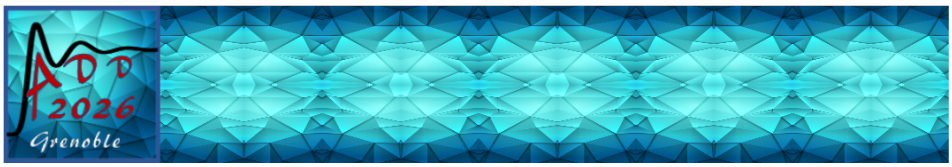

Abstract ID : **12**

RMCProfile: Local structure of crystalline to amorphous materials

Content

Many of the useful materials that make modern life possible are crystalline. Quartz keeps our watches on time, perovskites are widely used in consumer electronics and solid oxide fuel cells may help to power the future.
The importance of local structure and disorder in crystalline materials is being recognised more and more as a key property of many functional materials. From negative thermal expansion to solid state amorphisation and the 'nanoscale' problem to improved fuel cell technology, a clear picture of the local atomic structure is essential to understanding these phenomena and solving the associated problems.
Total scattering, an extension of the powder diffraction method, is increasingly being used to study crystalline materials. The unique combination of Bragg and diffuse scattering can be used to determine both the average structure and the short-range fluctuations from this average within a single experiment. To maximise the structural information from such data, three-dimensional atomic models consistent with all aspects of the data are required.
RMCProfile [1] expands the reverse Monte Carlo (RMC) modelling technique [2] to take explicit account of the Bragg intensity profile from crystalline materials. Analysis of the RMCProfile-generated atomic models gives more detailed information than is available directly from the data alone. We will give several examples where RMCProfile has been used to successfully study the structure and disorder of crystalline materials to illustrate its potential. Also, since the original RMC technique was designed to study amorphous materials, we will give examples where RMCProfile has been used to model amorphous structures that derive from crystalline materials.

[1] see www.rmcprofile.org; M G Tucker, D A Keen, M T Dove, A L Goodwin and Q Hui, *J. Phys. Condens. Matter* **19**, 335218 (2007).
[2] R L McGreevy amd L Pusztai, *Mol. Simul.* **1**, 359 (1988).

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