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

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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

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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

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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

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X-ray layout and radiation properties of the European XFEL

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