

USE OF *IN-SITU* XRD TO DEVELOP CONDUCTING CERAMICS WITH THE AURIVILLIUS CRYSTAL STRUCTURE

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In-situ X-ray diffraction and impedance spectroscopy have been employed to investigate ceramic oxides with the Aurivillius crystal structure and their potential as oxygen ion conductors in electrochemical devices such as fuel cells.

Many ceramics with the Aurivillius crystal structure undergo phase transformations at elevated temperatures. In some such oxides, this transformation appears to have significant impact on conductivity. For example, $\text{BaBi}_4\text{Ti}_3\text{ScO}_{14.5}$ and $\text{BaBi}_4\text{Ti}_3\text{InO}_{14.5}$ become fast ion conductors when this transformation occurs.

The Aurivillius structure consists of perovskite-type blocks layered between $\text{Bi}_2\text{O}_2^{2+}$ sheets, described by the notation $\text{Bi}_2\text{O}_2 \cdot A_{n-1}\text{B}_n\text{O}_{3n+1}$. This study focuses on Aurivillius phases with $n = 3$ and 4 , where n effectively indicates the number of perovskite-type layers between the bismuth oxide layers. Bi, Ba, La, and Sr have been varied on the A site; and Ti, In, Nb, and Fe have been varied on the B site. A thorough crystallographic understanding of these phases is being pursued to facilitate the development of better ionic and mixed conductors. *In-situ* X-ray diffraction has been employed to study phase transformations in these materials and their correspondence to ionic conductivity. Crystal structure solutions of these phases have been developed. Atomistic computer simulations based on these structural solutions are being attempted. This information is used to develop new compositions that might better optimize conductivity and transformation temperature.