PREFACE

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PREFACE

The first 21 years of reverse Monte Carlo modelling—a workshop held in Budapest, Hungary (1–3 October 2009)

Guest Editors

David A Keen
ISIS Facility, Rutherford Appleton Laboratory, UK

László Pusztai
Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, Hungary

This special issue contains a collection of papers reflecting the content of the fourth workshop on reverse Monte Carlo (RMC) methods, held in a hotel on hills overlooking Budapest at the start of October 2009. At this meeting around sixty participants gathered to hear talks and discuss a broad range of science based on the RMC technique in very convivial surroundings.

Reverse Monte Carlo modelling is a method for producing three-dimensional disordered structural models in quantitative agreement with experimental data. The method was developed in the late 1980s and has since achieved wide acceptance within the scientific community [1], producing on average over seventy papers and 1000 citations per year in the last five years. It is particularly suitable for studies of the structures of liquid and amorphous materials, as well as the structural analysis of disordered crystalline systems. The principal experimental data that are modelled are obtained from total x-ray or neutron scattering experiments, using the reciprocal space structure factor and/or the real space pair distribution function (PDF). Additional data might be included from extended x-ray absorption fine structure (EXAFS) spectroscopy, Bragg peak intensities or indeed any measured data that can be calculated from a three-dimensional atomistic model. It is this use of total scattering (diffuse and Bragg), rather than just the Bragg peak intensities more commonly used for crystalline structure analysis, which enables RMC modelling to probe the often important deviations from the average crystal structure, to probe the structures of poorly crystalline materials, and the local structures of non-crystalline materials where only diffuse scattering is observed. This flexibility across various condensed matter structure-types has made the RMC method very attractive in a wide range of disciplines, as borne out in the contents of this special issue. It is, however, important to point out that since the method is akin to a structural refinement method (albeit with some inbuilt Monte Carlo ‘randomness’) high-quality data are needed to yield the best structural models. In this regard it is particularly pleasing to see the recent (planned and actual) growth in diffractometers at neutron and synchrotron x-ray facilities that have been designed with total scattering in mind.

Since the previous RMC workshop in 2006 [2] (and indeed the earlier workshop in 2003 [3]) there have been several developments in the technique and in the range of its application. On the technical side, the method has been used in conjunction with ‘standard’ Monte Carlo [4] and molecular dynamics [5] simulations and lattice dynamical calculations [6]; bond valence functionality [7] has been built into the RMCProfile code as well as more general calculations of molecular geometry constraints. Furthermore, existing RMC modelling codes have been updated and improved and made more ‘user-friendly’ [8]. Although the majority of RMC applications are still concerned with the structures of liquid and amorphous materials (see, for example, [9])—where atomistic modelling is the main method for obtaining three-dimensional structural information—there are
now a significant number of papers each year which use RMC to investigate disorder within crystalline materials, to understand the structure of nano-materials and thin films, to characterize magnetic structure and to use RMC analysis of small-angle scattering data to investigate longer-range structural fluctuations.

The RMC workshop was particularly beneficial, providing a forum for those workers in the field to take stock of past achievements and to look forward to future developments. It also enabled students and other young researchers to gain a deeper understanding of the RMC method at the start of their scientific careers. It is our hope that the collection of research papers within this special issue will communicate the vibrancy of this field to the wider scientific community by showing the current state-of-the-art research opportunities using the RMC method. Furthermore, by including a small number of papers from colleagues working on similar disordered problems with complementary analysis techniques, we hope that the RMC method may be placed in a broader scientific context. The papers have been arranged in order of increasing structural disorder, starting with studies of crystalline systems, through to amorphous materials and liquids, and ending with RMC developments using small-angle scattering.

We are very grateful to IOP Publishing for their willingness to publish this collection of papers which celebrates the 21st anniversary of the first RMC publication in a special issue of Journal of Physics: Condensed Matter and for their co-ordination of the refereeing process.

References