EDITORIAL

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Editorial

Focus issue on studies of structural disorder using reverse Monte Carlo methods

David A Keen
ISIS Facility, Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxfordshire OX11 0QX, United Kingdom

Understanding how structure underpins the physical properties of materials continues to be an active area of research worldwide. Increasingly those working in this area are required to not just investigate structures with regular atomic arrangements but to also develop and use methods and protocols for interrogating systems where the structure is disordered and not amenable to regular crystallographic techniques. The reverse Monte Carlo (RMC) method is one such technique; it has been developed over the last 27 years and is capable of determining the disordered atomic arrangements of liquids, glasses and crystalline systems from routine diffraction measurements. The method uses a Monte Carlo minimisation protocol, but instead of reducing the overall energy of the system, it aims to reduce the disagreement between functions that have been measured experimentally and those which can be calculated from a large configuration of atoms. These functions can be very varied but are typically some or all of the following: Bragg diffraction patterns from powders, total scattering structure factors, pair distribution functions and/or EXAFS spectra. Although the flexibility of the RMC method is a considerable strength it can also be a weakness and, as ever more complex systems are being studied, data-sets from x-ray, neutron and electron diffraction measurements are increasingly being refined simultaneously in order to build up a complete and detailed description of the disordered structure under study.

Every three years the RMC community meets in Budapest to discuss current work and to encourage each other in new endeavours. The community is broad, with representatives from within physics, chemistry and materials science, each working in areas of direct relevance to their discipline. The invited papers presented in this focus issue are a flavour of the original research that was discussed during the most recent meeting in September 2015 (see the RMC Conference: www.szfki.hu/~nphys/rmc6/). In these papers [1–8], we see the broad interests of those who are using RMC methods, from those studying disordered crystal structures and oxide and metallic glasses, to those interested in liquids and magnetic structure. A variety of experimental data are refined—often simultaneously—and the RMC method is used in tandem with other techniques such as molecular dynamics (MD) or by incorporating evolutionary algorithms.

For readers interested in finding out more about the basics of the RMC method I would recommend Pethes *et al* [4] and Timm *et al* [6]. The former shows how a variety of data and the RMC++ code might be used to refine a single 30 000-atom model of $Pd_{81}Ge_{19}$ glass and the latter uses neutron diffraction and the RMCProfile code to refine the magnetic structure of large crystalline supercells of NiO and CoO. Alternatively the popular (based on total downloads to date) open access paper by Clark *et al* [8] would provide a good introduction to the method. Finally—and I am showing my own personal bias for studies of disordered crystal structure here—I'd like to highlight the work on the A-site vacant perovskite FeF_3 (Jonane *et al* [3]) and scheelite-type AWO_4 (Kalinko *et al* [5]), both of which use a combination of RMC and MD in the analysis of the structural disorder. Notwithstanding my above stated bias, I commend *all* the papers in this Focus Issue to you.

References

[1] Timoshenko J *et al* 2016 Local structure of copper nitride revealed by EXAFS spectroscopy and a reverse Monte Carlo/evolutionary algorithm approach *Phys. Scr.* **91** 054003

[2] Fábián M and Araczki C 2016 Basic network structure of SiO_2–B_2O_3–Na_2O glasses from diffraction and reverse Monte Carlo simulation *Phys. Scr.* **91** 054004

[3] Jonane I *et al* 2016 Atomistic simulations of the Fe *K*-edge EXAFS in FeF_3 using molecular dynamics and reverse Monte Carlo methods *Phys. Scr.* **91** 104001

[4] Pethes I *et al* 2016 Chemical ordering in $Pd_{81}Ge_{19}$ metallic glass studied by reverse Monte-Carlo modelling of XRD, ND and EXAFS experimental data *Phys. Scr.* **91** 104004

[5] Kalinko A *et al* 2016 Molecular dynamics and reverse Monte Carlo modeling of scheelite-type AWO_4 (A = Ca, Sr, Ba) W L_3-edge EXAFS spectra *Phys. Scr.* **91** 114001

[6] Timm L *et al* 2016 Exploration of antiferromagnetic CoO and NiO using reverse Monte Carlo total neutron scattering refinements *Phys. Scr.* **91** 114004

[7] Steinczinger Z *et al* 2017 Comparison of interatomic potentials of water via structure factors reconstructed from simulated partial radial distribution functions: a reverse Monte Carlo based approach *Phys. Scr.* **92** 014001

[8] Clark A H *et al* 2017 Reverse Monte Carlo studies of CeO_2 using neutron and synchrotron radiation techniques *Phys. Scr.* **92** 034002