Getting the most from Total Scattering

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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. Here I present a technique for producing such models based on the reverse Monte Carlo (RMC) method. The existing RMC method has been expanded to take explicit account of the Bragg intensity profile from crystalline materials[1].

Analysis of the RMC-generated atomic models gives much more detailed information than is available directly from the data. I will give several examples where this method has been used to successfully study the structure and dynamical disorder of materials including those with the perovskite structure[2], those showing negative thermal expansion and molecular crystals. I will also show examples of low-energy phonon dispersion curves obtained from the models[3].

[1] Keen D. A., et al, *J. Phys.: Cond. Matt*, 2005, **17**, S15. [2] Hui Q., et al, *J. Phys.: Cond. Matt*, 2005, **17**, S111. [3] Goodwin A. L., et al *Phys. Rev. Lett.* **93**, 075502, 2004.

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