ESS Science Symposium 2014

Future Engineering Diffraction Research in Materials Processing and Testing

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November 17-18, 2014,
Vila Lanna, Prague, Czech Republic

Organised by
Institute of Physics of the ASCR

Program and Abstracts

Program

Day	Time	Speaker	Talk title	Topic
	11.00-13.00	**Welcome**		
Monday, Nov 17	13.00-13.10	Petr Lukáš	Welcome and ESS project update	ESS and BEER diffractometer update Chair: P.Šittner
	13.10-13.25	Michelle Everett	ESS instruments update	
	13.25-13.40	Andreas Schreyer	BEER project update	
	13.40-14.00	Jan Šaroun	BEER diffractometer update – neutron optics	
	14.00-14.20	Jan Pilch	BEER diffractometer update - sample environment for in-situ experiments	
	14.20-14.40	Jochen Fenske	BEER diffractometer update - sample environment for other experiments	
	14.40-15.05	**Questions & Discussion on BEER project** **Chair:** Helena Van Swygenhoven-Moens		
	15.05-15.30	Florian Pyczak	TiAl Research with photon and neutron sources – present and future	Material testing experiments Chair: P.Staron
	15.30 -15.55	David Rafaja	Stacking fault energy determination by using in situ diffraction	
	15.55 -16.20	Tobias Panzner	In-situ biaxial mechanical testing at the neutron time-of-flight diffractometer POLDI	
		COFFEE BREAK		
	16. 50-17.15	Christian Máthis	Exploring deformation mechanisms in magnesium alloys using in-situ neutron diffraction and acoustic emission techniques	
	17.15-17.35	Andreas Stark	In situ synchrotron experiments using a quenching and deformation dilatometer	Material processing experiments Chair: P.Strunz
	17.35-18.00	Grzegorz Korpała	Experimental modelling and numerical interpretation of experiment using GPU-calculation	
	18.00-18.25	Debashis Mukherji	Measurement with neutron and synchrotron helps high temperature Co-Re alloy development	
	20.00-22.00	**ESSS Dinner**		

The European Spallation Source

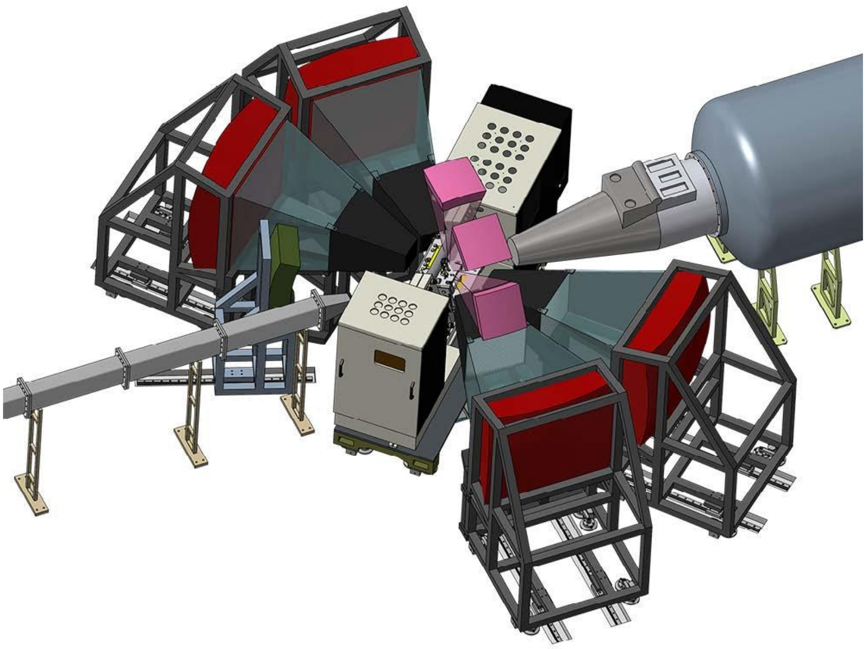
http://europeanspallationsource.se/

The Beamline for European Engineering Materials Research (BEER)

Nuclear Physics Institute ASCR, Czech Republic

Helmholtz-Zentrum Geesthacht, Germany.

Tuesday, Nov 18	9.00-9.25	Shu Yan Zhang	Neutrons for Materials Science and Engineering Research at ISIS: Recent studies and future possibilities	Research at TOF diffractometers Chair: P. Beran
	9.25-9.50	Ke An	Fatigue Deformation Behavior of HCP Alloys by Real-time in-situ Neutron Diffraction	
	9.50-10.15	Stefanus Harjo	Trials of in-situ materials processing at TAKUMI	
		COFFEE BREAK		
	10.45-11.10	Arne Kromm	Capabilities of Diffraction Techniques in Welding Research	In-operandi experiments Chair G. Nowak
	11.10-11.35	Anatoliy Senyshyn	In situ neutron scattering on Li-ion batteries	
	11.35-12.00	David Dye	SANS, SAXS and synchrotron X-ray studies in super elastic Beta-Ti alloys	
	13.00-12.25	Michael Preuss (**via Internet**)	In situ studies of texture evolution during heat treatment of Ti alloys	
		LUNCH		
	14.00-14.25	Luca Lutterotti	Rietveld Texture Analysis of Materials by Neutron Diffraction	Methods for reconstruction of microstructure info. Chair M.Strobl
	14.25- 14.50	Michael Wedel	Neutron time of flight data analysis at POLDI: implementation in Mantid	
	14.50-15.15	Soren Schmidt (**via Internet**)	Tbd.	
	15.15-15.40	Robin Woracek (**via Internet**)	Applications of neutron Bragg edge imaging & torsional deformation studies using neutron diffraction	
	15.40-16.05	Aaron Stebner (**via Internet**)	In-situ neutron diffraction for advancing constitutive models of shape memory alloys	
	16.05-16.30	**Discussion and Closure of the Symposium** **Chair:** Marcus Strobl		



Materials Engineering Diffractometer BEER for ESS

Abstracts

TiAl Research with photon and neutron sources – present and future

Florian PYCZAK, Li WANG, Marcus RACKEL, Andreas STARK, Andreas SCHREYER
Helmholtz-Zentrum Geesthacht, Germany
Monday 15.05-15.30

TiAl alloys are new lightweight materials for high temperature applications. Nevertheless, phase constitution, microstructure formation and their effects on properties are far from understood. Diffraction by photons and neutrons, especially combined with in-situ specimen environments, is a powerful tool to shed light on until now unresolved questions of TiAl. The talk will present diffraction investigations of an additional orthorhombic phase in a high niobium TiAl alloy. It's character, parent phase and formation path were uncertain. Unambiguous phase identification may be helped by neutron and photon diffraction combined to benefit from different contrast mechanisms. Carbon improves the high temperature strength of TiAl alloys. Our investigations on carbide precipitation show how transmission electron microscopy (TEM) and diffraction complement each other. TEM is more sensitive to detect small carbides while diffraction can distinguish between carbide dissolution and rearrangement. Neutron diffraction can help to monitor such processes in specimens closer to the size of real components.

Stacking fault energy determination using in situ diffraction

David RAFAJA
Institute of Materials Science, TU Bergakademie Freiberg, Germany
Monday 15.30 -15.55

A method is presented, which determines the stacking fault energy in face centred cubic materials from a critical stress that is induced via sample bending in early stages of the plastic deformation and gauged by in situ diffraction methods during the sample bending. Furthermore, the method monitors the separation of partial dislocations and the corresponding triggering stress, and indicates the possible interactions between stacking faults present on equivalent lattice planes and the interactions of the stacking faults with other microstructure defects. The capability of the proposed method was tested on highly alloyed austenitic steels containing chromium (approx. 16 wt%), manganese (approx. 7 wt%) and nickel as the main alloying elements. For the steels containing 5.9 wt% Ni and 3.7 wt% Ni, the stacking fault energies of (17.5 +/- 1.4) mJ/m² and (8.1 +/- 0.9) mJ/m² were obtained, respectively.

In-situ biaxial mechanical testing at the neutron time-of-flight diffractometer POLDI

Tobias PANZNER
Paul Scherrer Institut, Switzerland
Monday 15.55 -16.25

Tbd.

Exploring deformation mechanisms in magnesium alloys using in-situ neutron diffraction and acoustic emission techniques

Kristián MÁTHIS, Jan ČAPEK, Bjorn CLAUSEN, Petr LUKÁŠ
Faculty of Mathematics and Physics, Charles University, Prague
Monday 16.50 -17.15

Having a hexagonal closed packed (hcp) structure and ratio of the crystallographic axes c/a close to ideal, the deformation behavior of magnesium alloys is rather different from other (e.g. fcc or bcc) metals. In the identification of the particular deformation mechanisms in magnesium the non-destructive in-situ methods play an important role. In this talk the potential of acoustic emission (AE) and neutron diffraction (ND) methods in study of deformation twinning and dislocation slip is presented. It is shown that the concurrent application of these two methods can result in a complex description of the dependence of the twinning mechanism on the experimental parameters (strain path, temperature etc.). Furthermore the activity of the various slip systems discovered by statistical analysis of AE waveform streaming data is discussed in detail.

In situ synchrotron experiments using a quenching and deformation dilatometer

Andreas STARK, Michael OEHRING, Florian PYCZAK, Marcus RACKEL, Andreas SCHREYER
Helmholtz-Zentrum Geesthacht, Germany
Monday 17.15-17.35

Thermo-mechanical treatments are well established metallurgical processes to improve mechanical properties. Several microstructure parameters change during processing like phase fractions or crystallographic texture. However with conventional analysis technics the changing mechanisms can only be inferred from post process metallographic studies in which the real high temperature conditions are often masked. We used a quenching and deformation dilatometer (DIL 805A/D) as an advanced engineering sample environment for in situ high-energy X-ray diffraction (HEXRD) experiments. This setup enables the continuous monitoring of the interaction and evolution of different microstructure parameters during processing, while simultaneously recording the process parameters. The talk will present results of several in situ HEXRD experiments using the dilatometer. For example the texture formation of a multiphase Nb-rich TiAl alloy was observed during hot forming in different phase fields.

Experimental modelling and numerical interpretation of experiment using GPU-calculation

Grzegorz KORPALA
Institute of Metal Forming TU Bergakademie Freiberg, Germany
Monday 17.35-18.00

Modern Graphic Processing Units (GPU) provide in combination with a very fast Video Random Access Memory (VRAM) very high computational potential, outrunning the conventional combination of a Central Processing Unit (CPU) and Random Access Memory (RAM) in terms of parallel computing and calculation. Numerical calculations based on a combined GPU/CPU approach have a big potential for use in material science, as a large amount of data can be calculated to investigate material phenomenon. A numerical GPU/CPU model is presented, which is based of models for diffusion, stress field and deformation. This model is used to calculate the flow curve testing by different models, such as tension, compression and torsion testing. The results of the numerical simulation are compared with experimental data, showing that the physically based GPU/CPU model is able to simulate those testing methods in detail with a good representation of physical phenomenon being also observer in the experiment.

Measurement With Neutron And Synchrotron Helps High Temperature Co-Re Alloy Development

Debashis MUKHERJI, Joachim RöSLER
Technische Universität Braunschweig, Institut für Werkstoffe, Germany
Monday 18.00-18.25

Amongst new alloy systems being developed to supplement Ni-superalloys in future gas turbines, the Co-Re alloy is a promising candidate. The alloy designed at TU Braunschweig in 2007 is presently being studied in a joint collaborative project with MLZ, Garching, Germany. The Co-Re alloys are stabilized by Ta and Cr carbides for creep strength. Cr also provides the resistance to oxidation and corrosion. The TaC phase with a much higher temperature stability than the Cr23C6 carbides forms the main strengthening precipitate. An important open question is how C is shared between the Cr and Ta carbides. In-situ measurements at high temperatures by synchrotron and neutron scattering are ideal tools to study these new alloys. In Co-Re alloy development program we use these tools extensively to study phase evolution and transformation. They are guiding the alloy development. Selected results of microstructural characterizations by neutron and X-ray measurements are presented here.

Neutrons for Materials Science and Engineering Research at ISIS: Recent studies and future possibilities

Shu Yan ZHANG, UK
ISIS, STFC
Tuesday 9.00-9.25

The Engin-X instrument at ISIS is a world leading neutron diffractometer purpose-built for stress evaluation in the context of materials science and engineering research. Over the past 11 years Engin-X has continually redefined the frontier of stress measurement capability through investment in state-of-the-art equipment to alter the conditions under which experiments are carried out. These include a rotation robot, furnaces, cryostats, and hydraulic stress-rigs for testing material performance under simulated in-service loading. Engin-X has attracted academic and industrial users to address a wide range of engineering problems. Some recent science highlights will be reviewed, including: assessment of fracture mechanics in collaboration with TWI, tomography driven diffraction, investigation of transformation plasticity in TRIP steels under cryogenic temperature, stress relaxation through ageing heat treatment, etc. In order to meet the user demand and increase our capability, we are developing new sample environments: tomography loading rig and long term creep rig. We are also looking for matching funding to build a new engineering beamline.

Fatigue Deformation Behavior of HCP Alloys by Real-time in-situ Neutron Diffraction

Ke AN
Oak Ridge National Laboratory, USA
Tuesday 9.25-9.50

Thanks to the high power of the Spallation Neutron Source, the deformation mechanisms of rolled HCP magnesium alloys were investigated under continuous cyclic loading using the real-time in-situ neutron diffraction. The relationship between the macroscopic cyclic deformation behavior and the microscopic response at the grain level has been established. The neutron diffraction results indicate that more and more grains are involved in the twinning and detwinning deformation process with the increase of fatigue cycles. The residual twins appear in the early fatigue life, which is responsible for the cyclic hardening behavior. The asymmetric shape of the hysteresis loop is attributed to the early exhaustion of the detwinning process during compression, which leads to the activation of dislocation slips and rapid strain hardening. In the cycle before the sample fractured, the dislocation slips became active in tension, although the sample was not fully twinned.

Trials of in-situ materials processing at TAKUMI

Stefanus HARJO
J-PARC Center, JAEA, Japan
Tuesday 9.50-10.15

TAKUMI is a TOF neutron diffractometer for engineering science at Materials and Life Science Facility of J-PARC. A new sample environmental device dedicated for material processing (thermec-mastor) has been developed in the collaboration between a research group in Kyoto University and TAKUMI, within a project of Elements Strategy Initiative for Structural Materials (Ministry of Education, Culture, Sports, Science and Technology). The basic design and the commissioning progress of the thermic-mastor will be briefly introduced together with hopefully the first neutron data. Preliminary results on a hot compression experiment of Fe-32Ni alloy using a standard load frame added with a halogen lamp furnace will be also introduced to show what we can expect from in situ neutron diffraction during materials processing.

Capabilities of Diffraction Techniques in Welding Research

Arne KROMM, Thomas KANNENGIESSER
BAM Federal Institute for Materials Research and Testing, Germany
Tuesday 10.45-11.10

Nowadays engineering calls for tailored materials used on their design limits featuring specific microstructures. Special material characteristics can be adjusted by complex thermo-mechanical processes. Nevertheless, welding of such structures is more and more challenging as a degradation of the material properties has to be avoided. This is the reason why welding calls for substantially improved understanding of the relationships between microstructure, residual stresses and cracking to evaluate the influence on the integrity of high performance joints. Examples will be presented showing how diffraction as well as tomography can be utilized for the characterization of diverse welding specific phenomena. The results show that in-situ techniques are an ideal tool for investigating microscopic as well as macroscopic behavior with the purpose of improving material models.

In situ neutron scattering on Li-ion batteries

Anatoliy SENYSHYN
Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany
Tuesday 11.10-11.35

Lithium-ion batteries are now considered the major energy storage media for portable electronics and electric vehicles. However despite its popularity the Li-ion technology possesses a number of drawbacks requiring systematic and research at real operating conditions. The neutron scattering (due to its unique and well-known advantages) is a well-suited tool for non-destructive studies of sophisticated electrochemical devices, like Li-ion batteries. In the current contribution the combination of three neutron-based techniques, namely computed neutron tomography, high-resolution and spatially-resolved neutron powder diffraction, applied for studies on commercial Li-ion cells of the 18650-type (with graphite and $LiCoO_2$ used as anode and cathode, respectively) will be presented. The details of the cell organization on different length scales and its evolution on state of charge and fatigue will be discussed along with the future needs for spatially-resolved diffraction.

SANS, SAXS and synchrotron X-ray studies in superelastic Beta-Ti alloys

David DYE
Imperial College, UK
Tuesday 11.35-12.00

Superelastic beta-titanium alloys are a class of alloys that can undergo a stress-induced phase transformation from the bcc phase to an orthorhombic martensite. However, these alloys may also be unstable with respect to the formation of the hexagonal close packed omega phase. Recent work on the Ti-Mo-Al-O system will be highlighted, showing how these alloys respond to deformation. Informed by the phenomenological theory of martensite transformations, it becomes clear that the stress-induced transformation will only be perfectly reversible if the interface strains are minimised, by matching the lattice parameters of the two phases. Unfortunately, this means that the dominant martensite peaks then perfectly overlap with the parent bcc peaks. To some extent, this can be mitigated through improved resolution, but in certain cases it will be shown that the orientation relationships can also be exploited. Separately, the in situ observation of omega formation will be examined using a combination of SAXS, SANS and atom probe to determine the omega volume fractions and compositions.

In situ studies of texture evolution during heat treatment of Ti alloys

Michael PREUSS
University of Manchester, UK
Tuesday 13.00-12.25 **Via internet**

Tbd.

Rietveld Texture Analysis of Materials by Neutron Diffraction

Luca LUTTEROTTI
University of Trento, Department of Industrial Engineering, Italy
Tuesday 14.00-14.25

Diffraction is one of the best techniques to obtain the full orientation distribution function (ODF) and with neutron we can study the texture of large, thick or complex objects. In particular neutron TOF are suitable for rapid collection times using multiple detector banks arranged spatially around the sample. The technique allows us to collect rapidly one entire spectrum per orientation and is well suited for an analysis based on inverse pole figures like the Rietveld texture analysis. In such case, instead of using full covered pole figures of few reflections, we make use of several reflections and few orientations. To obtain the ODF from the spectra using the Rietveld method we have two possibilities: in the first case we approximate the OD with some mathematical functions (spherical harmonics or standard functions) fitting their coefficients, in the second case we discretize the OD in cells using a suitable space and we derive the orientation probability of each cell (WIMV, EWIMV). We are going to present some special cases, problems and solution with neutron diffraction applied to texture analysis in material science, geology and cultural heritage fields.

Neutron time of flight data analysis at POLDI: implementation in Mantid

Michael WEDEL
Paul Scherrer Institut, Switzerland
Tuesday 14.25- 14.50

Tbd.

Tbd.

Soren SCHMIDT
Technical University of Denmark, Denmark
Tuesday 14.50-15.15 **Via internet**

Tbd.

Applications Of Neutron Bragg Edge Imaging & Torsional Deformation Studies Using Neutron Diffraction

Robin WORACEK, Dayakar PENUMADU
University of Tennessee Knoxville, USA
Tuesday 15.15-15.40 **Via internet**

The presentation will be twofold: The first part will describe the measurement of lattice strains under applied torsion (pure shear) and a combination of tension and torsion. This is accomplished using a (traditional) neutron diffractometer instrument, in conjunction with special alignment procedures and a specifically designed loading system. [Woracek et al., Appl. Phys. Lett. 100, 191904 (2012)]. The second part will highlight accomplishments and future needs for wavelength dependent neutron transmission imaging, which is capable of spatially resolving texture, crystallographic phase and lattice strain, by analysis of Bragg Edges. Examples will be given for spallation and reactor sources. Highlights include recent results, where a 3D tomographic reconstruction reveals phase fractions and inhomogeneities in samples exhibiting the TRansfomation Induced Plasticity (TRIP) effect, which remain undetected by other techniques. [R. Woracek et al., Adv. Mater., 26: 4069–4073 (2014)]. The research results to be discussed have been performed in collaboration with the Helmholtz Zentrum Berlin (N. Kardjlov, A. Hilger, I. Manke, M. Boin, M. Strobl), the University of Berkely (A. Tremsin), Rutherford Appleton Laboratory (J. Kelleher, W. Kockelmann), the Los Alamos Neutron Science Center (B. Clausen, S. Vogel), NIST (D. Hussey, D. Jacobson), and the Oak Ridge National Laboratory (J. Bunn, A. Pyzant, C. Hubbard).

In-situ neutron diffraction for advancing constitutive models of shape memory alloys

Aaron STEBNER
Colorado School of Mines, USA
Tuesday 15.40-16.05 **Via internet**

It is generally accepted that development of physics-based constitutive models implemented in the form of engineering tools and methodologies to the same extent such means exist to design with traditional solid materials will contribute to market expansion for SMAs. To develop such models, physics-based understanding of the coupled chemical, thermal, and mechanical physics of the elastic, phase transformation, and plastic interactions within SMA microstructures that lead to shape memory behaviors is required. Afforded by in-situ neutron diffraction, an ability to make empirical measurements to quantify relationships between microstructure and macroscopic thermo-mechanical responses of SMAs has helped elucidate such micromechanical understanding of SMA physics in recent years. Specifically, work performed on the SMARTS and HIPPO diffractometers at LANSCE has played a critical role. In this presentation, key fundamental physical understandings and modeling capabilities of SMAs that have been enabled and accelerated by neutrons will be reviewed.

List of participants

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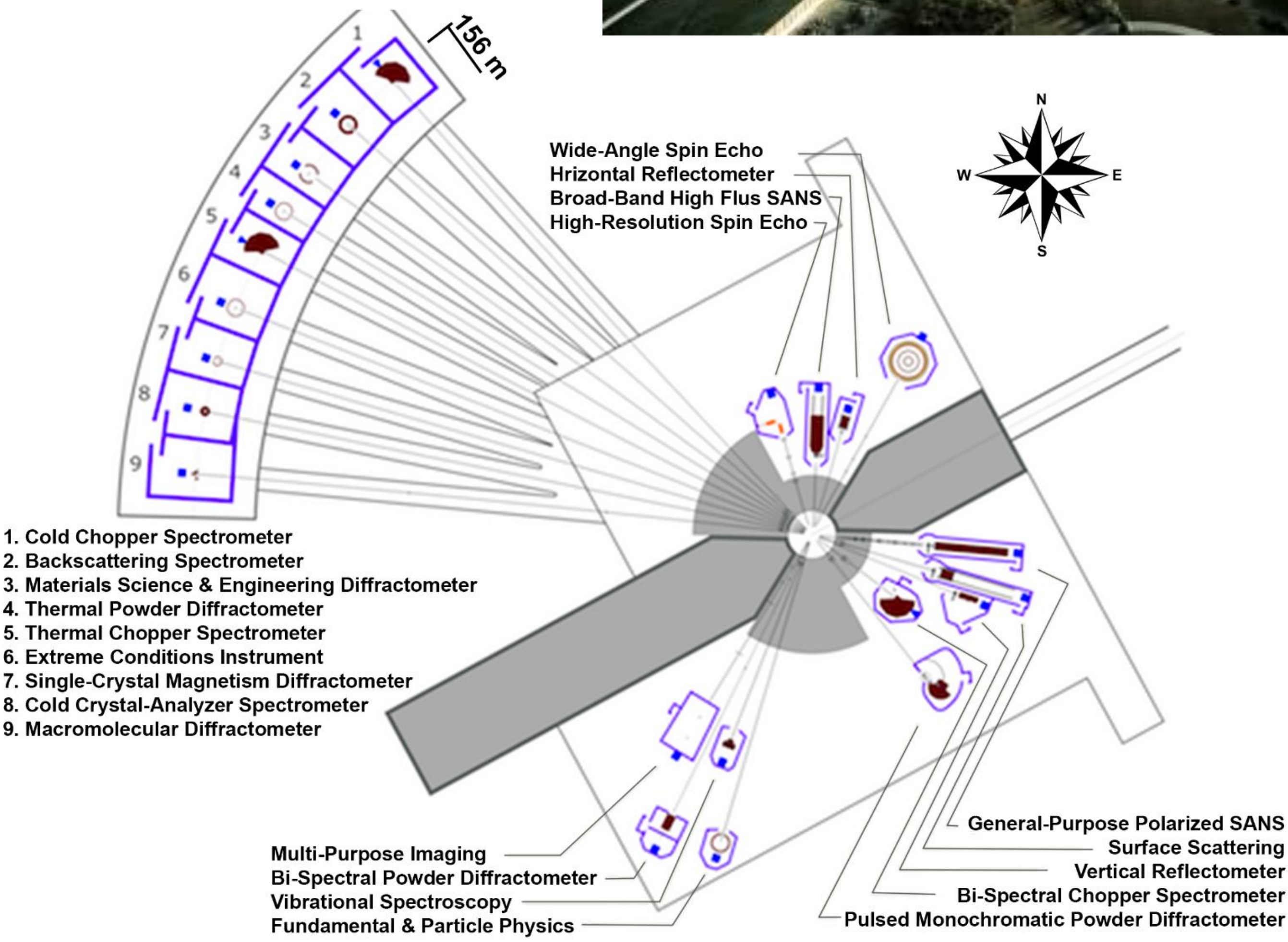
The European Spallation Source (ESS) is a multi-disciplinary research centre currently under construction in Lund, Sweden based on the world's most powerful neutron source - around 30 times brighter than today's leading neutron facilities.

A total of 22 instruments will be built at the ESS to serve the neutron user community, with the aim of having the initial seven instruments commissioned by 2020.



Neutron Instruments for ESS