

Version xxx: 22 September 2006
(still may be changing!)

Programme of the 3rd RMC Conference (RMC-3)
'THE FIRST 18 YEARS OF REVERSE MONTE CARLO MODELLING'
(26-)28-30 September, 2006
Hotel Normafa, Budapest, Hungary

26 September (Tuesday)

Reverse Monte Carlo tutorial, organised by L. Pusztai (Hotel Normafa)

We meet in the Hotel lobby at 1:00 pm.

Lecture(s) - practical introduction (the method, algorithm details, possible applications)
(L. Pusztai)

27 September (Wednesday)

09:00 Morning session: *How to run RMC? Demonstration of several applications (basic RMCA; molecular systems; the new C++ code)*
(L. Pusztai and Co.)

13:00 Lunch (in the Hotel)

14:30 Afternoon session: *Disorder in crystals: modelling total scattering data using RMC methods* (under the supervision of Matt Tucker (ISIS, UK))

28 September (Thursday)

08:50 Opening and introduction (L. Pusztai, RISSPO HAS, Budapest)

09:00 Pál JÓVÁRI (RISSPO HAS, Hungary): On the structure of some covalent glasses: neutron and X-ray diffraction and EXAFS + RMC modelling

09:45 Toshio KAWAHARA (University of Osaka, Japan): Possibility of Reverse Monte Carlo Modelling of Amorphous Si Deposited on the Reactive Ion Etched Si Substrate

10:15 Erzsébet SVÁB (RISPPPO HAS, Hungary): Network structure of multi-component borosilicate waste glasses from high Q neutron diffraction study and RMC modelling

10:45 Coffee (and first glimpses at the POSTERS!)

11:15 Takashi ARAI (National Defence Academy, Japan) Structural changes of c/a-Ge₂Sb₂Te₅ due to RMC analysis with EXAFS and XRD data

11:45 Sándor KUGLER (TU Budapest, Hungary): Amorphous selenium – molecular dynamics vs. RMC (... exact title to be announced...)

12:15 János LÁBÁR (RITPM HAS, Budapest): Electron diffraction: a possible open field for structural modelling?

13:00 Lunch

14:30 Matt TUCKER (ISIS, UK): Determining disorder in crystalline materials using RMCprofile

15:00 Martin DOVE (Cambridge Univ., UK): Understanding substitutional disorder in perovskites

15:30 Dave KEEN (ISIS, UK): Local structural disorder associated with negative thermal expansion and piezoelectricity

16:00 Coffee with POSTERS (Posters by Shuta TAHARA (JAP), László TEMLEITNER (HU), Ivan KABAN (D), Joanna ROPKA (CH), Ádám LŐRINCZI (RO), Viviana CRISTIGLIO (F), Szilvia POTHOCZKI (HU), Thor WIKFELDT (S), Yixin CHEN (UK), Vicky FITZGERALD (UK), Katsumi HAGITA (JAP), Gergely TÓTH (HU), Helen THOMPSON (UK), Margit FÁBIÁN (HU), ...)

17:00 Andrew GOODWIN (University of Cambridge, UK): Lattice and spin dynamics from diffraction

17:30 Simon BILLINGE (Michigan State University, USA) Real Space Rietveld and other PDF profile refinement strategies

29 September (Friday)

09:00 Gergely TÓTH (Eötvös University, Hungary): Interactions from structural data: historical overview of simulation assisted methods

09:30 Alan SOPER (ISIS, UK): Empirical potential structure refinement: where it came from, what it does, and why

10:15 Sylvia McLAIN (ISIS, UK): The structure of amino acids in aqueous solution: A combined neutron diffraction and empirical potential structure refinement study

10:45 Coffee

11:15 Ildikó HARSÁNYI (RISSPO HAS, Hungary) The structure of aqueous Rb and Cs salt solutions by RMC modelling

11:45 Barbara Gabrys (University of Oxford, UK): On the structure of liquid phosphorous tribromide (PBr₃)

12:15 László TEMLEITNER (RISSPO HAS, Hungary): The structure of fluid phases of carbon dioxide (CO₂)

13:00 Lunch

14:30 László PUSZTAI (RISSPO HAS, Hungary): Water structure: do polarised neutrons help?

15:00 Yukinobu KAWAKITA (Kyushu University, Japan) RMC analysis of the local structure of eutectic liquid alloys between noble metals and IVb elements

15:30 Coffee with POSTERS

16:30 Discussion (proceedings, RMC-4 (!!))

17:30 ... free slots ... (or maybe a FREE EVENING ???)

30 September (Saturday)

09:00 Orsolya GEREBEN (HU): RMCT – modelling the dynamic structure factor via RMC methods

09:45 Frederick BERNARDIN (MIT, USA): ...title to be announced later..

10:15 Per ZETTERSTRÖM (CSIC, Spain): A study of nano-porous carbon using neutron diffraction and RMC

10:45 Coffee

11:15 Sascha Gruner (TU Chemnitz, Germany) Determination of partial structure factors in multi-component alloys

11:45 ... (possible) free slot

12:15 Robert McGREEVY (ISIS, UK): RMC: past, present, future (Conference summary)

13:00 CLOSING and lunch