



Symmetry-Adapted Pair Distribution Function Analysis

Tobias Bird

Symmetry-Adapted Pair Distribution Function Analysis (SAPA)^[1] is a novel technique for obtaining information on local dynamics and disorder from pair distribution function (PDF) data. In the SAPA method, the crystal structure is expanded to a supercell of a given size and then broken down into a symmetry-mode basis using the *ISODISTORT* online software. Using the *TOPAS* command line functionality, groups of modes transforming as the same irreducible representation can be tested in turn, in order to find the modes most responsible for any deviation of the local structure from the average. With the python programming language, this technique can be performed as an automated process. Using this method, it has been possible to elucidate the underlying symmetry of the successive ferroelectric phase transitions in BaTiO₃^[2] and have highlighted the importance of structural flexibility in determining the range and magnitude of negative thermal expansion in ReO₃^[3] and related structures^[4].

[1] T. A. Bird, A. Herlihy and M. S. Senn, *J. Appl. Cryst.*, **54** (2021), 1514-1520

[2] M. S. Senn, D. A. Keen, T. C. A. Lucas, J. A. Hriljac and A. L. Goodwin, *Phys. Rev. Lett.*, **116** (2016), 207602

[3] T. A. Bird, M. G. L. Wilkinson, D. A. Keen, R. I. Smith, N. C. Bristowe, M. T. Dove, A. E. Phillips and M. S. Senn, *Phys. Rev. B*, **104** (2021), 214102

[4] T. A. Bird, J. Woodland-Scott, L. Hu, M. T. Wharmby, J. Chen, A. L. Goodwin and M. S. Senn, *Phys. Rev. B*, **101** (2020), 064306

Primary author(s) : Dr. BIRD, Tobias (Diamond Light Source)

Co-author(s) : Dr. CHATER, Philip (Diamond Light Source); Dr. SENN, Mark (University of Warwick)