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Reconsidering the magnetic structure in $NiS_{2-x}Se_x$ SHINICHIRO YANO, DESPINA LOUCA, UTPAL CHATTERJEE , Univ of Virginia, DUCK YOUNG CHUNG, DANIEL E. BUGARIS, MERCOURI KANATZIDIS, Argonne National Laboratory, JOERG C. NEUEFEIND, MIKHAIL FEYGENSON, Oak Ridge National Laboratory — The Mott metal-insulator transition (MIT) has been at the forefront of condensed matter research for decades. A Mott insulator is associated with antiferromagnetism (AFM) as well as an energy gap. The AFM order parameter can be directly traced by neutron scattering measurements. We focused on the study of MIT on the $NiS_{2-2x}Se_x$ system. With increase in x where x corresponds to the atomic volume of S that is replaced by Se, the system undergoes an AFM insulator to an AFM metalic transition at $x = 0.43$ at $T = 0$. Although $NiS_{2-2x}Se_x$ has been previously studied, the magnetic structure is not well understood. We measured the powder neutron diffraction for 4 compositions, $x = 0$, 0.4, 0.6, and 0.8, as a function of temperature. At T = 2K, we observed a clear composition dependence of the magnetic structure. While NiS_2 (x = 0) has two magnetic propagation vectors, M1 = (000) and M2 = (0.5 0.5 0.5), $NiS_{1.6}Se_{0.4}$ and $NiS_{1.4}Se_{0.6}$ have only one magnetic phase, M1. However, the M1 structure vanishes by $NiS_{1.2}Se_{0.8}$. While the two magnetic phases have been previously reported, we determined the magnetic structures by using representation analysis.the magnetic structure and physical properties of this system will be discussed.

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