

W0014

Collective Properties from RMC Analysis of Total Scattering Data: Excitations, Modulations and Some Limitations. A.L. Goodwin¹, M.T. Dove¹, E.R. Cope¹, M.G. Tucker², D.A. Keen², ¹Dept of Earth Sciences, Cambridge Univ., Cambridge CB2 3EQ UK ²ISIS Facility, Rutherford Appleton Laboratory, Oxon OX11 0QX UK.

The reverse Monte Carlo (RMC) structural refinement method provides a powerful means of generating atomistic configurations from total scattering data. These configurations represent at once both elastic and inelastic contributions to the scattering process: the former is reflected in the average periodic structure of the configuration, and the latter in local deviations from this average structure. Inelastic scattering from collective excitations such as phonons will then enter the RMC configurations in the form of correlated atomic displacements. This talk will describe how information regarding the phonon spectrum can be retrieved from analysis of large numbers of RMC configurations, enabling the calculation of phonon dispersion curves from powder diffraction data. The known limitations of the approach will be discussed. The extension of the RMCProfile implementation to allow refinement of magnetic structures will also be described, together with its role in the discovery of structural modulations in the benchmark antiferromagnet MnO. Finally, it will be shown that spin-wave dispersion curves can be recovered from these magnetic RMC configurations.