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PII: S0022-4596(13)00233-8
DOI: http://dx.doi.org/10.1016/j.jssc.2013.04.039
Reference: YJSSC18008

To appear in: *Journal of Solid State Chemistry*

Received date: 12 March 2013
Revised date: 24 April 2013
Accepted date: 25 April 2013

Cite this article as: Fengxia Wei, Tim Williams, Tao An, Tom Baikie, Christian Kloc, Jun Wei, Tim White, Observation of Atomic Scale Compositional and Displacive Modulations in Incommensurate Melilite Electrolytes, *Journal of Solid State Chemistry,* http://dx.doi.org/10.1016/j.jssc.2013.04.039

Observation of Atomic Scale Compositional and Displacive Modulations in Incommensurate Melilite Electrolytes

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Abstract

The paradigm that functional materials are adequately described as three dimensional crystal structures is not universally tenable. Gallate melilites are efficient oxide ion conductors at intermediate temperatures (~750°C) with non-rational crystallographic modulations presumed to play a key role in significantly enhancing oxygen mobility. Lattice distortions associated with incommensuration are usually extrapolated from diffraction analysis of volumes greatly exceeding the scale of modulation. Therefore, opportunities for making direct nanometric measurements are exceptionally valuable for correlating structure with function. In $[CaLn]_2[Ga]_2[Ga_2O_7]_2$ (*Ln* = Nd, La) melilites, atomic displacive and compositional modulation waves can be imaged by high angle annular dark field and bright field scanning transmission electron microscopy with contrast quantified through electron scattering simulation. Here, we present atomic scale observations of (3+2)-dimensional modulations in gallate melilites which expands our understanding of the ion conduction mechanism and provides guidance for enhancing the performance of solid oxide fuel cells through crystal chemical tailoring.