Session IV - Neutron scattering, Tuesday, June 21

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FIRST SCIENCE ON THE ESS INSTRUMENT SUITE

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The European Spallation Source currently under construction in Lund, Sweden is designed to become the world's most powerful neutron spallation source, opening up new scientific opportunities.

An overview of the progress of the construction project will be given, the time to starting user operation will be discussed and new scientific opportunities will be highlighted.

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EUROPEAN SPALLATION SOURCE - CONTRIBUTION OF THE CZECH REPUBLIC

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European Spallation Source (ESS) is the world's most powerful neutron source under construction in Lund (Sweden), which will offer about 4000 beam days annually to scientists from Europe when built to its planned capacity of 22 instruments. Even with just the 15 instruments to be built within the ESS construction scope, ESS will greatly increase the capacity of the European network of neutron sources by opening new opportunities for breakthrough research with neutrons thanks to the unprecedented neutron beam brightness accompanied by world-class instrumentation and novel experimental methods developed for the long-pulse neutron source.

The Czech Republic became one of the 13 founding members of the ESS ERIC consortium in 2015 with the planned 2% contribution to the ESS construction, which should ensure a proportional share of beam capacity for Czech users after ESS is put into operation. This step is of great importance for the Czech user community when considering the fading capacity of neutron sources in Europe: several research reactors which used to serve our user community were shut down recently, while others are approaching the end of their lifetime, including the research reactor LVR-15 in Řež and ILL Grenoble.

In-kind contributions make a significant part of the ESS construction. The Nuclear Physics Institute, CAS (NPI) in Řež has the task of implementing several of these contributions:

The supply of systems for the ESS target station includes the helium cooling loop, water cooling of the target and HVAC (Heating, Ventilation, Air Conditioning) of the target station building. These technologies have already been delivered, and their installation is being finalized.

NPI, together with Helmholtz Zentrum Hereon in Geesthacht, develops and builds one of the neutron scattering instruments – the Beamline for European Materials Engineering Research (BEER). According to the current schedule, BEER is supposed to be ready for hot commissioning in early 2024 and enter into the user regime during the ESS operation ramp-up between 2025 and 2027. BEER has been developed in cooperation with neutron users from the material research and engineering areas. On the Czech side, teams from the Faculty of Mathematics and Physics of the Charles University and the Institute of Physics, CAS, largely contributed to the instrument concept and actively participated in the development of a sample environment for in-situ measurements and novel methods to be tested during early operation. Such a collaboration is vitally important for a successful start of the user program at BEER, and neutron users are encouraged to collaborate with the instrument team on the preparation of the early operation program.

The contribution of the Czech Republic to the ESS construction has been supported by the Czech Ministry of Education, Youth and Sports through the project of large infrastructure ESS Scandinavia-CZ (project LM2018111) and by EU Structural Funds (Reg. No. CZ.02.1.01/0.0/0.0/16_013/0001794).

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BEER - SCIENCE CASE AND STATUS

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The time-of-flight engineering diffractometer BEER [1] (Beamline for European Materials Engineering Research), which is under construction at the European Spallation Source (ESS), will offer new opportunities for investigations of microstructures, residual stress evolutions and in-situ phase transformations under near-processing conditions. The layout of the instrument is depicted in Figure 1 and the basic parameters are listed in Table 1.

The construction of the instrument is divided into two stages called *Day-1* (coloured parts in Figure 1) and *Full-scope* (white parts in Fig. 1). The *Day-1* instrument will provide reduced capabilities mainly in the detector coverage, SANS option and variability of chopper cascade but will be fully operational and comparable with the current engineering instruments worldwide.

BEER combines the high brilliance of the ESS source with large instrument flexibility. The diffractometer includes a novel beam-shaping technique, the so-called modulation technique (see Figure 2) [2]. By a time-encoded extraction of several short pulses from the long ESS pulse, a substantial intensity gain of up to an order of magnitude compared to a pulse shaping method (one pulse extraction) for high-crystal-symmetry materials can be achieved without compromising the resolution. More complex crystal symmetries or multi-phase materials can be investigated by the standard pulse shaping method. The variable chopper set-ups and advanced extracting techniques [3] offer broad intensity/resolution ranges that can be adjusted for the experiment's needs. This flexibility opens up new possibilities for in-situ experiments studying materials processing and performance under operating conditions.

Table 1 - Basic facts about the BEER instrument

Instrument Class	Engineering Diffraction
Moderator	Bispectral
Primary Flightpath	158 m
Secondary Flightpath	2 m
Wavelength Range	0.8 – 6 Å
Bandwidth	1.7 Å
d-spacing Range	0.6 – 7 Å
Pulse-Shaping Mode	
Resolution d/d	0.15 – 0.6 %
Flux at Sample at 2MW	0.18 – 1.4•10^8 n s^{-1} cm^{-2}
Modulation Mode	
Resolution d/d	0.1 – 0.3 %
Flux at Sample at 2MW	0.18 – 0.87•10^8 n s^{-1} cm^{-2}

Advanced sample environments dedicated to thermo-mechanical processing are foreseen to fulfil this

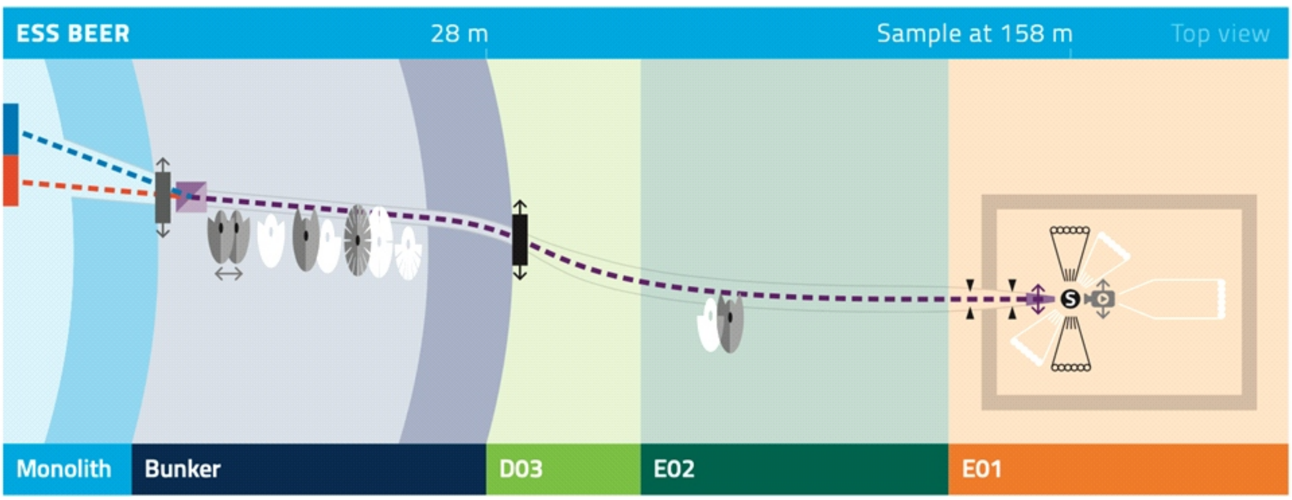

Figure 1. The BEER instrument schematic layout

task, e.g. a quenching and deformation dilatometer, and various deformation rigs.

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2. M. Rouijaa, R. Kampmann, J. Šaroun, J. Fenske, P. Beran, M. Müller, P. Lukáš, A. Schreyer, Beam modulation: A novel ToF-technique for high resolution diffraction at the Beamline for European Materials Engineering Research (BEER), *Nuclear Instruments and Methods in Physics Research, Section A.* **889**, (2018), 7–15.
3. J. Šaroun, J. Fenske, M. Rouijaa, P. Beran, J. Navrátil, P. Lukáš, A. Schreyer, M. Strobl, Neutron optics concept for the materials engineering diffractometer at the ESS, *J. Phys.: Conf. Ser.* **746**, (2016), 012011.

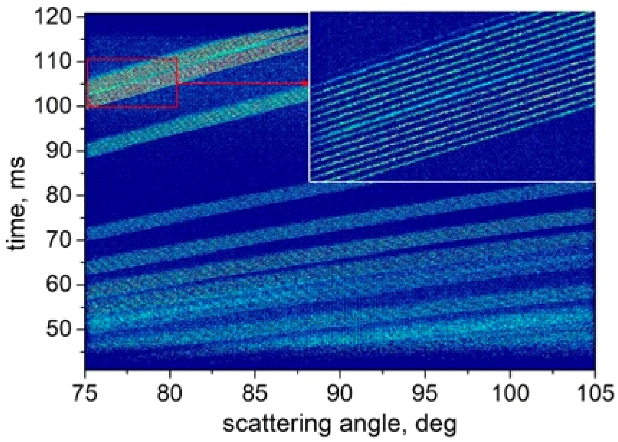

Figure 2. Simulated time-of-flight diffraction pattern of a duplex-steel for +90° detector showing the splitting of the Bragg reflections when modulation technique is used [2].

Session V - Neutron scattering, Tuesday, June 21

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SANS INVESTIGATION OF MICROSTRUCTURE EVOLUTION IN SINGLE CRYSTAL Ti-15Mo METASTABLE -Ti ALLOY AT ELEVATED TEMPERATURES

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Titanium alloys have a plenty of applications in industry and medicine [1] due to unique combination of high strength, low density and excellent biocompatibility. Ti-15Mo alloy is a metastable -Ti alloy containing (hexagonal) and (hcp) precipitates in -phase matrix. Particular microstructure resulting from the heat treatment has a large impact on mechanical properties and thermal stability of the alloy. One of the techniques able to deliver bulk information on the precipitate evolution directly at elevated temperatures is Small-Angle Neutron Scattering (SANS). V4 SANS facility of HZB Berlin [2] was used for investigation of Ti-15Mo (wt.%) alloy. SANS data were acquired in-situ up to 600°C at three orientations of the single crystal sample – with <111>, <110> and <100> directions of -phase parallel to the neutron beam. The rate of 1 K/min was used for the in-situ heating during SANS measurement. The orientation of the crystal in this case was <110> direction of the -phase matrix parallel to the neutron beam.

Strongly anisotropic scattering pattern, moreover evolving with temperature increase, was detected. Observed 2D intensity distribution at temperatures 400-530 °C originated from isothermal prolate-spheroidal precipitates arranged on a simple cubic-like grid. When heating above 400 °C, the mean size and interparticle distance of particles gradually increased. Initially, volume fraction times scattering contrast of -phase increases up to 443 °C, and it then gradually decreases up to 530 °C.

In the temperature range 531-538 °C, both -phase ordered spheroids and a population of plates is needed to fit the observed SANS patterns well. Fig. 1 (left side) shows an example with already well visible -phase streaks (near the edge of the detector), but with still present major part of the scattering (including interparticle-interference maxima near the detector centre) originating from the spheroids.

Above 538 °C, no more scattering from particles exists; nevertheless, the scattering coming from the population of plates remains. Moreover, a second type of streaks appears, which has orientation clearly distinguished from the first ones caused by plates. The two types of streaks in the scattering pattern can be seen in Fig. 1, right side. The cause of the second type of streaks can be a formation of a second population of plates which has orientation clearly distinguished from the first population of plates. The data were evaluated and interpreted using this hypothesis.

In the initial stage after their appearance, the scattering intensity from both -phase populations gradually increases on temperature increase. Both phase populations