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RMCProfile: A step towards complex modelling

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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 improved fuel cell technology and solid state amorphisation to the 'nanoscale' problem, 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] (see www.rmcprofile.org) 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. I will give several examples where RMCProfile has been used to successfully study the structure and disorder of crystalline materials to illustrate its potential. As the systems being studied become more complex, the information from many experimental techniques and any prior chemical knowledge needs to be combined into one consistent atomic model. The continued development of RMCProfile and its new capabilities is moving us closer to the complex modelling paradigm[3] required to drive the discovery of new functional materials.

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