Proposal:	5-14-276			Council: 10/2020			
Title:	Structu	cture of the candidate Weyl semi-metal Mn3Ge					
Research area: Physics							
This proposal is a continuation of 5-41-975							
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Samples: Mn3Ge							
Instrument			Requested days	Allocated days	From	То	
D9			3	3	31/05/2021	03/06/2021	
Abstract: We propose to investigate the crystal structure of antiferromagnetic Mn3Ge, which has been predicted to host relativistic quasi-particles							

We propose to investigate the crystal structure of antiferromagnetic Mn3Ge, which has been predicted to host relativistic quasi-particles called Weyl fermions. However, the Mn3Ge single crystals obtained from the melt are very prone to being off-stoichiometric (up to 10%). We have synthesized Mn3Ge crystals via the flux-growth method. This is the first reported flux-grown single crystal of Mn3Ge. Specifically, we want to find out whether the stoichiometry and site occupation of flux-grown crystals is different from melt-grown crystals.

Recently, Mn3Ge was found to display a large anomalous Hall effect (AHE) of ~50 Ω -1cm-1 at room temperature. This finding was surprising because Mn3Ge is an antiferromagnetic (AFM) metal, and a large AHE is usually restricted to ferromagnetic metals. Moreover, the spontaneous AHE in Mn3Ge is strongly anisotropic, and can be switched with a small applied magnetic field. From a technological standpoint, the concept of an AFM memory device that can be switched is very attractive as there is no demagnetization field, which limits the size of ferromagnetic materials. The prospect of scaling down the size of magnetic devices has prompted many studies of thin-film Mn3Ge, and the initial results look promising.

The hexagonal unit cell of Mn3Ge can be described by the P63/mmc space group (No. 194). The atoms that reside on the 6h Wyckoff site are arranged in a Kagomé pattern, with two Kagomé layers per unit cell stacked along the c axis with an in-plane displacement. Antiferromagnetic order of the Mn spins sets in at TN = 380 K, and below roughly the same temperature weak ferromagnetism in the basal plane is observed in the magnetization measurements, with a zero-field remnant moment of about 0.006 μ B per Mn at low temperature.

Up until recently, all of the reported bulk Mn3Ge crystals were grown from the melt. In practice, a small excess of Mn is needed to stabilize the hexagonal phase, so that the true chemical formula is Mn3+xGe, with x = 0.1-0.44. The Mn atoms are found to generally reside on the 6h site and the Ge atoms on the 2c site respectively. Yet, the off-stoichiometry in these samples suggest that the excess Mn might occupy the 2c site and perhaps account for the small ferromagnetism. There is an imperative need to explore other methods of growing bulk Mn3Ge.

To determine the stoichiometry of Mn3Ge crystals obtained from flux growth, we measured a large set of high quality and refinable data set on the D9 diffractometer. Since the X-ray structure factor of Mn and Ge are very similar, neutrons are required to obtain a good structure refinement. Measurements were performed at 400 K, well above the magnetic ordering temperature of 380 K. The refinement of the data is currently underway and is indicative of a slight excess of Mn.

To study the Mn3Ge single crystal on the D9, we used the OrientExpress Laue diffractometer to align the crystal to within 1 degrees.