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Structural Disorder in the Negative Thermal Expansion Material ZrW_2O_8 and Quartz-based Piezoelectrics: An RMC Analysis of Total Scattering Data. D.A. Keen[1], M.G. Tucker[1], M.T. Dove[2], A.L. Goodwin[2], S.A. Wells[3], J.S.O. Evans[4], J. Haines[5], O. Cambon[5], [1]ISIS Facility, Rutherford Appleton Laboratory, Oxon OX11 0QX UK, [2]Earth Sciences Dept., Cambridge Univ., Cambridge CB2 3EQ UK, [3]Biological Physics, Arizona State Univ., Tempe, AZ 85287 USA, [4]Chemistry Dept., Durham Univ., Durham DH1 3LE UK, [5]UMR CNRS 5617, Univ. Montpellier II, 34095 Montpellier 5, France.

Total scattering data from disordered crystals gives information on the long-range average structure via the Bragg intensities and local deviations from this average via the pair distribution function. The reverse Monte Carlo (RMC) method is an ideal way to analyse these data to provide self-consistent structural models. Disorder plays an important role in the NTE behaviour of ZrW_2O_8 and the reduced piezoelectric performance in a-quartz SiO_2 and a-berlinite $GaPO_4$ resonators at high temperature. This talk will describe how results from RMC analysis of total scattering have been able to identify local structural features which are responsible for the observed macroscopic behaviour in these two materials. In particular, it is found that complex motion of “rigid” structural units provides the mechanism for thermally induced contraction of ZrW_2O_8 and the dissipation of induced dipoles in SiO_2 and $GaPO_4$.