



Figure 1. (left) crystal structure of $(\text{C}_6\text{H}_{11}\text{NH}_3)_2[\text{PbI}_4]$. (right) commensurate-incommensurate structural phase transition.

Keywords: hybrid perovskite, phase transition, incommensurate structure

MS26-O4 Probing the nuclear and magnetic structure of a complex ferromagnetic semiconductor

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The large diversity of structural, electronic, and magnetic phases offered by compounds made up of two or more interpenetrating sublattices (composite structure) such as misfit layer chalcogenides offer the possibility to tune materials functionality using crystal chemistry concepts [1]. The structural and physical properties of the columnar composite crystal $\text{A}_p\text{Cr}_2\text{X}_6$ ($\text{A} = \text{Ba}, \text{Sr}, \text{Eu}, \text{Pb}$; $\text{X} = \text{S}, \text{Se}$; $p \approx 0.29$) have not been studied in details.[2] The difficulty in interpreting the observed physical properties and the uncertainty about the exact chemical composition led to the reinvestigation of the crystal structure by Brouwer and Jellinek [2]. They concluded that the crystal structure of this family of materials could be described as an intergrowth of three structural units which have a common hexagonal basal plane, but different c axes. A three-dimensional network (B_3X_{36}) of triply twined strips of CrX_6 octahedra with a lattice constant of c_0 creates hexagonal funnels containing $\text{A}_6\text{B}_2\text{X}_6$ chains with a lattice parameter c_6 and the triangular tunnels A_3X chains with a lattice parameter c_3 . Here we solve the crystal structure of the $\text{Ba}_{0.712}\text{Cr}_2\text{Se}_{3.712}$ in the superspace group $\text{P6/m}(00\gamma_1)s0(00\gamma_2)00$ (175.2.81.3 in the tables of Stokes and Campbell) using neutron powder diffraction, showing it is not a commensurate supercell but incommensurately modulated and study the evolution of the structural parameters on cooling through the magnetic transition observed at 110 K. This material is a ferromagnetic semiconductor at low temperature, with a measured Seebeck coefficients as large as 100 $\mu\text{V/K}$ at room temperature. It is thus likely to have low thermal conductivity on account of its complex structure and is thus of interest for thermoelectric applications.

[1] J. Rouxel, A. Meerschaut and G. A. Wiegiers, *J. Alloys Comp.*, 229 144 (1995)

[2] R. Brouwer and F. Jellinek, *J. Physique Colloque*, 38 C-7 (12) c7.36 (1977)

Keywords: composite phase, magnetic structure, incommensurate, neutron diffraction