Nuclear and Magnetic Structure of Ba$_{1-p}$Cr$_2$Se$_{4-p}$ an aperiodic ferrimagnetic semiconductor

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Keywords: Aperiodic, Ferrimagnet, Magnetic Structure

The family of compounds A$_{1-p}$Cr$_2$X$_{4-p}$ (A: Ba, Sr, Eu, Sn, Pb; X: S, Se)[1]. They established these compounds as a class of isotypic chromium sulphides and selenides. The structure is described as intergrowth of three different structural subsystems, including a host framework and two different chains that lie within, sharing a common hexagonal basal (a-b) plane but have different c axes.

The framework consists of CrX$_6$ octahedra, containing strips of edge sharing octahedra (Figure 1(a)) similar to those in rutile interconnected by face sharing octahedra. These form a framework which contain channels/tunnels centred on the threefold and sixfold axes (3/m and 6/m). The chains that occupy the triangular tunnels consist of A$_3$X units, whereas the chains that occupy the hexagonal tunnels consist of A$_6$Cr$_2$X$_6$ units.

We have re-examined the Barium selenide previously reported to be a commensurate superstructure, by X-ray single crystal and neutron powder diffraction. Single crystal measurements show that the first two subsystems are well ordered and described in super space group $P6/m(00\alpha)s0$ whilst the third subsystem is highly disordered giving rise to strong diffuse scattering (Figure 1 (b)).

Figure 1. (a) Projection of average structure along c. (b) Diffuse scattering in hk0.6 plane

Bellow 120 K the structure orders ferrimagnetically and refinement of the neutron powder diffraction at 10 K gives the best fit for magnetic structures which break inversion symmetry. These agree well with the measured moments and indicate that the material is multiferroic at low temperatures.


Acknowledgements: This work is supported from JSPS KAKENHI Grant Numbers JP19H05817 and JP19H05818.