

## Electron Diffraction of Germanane

Amanda Hanks<sup>1</sup>, Shishi Jiang<sup>2</sup>, Bryan D. Esser<sup>1</sup>, Joshua E. Goldberger<sup>2</sup>, and David W. McComb<sup>1</sup>

<sup>1</sup>Center for Electron Microscopy and Analysis, The Ohio State University, Columbus OH 43212, United States

<sup>2</sup>Department of Chemistry and Biochemistry, The Ohio State University, Columbus OH 43210, United States

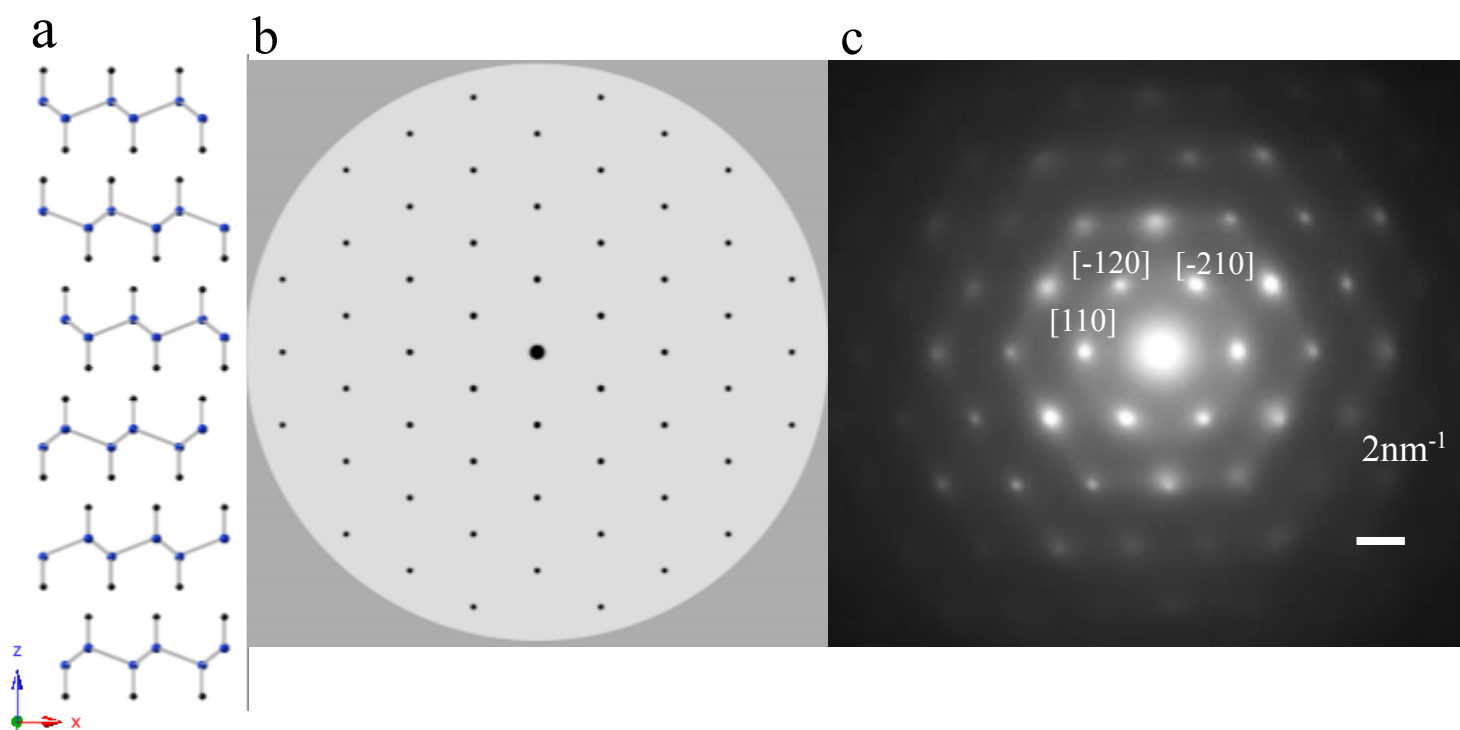
Differences in the physical phenomena exhibited by two-dimensional materials, compared with bulk materials, is the driver of significant interest in monolayers and bilayers of van der Waals layered materials. The ability to tune the properties and electronic structure of these layered materials via chemical functionalization opens numerous opportunities for novel applications and devices. For example, hydrogen terminated graphene, or graphane, has been extensively studied and used for a variety of applications. However, other two-dimensional materials that exhibit direct band gaps and high carrier mobilities are desired. Germanane, a group IV analogue of graphane, has recently been synthesized and exhibits a larger and direct band gap and higher electron mobility than that of bulk germanium [1-3]. However, while the electronic properties have been studied, the structure of the material remains largely unexplored. We have used electron diffraction in a transmission electron microscope (TEM) to investigate the structure of germanane on the nanometer scale.

Germanane (GeH) was synthesized by deintercalation of the the zintl phase  $\beta$ -CaGe<sub>2</sub>, resulting in a layered germanium honeycomb structure with hydrogen termination on each germanium atom as illustrated in Figure 1a. X-ray diffraction (XRD) and electron diffraction were used to confirm the hexagonal germanium lattice. However, both analyses indicate some disorder along the c-axis [1, 2]. The calculated electron diffraction pattern of perfectly crystalline germanane exhibits sharp, symmetric Bragg reflections as shown in Figure 1b. The experimental electron diffraction pattern of germanane exhibits the expected sharp Bragg spots but in most cases a diffuse halo is also observed. (Figure 1c) Typically such halos are associated with amorphous phases and are circularly symmetric. As shown in Figure 1c the diffuse halo in the diffraction pattern of germanane is not circular; it appears to have hexagonal symmetry with the intensity connecting the maxima in the diffraction pattern. This is unusual as it would correspond to a range of interplanar spacings in the layered structure coupled with some rotational disorder.

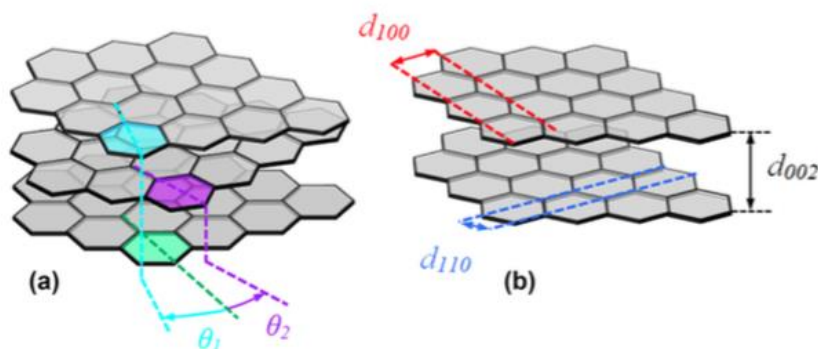
In order to fully understand the germanane structure the diffuse “hexagonal” halos are being investigated. It has been shown that graphite and other layered materials can also exhibit disorder along the c-axis that is referred to as turbostratic disorder. Turbostratic disorder is defined as random rotations and/or translations between layers as shown in Figure 2. This disorder can affect the electronic and magnetic properties by disrupting the pi-orbital hybridization and decoupling the layers or by eliminating interlayer epitaxial relationships [4-6]. Turbostratic graphite exhibits properties found in both bulk and single layer graphite which may suggest that similar properties could be observed in germanane. In this contribution, we will discuss the origins of this behavior in germanane and will show additional electron diffraction work to substantiate turbostratic disorder in this material.

## References

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**Figure 1:** (a) Schematic of structure of germanane looking down the (010) direction. (Ge: blue; H:Black) (b) Simulated electron diffraction pattern of single crystal of germanane. (c) Experimental diffraction pattern of germanane.



**Figure 2:** Model demonstrating turbostratic disorder in graphite with (a) being rotational and (b) being translational disorder along the z-axis [4].