Local structure of crystalline to amorphous materials

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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 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 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 gain the most useful information from total scattering data it is often necessary to produce atomistic models with computation methods. One such method is reverse Monte Carlo (RMC) [1], here a large box of atoms is constructed with the correct composition and density. Then atoms chosen at random, are moved by a random amount until the calculated total scattering matches the experimental data. This comparison back to the data rather than to an empirical potential makes this reverse rather than classical Monte Carlo. The resulting atomistic configuration can then be analysed to provide a more detailed understand of the environment around the various atom types.

As with the experimental technique we have been developing RMC methods for the study of crystalline materials over the past decade and produced the program RMCProfile [2]. However, since these methods are built on those originally developed for amorphous materials, the new developments can equally be applied to amorphous systems. I will give several examples of how the new methods have been used to study phenomena such as solid-state amorphisation and how they are moving us closer to a complex modeling regime [3].

References:

1. R. McGreevy, L. Pusztai, Mol. Simul., 1988, 1, 359

2. RMCProfile: reverse Monte Carlo for polycrystalline materials M G Tucker, D A Keen, M T Dove, A L Goodwin, Q Hui J. Phys.-Condes. Matter 19 335218 (2007) - also more information and the program available at www.rmcprofile.org

3. S. Billinge, I. Levin, Science, 2007, 316, 561-565