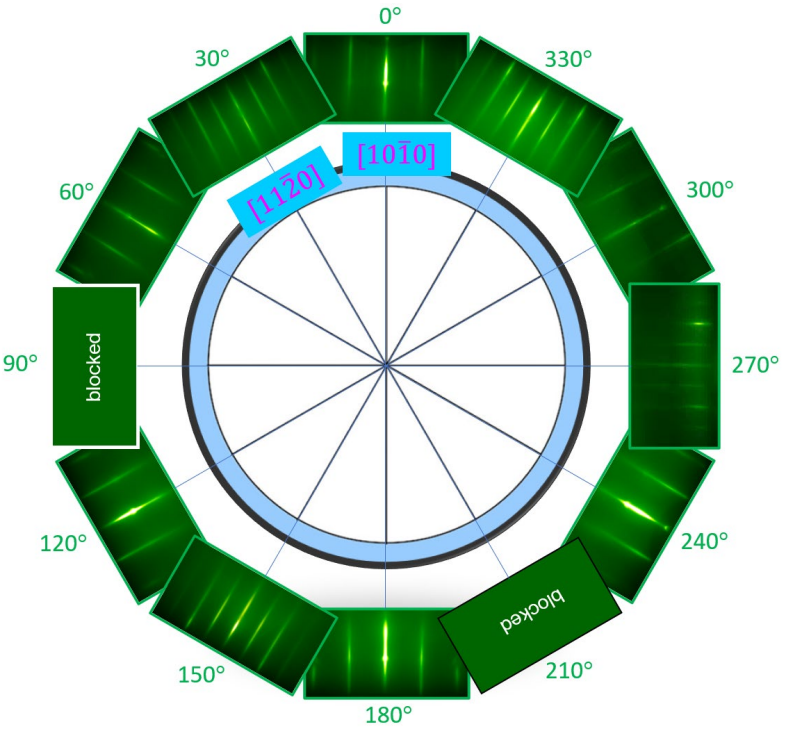

FIG. 3. 360° RHEED azimuth map for Mn_3Sn (0001). The patterns exhibit well-defined streaks, indicative of a well-ordered crystalline surface. A clear six-fold rotational symmetry is observed, consistent with the hexagonal crystal structure of Mn_3Sn. The primary crystallographic orientations, [11$\underline{2}$0] and [10$\underline{1}$0], are marked for reference. The 90° and 210° azimuths are blocked by the sample holder clips.

A preliminary UHV-STM image of a Mn_3Sn (0001) on *c*-plane GaN on Al_2O_3 (0001) surface showing a stepped terrace morphology is seen in Fig. 4(a). This image was acquired in constant current tunneling mode. One sees in the image a flat region at the top terrace together with atomic steps running from upper left to lower middle of the image area. As indicated by the line profile displayed in Fig. 4(b) the heights of the steps are consistent with single monolayers of Mn_3Sn of height *c*/2 (2.263 Å).

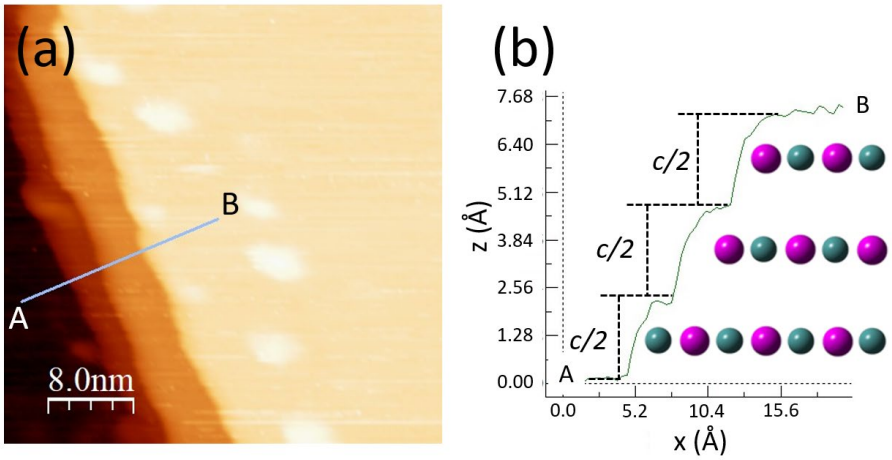

Fig. 4 *In-situ* UHV-STM image of Mn_3Sn/*w*-GaN/Al_2O_3 (0001) showing atomically smooth terraces and atomic layer height steps. The cross-section line profile A-B at the gray line is displayed in (b); model atoms are not to scale.