The First Eighteen Years of Reverse Monte Carlo Modelling, a workshop held in Budapest, Hungary (28–30th September 2006)

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PREFACE

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This Special Issue contains a collection of papers reflecting the content of the third workshop on reverse Monte Carlo (RMC) methods, held in a hotel on hills overlooking Budapest at the end of September 2006. Over forty 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]. It is particularly suitable for studies of the structures of liquid and amorphous materials, although it may also be applied effectively to the structural analysis of disordered crystalline systems. Since the previous RMC workshop in 2003 [2] there have been several developments in the technique, particularly as applied to crystals, and in the range of its application, most noticeable being the routine modelling of multiple data sets for a given problem; the latter growing through the increasing quality and availability of x-ray total scattering data from synchrotron x-ray sources. 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 is our hope that the collection of papers within this Special Issue will also communicate this to the wider scientific community, providing a balance between papers that have more of an introductory review flavour and those that concentrate on 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 within this special issue have been arranged into four groups: those concerning liquids (1–8), amorphous (9–13) and crystalline materials (14–17) and those of a more general nature (18–23). Within these groupings, there are descriptions of RMCProfile (18) and RMCt (23), programs which use RMC methods to analyse total scattering from crystalline materials and to model inelastic neutron scattering data, respectively. There is also work using the related EPSR (6) and PDFfit (19) techniques, developments of the RMC method for analysis of single crystal electron diffraction (16) or polarised neutron diffraction (7), and examples of simultaneous RMC modelling of neutron and x-ray total scattering and XAS data (13, 10).

We are very grateful to IoP Publishing for their willingness to publish the proceedings of this meeting in a Special Issue of *Journal of Physics: Condensed Matter*.

References

[1] McGreevy R L 2001 *J. Phys.: Cond. Matter* **13** R877
[2] RMC-2 Workshop Proceedings 2005 *J. Phys.: Cond. Matter* **17** S1–S174

David A Keen and László Pusztai