

Stabilizing Polar Polymorphs of Scandium Ferrite for Photovoltaics

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Metastability is no longer synonymous with unstable or unattainable. Although significant advancements have been made in stabilizing metastable polymorphs (materials with the same stoichiometry but a different crystal structure than the ground state) further work is needed to enable the next generation of ferroelectric photovoltaics. Here we will discuss the stabilization of the $P6_3cm$ phase of $ScFeO_3$ through precursor control and interface engineering. The $P6_3cm$ phase has potential for lead-free piezoelectric, photoferroics, and ferroelectric applications. Unfortunately, this phase is in competition with four other known polymorphs that are similar in structure and energy, and there is not a well matched epitaxial substrate. By controlling the atomic layering of the precursor structure and the deposition timing we were able to stabilize the $P6_3cm$ phase under conditions that previously lead to the ground state in the absence of layering. The film structure was verified by transmission electron microscopy, x-ray diffraction, and reflective high energy electron diffraction. *Ab initio* calculations confirm that layered growth stabilizes the metastable phase and highlights the importance of the variable oxidation state of iron, the high activation energy against diffusion, and the surface termination of the substrate in designing a stabilization approach. The growth approach highlighted here opens doors to accessing new materials or translating established materials into new device architectures.