with data to 2.5 Å or better.

Xsolve, a Java Message Service (JMS) based control system, can run on a Linux cluster different processing strategies in parallel, e.g. the data can be processed in several different space groups or MAD/SAD structure determination can be attempted using various wavelength combinations.

Xsolve supports a wide range of crystallography software programs, which can be used in parallel: data reduction with Mosflm, Denzo/HKL2000, XDS and Scala; heavy atom solution and phase determination with Solve, SHELXD/E and Sharp; phase improvement with Resolve and model building with Resolve and ARP/wARP.

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Keywords: automatic structure solution, MAD, software

MS41.26.3

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Iterative Model Building and Evaluation with Statistical Density Modification

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Automated model-building beginning with an FFT-based search for helices and sheets and followed by chain extension using tripeptide fragments from high-resolution structures and pattern-based probabilistic identification of side chains has been successful in automated model building for maps with resolution as low as 3 A. Model-building can be combined with refinement and statistical density modification to improve the quality and completeness of atomic models of macromolecules and to evaluate the quality of atomic models. A useful tool in removing model bias is prime-and-switch phasing. In this technique a substantially correct model containing some atoms in incorrect positions is used to estimate ("prime" initial phases, and a second source of phase information such as a flat solvent region is used without reference to the original phase probabilities in density modification. After prime-and-switch phasing the density at incorrect atomic positions is often considerably decreased compared to that at correct positions. This technique has been incorporated as an integral part of iterative model-building and refinement in the PHENIX software (http:www.phenix-online.org).

Keywords: model building, PHENIX, atomic models

MS41.26.4

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Automated Operation of Protein Crystallography Beamlines at the SPring-8

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RIKEN Structural Genomics Beamlines (BL26B1&B2) at the SPring-8 have been constructed for high throughput protein crystallography. The beamline operation is automated cooperating with the sample changer robot named SPACE (SPring-8 Precise Automatic Cryo-sample Exchanger) [1].

Since April 2004, BL26B2 has been continuously operated with the sample changer. More than twenty-five crystals a day have been constantly delivered by sample-tray to the beamline. The crystal screening at the beamline can be finished within ten minutes per a sample. For qualified crystals, unattended data collections have been perpetually performed. The sample-tray is portable with a Dewar and experimental conditions are uploaded to the web site, which have been developed considering the mail-in data collection.

The operation software BSS (Beamline Scheduling Software) provides the intuitive GUI and unified control of beamline instruments with the networked client-server architecture. The software structure has flexibility to be implemented at other protein crystallography beamlines. Other than BL26B1 and B2, three other beamlines have already adopted BSS. Further application to other beamlines is progressing to achieve the unified and user-friendly environment among all beamlines at the SPring-8.

[1] Ueno G., Hirose R., Ida K., Kumasaka T., Yamamoto M., *J. Appl. Cryst*.,2004, **37**, 867-873.

Keywords: automated data collection, high-throughput protein crystallography, mail-in data collection

MS41.26.5

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Automated Protein Structure Determination with *BnP*

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BnP[1] is a protein structure determination package with a graphical user interface suitable for both manual and automated operation. *BnP*'s main function is to couple the direct-methods program *SnB*, used to determine heavy atom/anomalous scatterer substructures, with the protein-phasing package *PHASES*, used for heavy atom refinement, protein phasing, density modification, and skeletonization. It also creates data and scripts for external programs required for automated chain tracing, graphical visualization, and refinement. In addition to seamlessly interfacing the various packages, near total automation is implemented such that one needs only to specify a few parameters, and the entire phasing process starting with diffraction data and resulting in interpretable electron-density maps is carried out by clicking a single button. With a couple of additional button clicks external programs for automated chain tracing or chain tracing/refinement can then be launched. The overall strategies and methodology employed will be described, with emphasis on those aspects required to facilitate automation and recent developments simplifying user input. Extensive test results verify the package's effectiveness. This work was supported by NIH grant EB002057.

[1] C. M. Weeks et. al., *Z. Kristallogr*., 2002, **217**, 686-693.

Keywords: automated structure determination, high-throughput, phasing methods

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MS42 COMPLEMENTARITIES OF NEUTRON AND X-RAYS METHODS IN MATERIAL SCIENCE

Chairpersons: Andreas Schreyer, Mark R. Daymond

MS42.26.1

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Integrated Use of Synchrotron and Neutron Diffraction to Monitor Residual Stress Evolution in Welded Aerospace Structures

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The factors controlling fatigue initiation and crack growth in welds are reasonably well understood and the importance of residual stress, HAZ hardness and microstructure is well known. However, previous access to reliable, spatially accurate residual stress field data has been limited. Recent advances in neutron and synchrotron diffraction allow a far more detailed picture of weld residual stress fields to be obtained which permits the development and use of predictive models that can be used for accurate design against fatigue in aircraft structures. This paper describes a fully integrated study of the 3D residual stress distribution accompanying state-of-the-art fusion welds in 2024 and 7150 aluminium aerospace alloys, and how they are affected by subsequent machining and service loading. A particular feature of this work has been the development of integrated neutron and synchrotron techniques allowing the non-destructive evaluation of the residual stress field in the full range of specimens used to provide the design data required for welded aircraft structures. This has included small bend specimens used to study initiation and short fatigue crack growth, centre-cracked panels used to study long fatigue crack growth, and large integral welded double stringer/skin mock-ups used to investigate the likely failure mode of welded wing-

skin assemblies.
Keywords: residual stress, welded structures, aerospace alloys

MS42.26.2
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Crystallographic Texture of Semi-finished Products
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Texture measurement is widely used to characterize any type of materials such as metals, ceramics and rocks. In the case of industrial applications not only the texture of the material itself described in the three dimensional orientation space is of importance but also texture gradients in real products. Commonly used techniques are based on sample destruction to prepare a set of ideal samples for a diffraction experiment, see for instance the EBSD orientation stereology by Bunge and Schwarzer [1] or the texture mapping of melt grown YBaCu samples by Jung and Brokmeier [2]. The investigation of semi-finished products or real components has to be carried out sometimes non-destructively. Thus, a beam with a high penetration power is necessary available at neutron or synchrotron sources. A number of experiments have been done at TEX-2 the neutron texture diffractometer at GeNF (GKSS-Research Center Geesthacht, Germany) and at the high energy beam line BW5 at HASYLAB (DESY, Hamburg, Germany). Due to the grains size, the sample geometry and the scattering behavior one has to use hard X-rays or neutrons to investigate tubes, rings, extrusion profiles, turbine blades, implants, etc.

[1] Bunge H.J., Schwarzer R.A., *Advanced Engineering Materials*, 2001, **3**, 25.
[2] Jung V., Brokmeier H.-G., *Crystal Research and Technology*, 2000, **35**, 321.
Keywords: texture analysis, neutron diffraction, synchrotron X-ray diffraction

MS42.26.3
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Dynamic Diffraction Effects in X-ray and Neutron Stress Analysis
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We present time-of-flight neutron and x-ray diffraction data from thick perfect Si single crystal samples showing dynamic double diffraction effects associated with finite crystal size. In this mode constructive interference occurs solely from thin layers bounded by the front (entry) and back (exit) surfaces of the sample with no scattering originating from the layers in between. This results in two distinct peaks for each reflection. If the instrument resolution is insufficient, these two peaks convolve and cause peak-shape aberrations which can cause significant errors in parameters obtained from diffraction analysis.
Keywords: dynamic diffraction, single crystals, stress analysis

MS42.26.4
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Charge Ordering and Magnetic Structure in Fe_3BO_5
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The structure of $(Fe^{2+})_2(Fe^{3+})O_2BO_3$ ludwigite (space group Pbam, a=9.462Å, b=12.308Å, c=3.075Å) is made of zigzag walls of edge-sharing FeO_6 octahedra, connected by BO_3 triangular groups. It contains two types of 3-leg ladders of Fe cations: ladder 1 with only Fe^{2+} cations and ladder 2 formed by Fe^{3+} cations with one additional electron per rung delocalized at high temperature. This leads to a quite complex physical behavior. Two magnetic ordering transitions are observed at 112K and 70K. Specific heat shows a plateau between ≈100K and 250K, and a change of slope of resistivity is observed close to room temperature. Using single crystal x-ray diffraction, we have shown that it is due to a partial localization of the Fe 3d electrons on ladder 2, accompanied by a superstructure doubling the c-axis.

We report here the investigation of the magnetic ordering, using neutron powder diffraction on I.L.L. D20 between 300K and 10K. Based on the superstructure found with x-rays, both magnetic structures were solved and refined by the Rietveld technique. Between 70K and 110K, only ladder 2 is ordered. The coupling is ferromagnetic in the rungs and antiferromagnetic between them. At 70K, ladder 1 orders as a canted antiferromagnet in the rungs which are ferromagnetically coupled. This also leads to a partial reorientation of the spins of ladder 2. A strong magnetic background increasing from room temperature to 110K could be related to short range correlations in both magnetic sub-units.
Keywords: magnetic structure determination, superstructure, spin ladder

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Determining Pb/Bi Distributions using High-Energy Resonant Scattering at K Edges
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Powder diffraction data collected at just below both the Pb and Bi K edges (88.005 keV and 90.526 keV respectively), and ~86 keV on an imaging plate detector have been used to examine the Pb/Bi distribution over the 11 crystallographically distinct sites in $Pb_5Bi_6Se_{14}$. Specialized x-ray optics with excellent energy resolution and stability were used for the experiment. Even with the relatively low scattering contrast that is available at the K edges, it was possible to determine the Pb/Bi distribution and probe the presence of cation site vacancies in the material. The current results indicated that resonant scattering measurements at high-energy K edges are a viable, and perhaps preferable, route to site occupancies when neutrons provide insufficient contrast and absorption from the sample or sample environment/container is a major barrier to the acquisition of high-quality resonant scattering data at lower energy edges.
Use of the Advance Photon Source was supported by the U.S. Department of Energy, Office of Sciences, Office of Basic Energy Sciences, under Contract No. W-31-109-Eng-38.
Keywords: synchrotron powder diffraction, anomalous scattering method, high-energy X-ray diffraction