Keynote Lecture

KN09

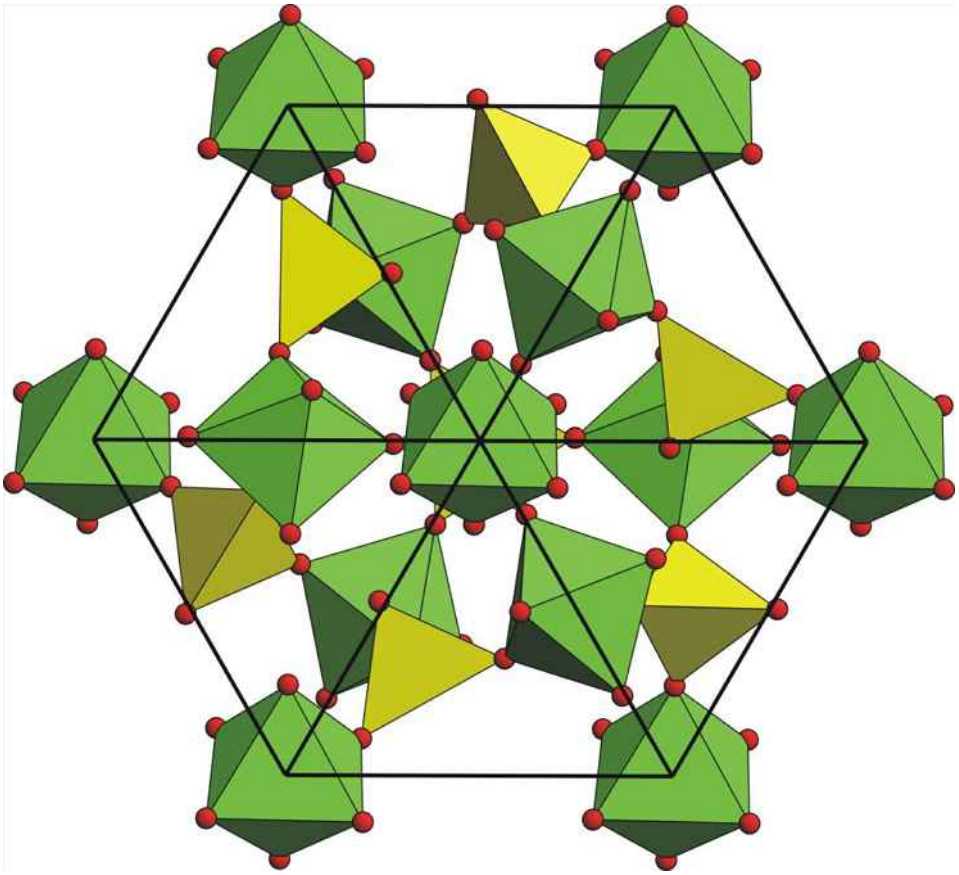
Put Your Trust in Powder: Negative and Zero Thermal Expansion Materials

J. Evans[1]

[1]*Durham University, Department of Chemistry, Durham, UK*

Powder diffraction is one of the most powerful structural probes available to the materials chemist. It invariably plays a critical role in the preparation of new phases and is increasingly exploited via in-situ studies to understand and control complex synthetic routes to fleetingly stable materials. Ab initio structure solution followed by Rietveld refinement frequently provides the first structural information on new functional materials, and powder diffraction is often the method of choice for probing structure-property relationships under non-ambient or in-operando conditions, or for following the structures of samples undergoing structural phase transitions. In this presentation I'll show how powder diffraction has been crucial in understanding the properties of so-called negative thermal expansion (NTE) materials – here inorganic oxides which contract on heating. Powder methods have provided key information on the thermodynamic stability of these materials, the low temperature synthetic routes required to prepare them, the average and local distortions that lead to NTE, and on the often complex phase transitions they undergo. I'll also discuss how powder diffraction can probe glass-like relaxation processes which occur over remarkably long timescales in some of these materials and how the synthetic control enabled by in-situ studies has led to the preparation of single-phase isotropic materials whose expansion properties can be systematically tuned from negative to zero to positive values (alpha –8 to +6 * 10–6 K–1) [1]. I'll emphasise how new techniques such as Parametric- [2] and Symmetry-Mode-Rietveld [3] refinement has been crucial in the study of these materials.

[1] *S.E. Tallentire, F. Child, I. Fall et al., Journal of the American Chemical Society, 2013, 135, 12849–12856.,* ***[2]*** *G.W. Stinton, J.S.O. Evans, Journal of Applied Crystallography, 2007, 40, 87–95.,* ***[3]*** *S. Kerman, B.J. Campbell, K.K. Satyavarapu et al., Acta Cryst., 2013, A68, 222–234.*



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