

Microsymposium

MS55.O02

Complexity in Cubic Crystals

D. Keen¹

¹*Rutherford Appleton Laboratory, ISIS Facility, Didcot, UK*

Cubic crystals have been studied in detail ever since the advent of X-ray crystallography 101 years ago when Lawrence Bragg first solved the cubic structure of rocksalt. Despite this long history they still hold a fascination with many topical materials such as C60, PbTe-based thermoelectrics, ZrW2O8-related negative thermal expansion materials and several ice phases, all crystallising into cubic structures. This talk will briefly outline the early heritage of (cubic) crystallography and will then highlight the key role of complexity on the physical properties of many cubic crystals. I define complexity as a local breaking of the overall crystal symmetry, rather than the creation of ever larger unit cells, and therefore accurate understanding cannot be gained through analysis of Bragg diffraction alone. Instead I will describe methods for quantifying this complexity via models refined by reverse Monte Carlo analysis of total scattering (pair distribution function) data and using a range of different examples, some taken from the list given above.

Keywords: Total Scattering, Ice, PbTe