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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.

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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

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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.

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