CSP methods generate hundreds or thousands of candidate crystal structures among which the structures that can be found experimentally are hopefully present. Usually the energy and density corresponding to predicted structures are guidelines for identifying polymorphs that are likely to be found. In many cases, however, these properties do not point unambiguously to the true structures.

When the true structure is known the set of predicted structures can be analyzed and verified by comparing the crystal structure data of true and predicted structure. For unknown crystal structures this is of course not possible. The only way to compare the predicted set of structures with reality is to match other experimental data (than crystal structure data) with theoretical data that can be deduced from a crystal structure model.

If an experimental powder diffraction pattern (PXRD) is available, this information can be used to select the true structure by comparing it to the simulated patterns of the predicted structures. A complication in doing so is that force fields often tend to induce (anisotropic) deformations in predicted structures, resulting in deformed simulated powder patterns. Powder pattern comparison is then far from straightforward: the true structure can be "hidden" in the predicted set or wrong structures can be selected by mistake.

The program IsoQuestCSP was developed to deal with this problem. It converts a set of predicted structures to a set of PXRD descriptors, compares an experimental pattern with this PXRD descriptor database and generates similarity matrices for predicted sets (suitable for cluster analysis) in an automated fashion. In this way the predicted structures can be analyzed in terms of structural diversity and candidates can be selected that are identical or close to the true structure.

Crucial to the success of the method is applying crosscorrelation functions in combination with (an)isotropic scaling.[1,2] The method is demonstrated for sets of predicted amino acid structures.

[1] R. de Gelder, R. Wehrens, J. Hageman *J. Comp. Chem.* **2001**, *22*, 273-289.
[2] R. de Gelder, *IUCr CompComm Newsletter*. **2006**, *7,* 59-69.

Keywords: crystal structure prediction, powder pattern comparison, structure determination

MS.07.1

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Pulsed neutron sources for neutron crystallography: new and future capabilities

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The last 5 years have seen a remarkable increase in the capabilities of pulsed neutron sources around the world. Although some smaller, older sources have closed (KENS, IPNS), they have been replaced by larger and more powerful facilities - SNS in the USA [1], MLF at J-PARC in Japan [2] and ISIS TS2 in the UK [3]. Within the next ten years there is the prospect of the world's first long pulse neutron source – the ESS in Sweden [4] – coming into operation. This presentation will review these new sources and their capabilities for diffraction studies of a range of materials including crystalline, disordered and large scale structures. It will also review the prospects for future development of both sources and techniques and the challenges that will be faced.

[1] http://neutrons.ornl.gov/facilities/SNS [2] http://j-parc.jp/MatLife/en/index.html [3] http://www.isis.stfc.ac.uk/about-isis/target-station-2 [4] http://ess-scandinavia.eu

Keywords: neutron, source, diffraction

MS.07.2

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Investigation of nanometer structures with soft X-ray FEL radiation at FLASH

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FLASH, the free electron laser (FEL) facility at DESY in Hamburg, is the first FEL for the vacuum ultraviolet and soft X-ray region in regular user operation. It is based on a superconducting linear accelerator that produces the high-density, low-emittance electron bunches required for driving the FEL. Since 2005, FLASH provides extremely bright, coherent light pulses which can be as short as 10 femtoseconds. After two upgrades in 2007 and 2009/10, FLASH covers a spectral range from 47 – 4.1 nm wavelength, i.e. it reaches the so-called water window which allows investigating biological samples with high contrast in their aqueous environment. These unique beam properties have allowed exploring new fields of science, such as non-linear processes in atoms and molecules, ultrafast electronic and magnetic phenomena in solids, and single-pulse imaging of biological samples or nanostructures.

This contribution gives an overview of the FLASH facility and its user programme, with an emphasis on structural investigations.

Keywords: free_electron_laser, soft_X-rays, X-ray_imaging

MS.07.3

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Linac Coherent Light Source: Status and Plans for Expansion†

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The Linac Coherent Light Source at SLAC is the first "hard" x-ray free-electron laser, providing x-rays in the spectral range 500-10,000 eV [1]. Experiment operations began in October 2009. LCLS will provide x-rays to six experiment stations, four of which are already in operation. Two of the four have been used for x-ray imaging of nanocrystals and single cells. Early results are very promising [2], [3]. The Department of Energy has approved a concept for a major expansion of the facility (the LCLS-II Project), to increase capacity and to expand its spectral coverage to 250-13,000 eV [4]. The upper end of the range was chosen to enable MAD techniques for structure determination. The presentation will report latest performance and results from LCLS and latest plans for the LCLS-II Project.

[1] P. Emma, et al., *Nature Photonics 4*, 641. [2] H.N. Chapman, et al., *Nature* **470**, 73–77. [3] J. Hajdu, et al., *Nature* **470**, 475-476. [4] Linac Coherent Light Source II Conceptual Design Report, https://slacspace.slac.stanford.edu/sites/slac_sci_controlled/PublishedLibrary/Controlled%20Documents/%5B060-003-000-00_LCLSIICDR_Index%5D.pdf

Keywords: free, electron, laser

MS.07.4

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X-ray layout and radiation properties of the European XFEL

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Following recent advances in the development of photo-injectors [1] and analysing results obtained at the Linac Coherent Light Source at SLAC, Stanford, U.S.A. [2], the electron beam parameters for the European XFEL accelerator have been refined. Variation of the electron bunch charge between 20 and 1000 pC and compression to nearly constant peak currents of order 5 kA allows at the same time to obtain very small normalized emittances between 0.4×10^{-6} and 1.0×10^{-6} m.rad, respectively. The x-ray pulse duration scales nearly linear with bunch charge from 2 to 107 fs. Analyzing the needs of the prioritized scientific instruments of the European XFEL showed that all hard x-ray instruments require the possibility to select the photon energy in a minimum range from 5 – 15 keV. Furthermore there have been strong requests to extend the photon energy to as small as 3 keV and to as high as beyond 20 keV. Simulations using the new electron beam parameters and a magnetic length of the undulators of 175 m with a period of 40 mm indicate that it should be possible to provide FEL radiation in the fundamental for this range and possibly beyond. For the two prioritized soft x-ray experiments an energy tunability from below the carbon K-edge up to 3 keV is desirable. Simulations indicate that an undulator with a magnetic length of 100 m and a period of 68 mm allows reaching saturation at 3 keV even in cases where the electron bunch has acquired additional energy spread of up to 15 MeV due to the SASE FEL process occurring in the preceding undulator. Parallel operation of three undulators and three scientific instruments is enabled by operation of the electron accelerator at defined energy working points of 10.5, 14.0 and 17.5 GeV. These energies enable optimized operation at soft and very hard x-rays, respectively. Tuning the photon energy for individual instruments is achieved by gap tuning of the undulators.

Simulation of the FEL radiation properties at saturation indicates that the peak brilliance is nearly constant for different bunch charges due to compensating effects in the variation of pulse duration and pulse energy. The pulse energy, number of photons per pulse and also the average brilliance increase with increasing bunch charge. In contrast, the degree of transverse coherence depends strongly on the emittance and decreases with increasing bunch charge. The full set of FEL parameters at saturation can be found in [3]. Operating the FEL sources deeply beyond saturation will increase the x-ray pulse energy, but may also affect other parameters like divergence, bandwidth, or degree of transverse coherence.

The x-ray layout foresees three scientific instruments per FEL source. In a first phase two of these will be built. FEL radiation will be steered by means of ultra-grazing incidence mirrors to them. Initially one instrument per FEL source and at a given time will receive beam. Each FEL beam transport will include a two mirror system off-setting the beam and a further mirror for deflection to the side station. Technical designs for beam focussing and allowing optional usage of monochromators are currently worked upon.

[1] S. Rimjaem et al., *Proceedings of FEL2010 conference,* Malmö, Aug 23-27, **2010**, 410-413. [2] P. Emma et al., *Nature Photonics* **2010**, *4*, 641-647. [3] E.A. Schneidmiller, M.V. Yurkov, *DESY Print TESLA-FEL* **2011**, *2011-01.*

Keywords: x-ray, synchrotron, coherence.

MS.07.5

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A multi-purpose neutron diffractometer at the ILL: the state-of-the-art of D19

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D19 is a four-circle monochromatic diffractometer installed on the thermal guide H11 at the Institute Laue-Langevin. It is a unique instrument that combines an intense thermal beam, a flexible monochromator/optical arrangement and a 120º horizontal by 30º vertical position sensitive ^{3}He detector, to produce a diffractometer that is easily optimised for neutron diffraction studies of large chemical systems, fiber diffraction studies of natural and synthetic polymers, and crystallographic studies of small molecular systems. The total refurbishment of the instrument, funded by EPSRC, was completed in 2007. Since then, D19 has been producing valuable data in both fundamental research and industrial applications. The new challenges that face D19 include: faster data acquisition (e.g. optimisation of the strategy for sampling reciprocal space), measurement of smaller and smaller samples and new sample environments (for example a N_2-cryostream for moderately low temperature measurements).

In order to illustrate the spread of science that can be studied on D19 few examples will be presented: i) the role of metal ions and hydrogen atoms in the reaction of D-xylose isomerase with sugar; ii) hydrogen bonds dynamics of ammonia on cellulose; iii) binding coordination and dynamics of dihydrogen ligands in transition metal catalytic systems; iv) the study of texture in submarine rocks.

Keywords: instrumentation, neutron, diffraction

MS.08.1

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The recognition of endocytic signal sequences by the AP2 complex

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Membrane proteins are packaged for transport between the different membrane compartments of eukaryotic cells into small vesicles formed by an elaborate system of cytoplasmic proteins. Selection of cargo for vesicle formation at the plasma membrane (endocytosis) is generally mediated directly or indirectly by the heterotetrameric clathrin adaptor complex AP2, which binds short sequence recognition motifs of two types, YxxΦ (tyrosine-based motif, where Φ is a hydrophobic residue) and [DE]xxxLL (acidic dileucine motif). The structure of the 200kDa AP2 "core" crystallised in the absence of peptides showed a closed conformation, with binding sites for both types of motifs blocked, and indeed AP2 in solution does not bind motif peptides. AP2 is activated by binding to negatively charged membranes containing phosphatidylinositol-(4,5)-bisphosphate. We were able to trap the activated "open" conformation in crystals grown with a YxxΦ peptide, and this structure shows a large conformational change compared to the closed "locked" conformation, with the YxxΦ-binding domain moving out of the "bowl" formed by the other subunits. This places both peptide sites on the positively-charged face of the complex, allowing simultaneous interaction with cargo motifs and the membrane. Thus AP2 functions as a plasma membrane-activated switch for endocytic cargo recognition.

[1] L.P. Jackson, B.T. Kelly, A.J. McCoy, Th. Gaffry, L.C. James, B.M. Collins, S. Höning, Ph.R. E., D.J. Owen *Cell* **2010**, *141,* 1220–1229.

Keywords: membrane associated proteins, protein-peptide interactions, conformational change