whatever means has been in focus. A dramatic step forwards was due to Ada Yonath 1980 when she managed to get the first crystals of ribosomal subunits. Numerous improvements of methodology and crystals led to the first structural results 1998. Year 2000 high resolution structures of both subunits became available and the year after a medium resolution structure of the whole ribosome. This has made the whole field flourish both biochemically and structurally like for all fields where the central molecules have been clarified by crystallography.

KN-6

The European spallation source ESS. Colin Carlile (Lund/SE)
E-Mail: colin.carlile@esss.se

KN-7

From hot to cool and more for less: new developments for Structural Biology. Elspeth F.Garman, *Department of Biochemistry, University of Oxford, South Parks Road, OXFORD, OX1 3QU, U.K.*
E-mail: elspeth.garman@bioch.ox.ac.uk

Structural biology relies on X-ray crystallography to provide much of the three dimensional information on macromolecules that informs biological function. To enable problems not previously accessible to structure solution to be tackled, improved methods must be developed. A notable example of this has been the progress in finding protocols to cryocool protein crystals prior to 100K data collection to reduce the rate of radiation damage by around a factor of 70 compared to that at room temperature (RT): from hot to cool and more for less. Radiation damage to the sample is an inherent problem when utilising ionising X-radiation in macromolecular crystallography (MX), and it is now known that radiation damage can also be a limiting factor for MX at 100K [1]. Following our measurement of 30 MGy (1 Gy =1 J/kg energy absorbed) for the experimental dose limit for 100K [2] protein crystals, we tried to determine a limit for RT samples. The unexpected discovery of an RT inverse dose rate effect over a limited dose rate range [3] led us to search for RT scavengers [4], which in turn has elucidated the radiation chemistry induced in protein crystals when irradiated at 100K. Current ongoing methods investigations that will be described include studies of 100K and RT radiation damage in macromolecular crystals in order to inform both our understanding and putative mitigation strategies, and the trace elemental analysis of liquid and crystalline proteins using microPIXE (particle induced X-ray emission), allowing determination of their stoichiometric ratio to an accuracy of between 10 and 20% [5].

[1] Ravelli, R.B.G.; Garman E.F *Current Opinion of Structural Biology* 2006, 16, 624-629. [2] Southworth-Davies, R.J.; Medina, M.A.; Carmichael, I.; & Garman, E.F. *Structure* 2007, 15**,** 1341-1351. [3] Owen, R.L.; Rudiño-Piñera, E.; Garman, E.F. *Proc. Nat. Acad. Sci.* 2006, 103, 4912-4917. [4] Barker, A.I.; Southworth-Davies, R.J.; Paithankar, K.S.; Carmichael. I.; Garman, E.F. *Journal Sync Rad.* 2009**,** 16, 205-216. [5] Garman, E.F.; Grime, G. *Progress in Biophysics and Molecular Biology* 2005, 89/2, 173-205.

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KN-8

Single Crystal Diffraction Studies at Multimegabar Pressures. Malcolm McMahon, *SUPA, School of Physics & Astronomy, and Centre for Science at Extreme Conditions, The University of Edinburgh, UK.*
E-mail: mim@ph.ed.ac.uk

By the late 1990s, it was clear that the structural complexity induced in simple materials by compression was such that powder-diffraction methods were no longer able to solve complex structures being observed. While single-crystal techniques offer the ability to solve such structures, attaining the necessary high-quality samples at pressures above 20 GPa, perhaps after passing though one or more phase transitions, is extremely difficult. But the remarkable behaviour of the alkali metals Li and Na at extreme pressures, coupled with techniques developed at the SRS and ESRF synchrotrons, has enables us to push single-crystal techniques first to 100 GPa [1] and, most recently, to 145 GPa [2]. We have found previously unimagined structural complexity in both Na and Li [3], and have also been able to collect high-quality data from weakly scattering samples such oxygen [4] and nitrogen [5], including at both high- and low-temperature studies.
In this talk I will review both the new techniques, and the results we have obtained recently on these simple systems. I will also look to the future, and give some pointers as to the kind of crystallographic experiments that might be conducted on the next, "4th", generation of light sources.

[1] McMahon, M.I.; Gregoryanz, E.; Lundegaard, L.F.; Loa, I.; Guillaume, C.; Nelmes, R.J.; Kleppe, A.K.; Amboage, M.; Wilhelm, H.; Jephcoat, A.P.; *Proc. Nat. Acad. Sci.* 2007 104, 17297. [2] Lundegaard, L.F.; Gregoryanz, E.; McMahon, M.I.; Guillaume, C.; Loa, I.; Nelmes, R.J.; *Phys. Rev. B* 2007 79, 064105. [3] Gregoryanz, E.; Lundegaard, L.F.; McMahon, M.I; Guillaume, C.; Nelmes, R.J.; Mezouar, M.; *Science* 2008 320, 1054. [4] Lundegaard, L.F.; Guillaume, C.; McMahon, M.I.; Gregoryanz, E.; Merlini, M.; *J. Chem. Phys*. 2009 130, 164516. [5] Stinton, G.W.; Loa, I.; Lundegaard, L.F.; McMahon, M.I.; *J. Chem. Phys*. 2009 131, 104511.

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KN-9

Symmetry breaking in complex molecular assemblies. Jürg Hulliger, *Department of Chemistry and Biochemistry, University of Berne, Switzerland*
E-mail: juerg.hulliger@iac.unibe.ch

A mechanism leading to effects of symmetry breaking in the solid state results from the fact that at the nutrient-crystal interface incoming building blocks interact under the influence of a lower symmetry [1] than in the bulk. In case the attachment state shows kinetic stability, symmetry breaking in particular growth sectors can occur. A process most investigated during the last ten years [2, 3] is 180° orientational disorder of incoming dipolar molecules. Because of selective recognition at growing surfaces, this kind of symmetry breaking can lead to polar property formation. The lecture is reviewing the field, including examples from supramolecular crystals, single component and solid solution molecular materials. Because of generality, the theory applies also to the formation of polar tissues [4].