

## Poster Presentation

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#### *Effect of Lone Pair Cations on the Orientation of Crystallographic Shear Planes in Anion-Deficient Perovskites*

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Anion deficiency in perovskite-based ferrites containing lone pair cations Pb<sup>2+</sup> and Bi<sup>3+</sup> can be accommodated by the formation of crystallographic shear (CS) planes. In this contribution, using (Pb<sub>1-z</sub>Sr<sub>z</sub>)<sub>1-x</sub>Fe<sub>1+x</sub>O<sub>3-y</sub> as a model system, we demonstrate that the lone pair cations are not only responsible for the formation of the CS planes, but also control their orientation. The isovalent substitution of Pb<sup>2+</sup> by stereochemically inactive Sr<sup>2+</sup> highlights the influence of the A-cation electronic structure owing to very close ionic radii of these cations. Employing a combination of transmission electron microscopy and X-ray and neutron powder diffraction, we have systematically investigated the structure evolution of the compounds with changing P/Sr ratio. Two compositional ranges with distinct orientations of the CS planes have been identified in the system:  $0.05 \leq z \leq 0.2$ , where the CS planes orientation systematically varies but stays close to (203)<sub>p</sub>, and  $0.3 \leq z \leq 0.45$  with the (101)<sub>p</sub> CS planes. The incommensurate structure of Pb<sub>0.792</sub>Sr<sub>0.168</sub>Fe<sub>1.040</sub>O<sub>2.529</sub>, a representative compound of the first range, has been refined from the neutron powder diffraction data (S.G. X2/m( $\alpha$ 0 $\gamma$ ), X = [1/2,1/2,1/2,1/2], a = 3.9512(1)Å, b = 3.9483(1)Å, c = 3.9165(1)Å,  $\beta$  = 93.268(2)°, q = 0.0879(1)a\* + 0.1276(1)c\*, RF = 0.023, RP = 0.029, T = 900K). Comparing the CS structures in both compositional ranges, we demonstrate that the orientation of the CS planes is primarily governed by a specific bonding configuration of the lone pair cations with the anions.

**Keywords:** perovskites, incommensurate compounds, TEM