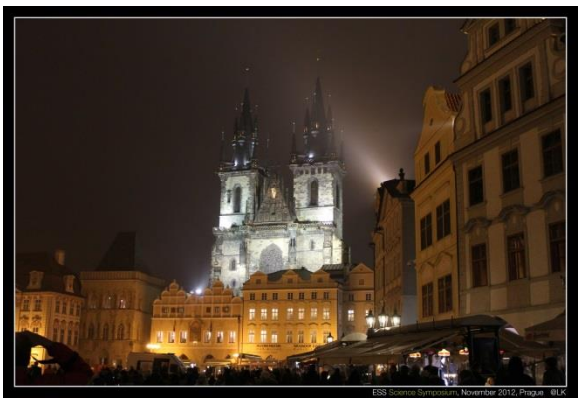
ESS Science Symposium 2012

Physical simulations of processes in engineering materials with in-situ neutron diffraction/imaging

15-16 November, 2012, Prague, Czech Republic

REPORT

http://ofm.fzu.cz/ess-prague



1. The scope of the Symposium

The ESS Science Symposium **„**Physical simulations of processes in engineering materials with in-situ neutron diffraction/imaging**“** was organised with the goal discuss with the specialists in the field the potential of the idea to carry out at ESS Spallation source a special kind of engineering diffraction research - **Physical simulation of materials fabrication, processing and/or testing under extreme loading conditions and complex loading histories.** It involves the exact reproduction of the thermal and mechanical processes in the laboratory that the material is subjected to in the actual fabrication, processing or end use. The concept was formally introduced into engineering metallurgy field by a company Dynamic System Inc. to explain the use of their equipment (special thermomechanical rigs Gleeble equipped with ultrafast heating and cooling, complex loadings, high temperature and vacuum chambers). The physical simulation concept can, however, be employed in many other fields and industries beyond the material engineering.

Physical simulator Gleeble brings a small piece of the material into the required material state by sequences of thermal and mechanical loads resembling as closely as possible the conditions the material is exposed to in the large scale fabrication process. Time evolution of macroscopic parameters as force, strain, temperature is recorded during the treatment. When the simulation is accurate (in the sense that of lab treated material exhibits desired microstructure and properties), the results can be readily transferred from the laboratory to the large scale production process. **Main goal of Physical Simulations in material engineering field is thus to develop new processing technology in laboratory scale and transfer it afterwards to the full scale industrial process.** The method is currently widely used by materials engineers to efficiently optimize the large scale material production routes used in the industry. It is essential to understand the difference between thermomechanical testing and physical simulation. While all physical simulations involve physical testing, the key difference is that physical simulation attempts to replicate real-world processes on a laboratory scale in a way that the resultant data can be used to solve real-world problems.

It is essential that the material follows during the physical simulation the same thermal and mechanical history that it would do in the full scale fabrication process. If this is the case, it can be reasonably assumed that microstructure and properties of the material evolve during the physical simulation as it would do in the large scale process. Since this is never guaranteed, researchers performing physical simulations always try **to follow the evolution of microstructure and properties of the material by conventional ex-situ metallurgical methods** (ex-situ metallography, SEM, TEM, hardness test etc.).

At the same time, mechanical engineers who help to design new better performing engineering materials simulate the materials processing by **numerical models which are capable of predicting the evolution of microstructure and properties of materials** with exactly same ultimate goal - to optimize the large scale production routes.

Evolution of microstructure - property in processed engineering materials thus play key role in both physical and numerical simulations of material processing. **It is the major benefit of neutron and high energy X-ray diffraction methods for material engineering field, that these methods can be employed to track down the evolution of material state (microstructure, internal stress, texture) in-situ during the physical simulation without disturbing the process.**

Although several X-ray/neutron diffractometers dedicated for engineering studies at large scale facilities (e.g. ENGIN-X, SMARTS, VULCAN, TAKUMI) have already been used for variety of "in-situ engineering studies" (time resolved characterization of deformation, phase transformation, residual stress, texture, and microstructure changes during material synthesis, processing, and service), these fell short of representing true Physical Simulations introduced above due to the limits posed by the installed environment - e.g. low deformation speed (forging simulations), low heating rates (welding simulations), low cooling rates (phase transformation during cooling), simple loading modes (rolling, forming) etc..

The above mentioned "In-situ engineering experiments" have been recently steadily gaining in importance and frequency at large scale neutron and high energy X-ray facilities. At the same time Physical Simulation experiments for industry seem to suffer from the lack of in-situ obtained information on evolution of microstructure and internal stresses during thermomechanical processing (currently used ex-situ metallography and electron microscopy is time consuming and frequently not does not provide actual information on the material state which existed in particular stages of the thermomechanical process). **If there is a dedicated material engineering beamline where Physical simulations with neutrons can be carried out, it would be a major step forward that would facilitate the optimization of large scale industrial production routes and better engineering materials could be possibly produced.**

Based on these facts, we have identified „Physical simulations of processes in engineering materials with in-situ neutron diffraction/imaging“ as a potential area for future neutron engineering research on material engineering beamline at ESS and decided to organize ESS Science Symposium on this topic as a brainstorming activity.

2. Preparation of the Symposium

In order to fulfill the goal of the symposium introduced above it was necessary to bring to the symposium representatives of the 3 relatively distinct R&D communities :

1) **engineers and material scientists involved in engineering material research using Gleeble simulators** (researchers carrying out physical simulations for industry) ,

2) **members of neutron diffraction community involved in engineering studies** (neutron instrument scientists, and instrument developers),

3) **material scientists who are actively involved in in-situ neutron and/or X-ray diffraction studies of advanced engineering materials** (typically academic researchers who recognized the power of X-ray and neutron diffraction/imaging to perform world class research in materials engineering field).

The symposium website, personal contacts and support of ESS helped us to assure interests of key representatives of the communities 2 and 3 (Appendix I) but they were not sufficient to attract sufficient interest from members of the community 1. In order to solve this problem, as well as to better understand the actual needs and prospects for physical simulations with neutron diffraction,

we have attended meetings of the community 1 – e.g. Workshop on Gleeble Welding Process Simulation held on February 27-28 in Graz Austria or Gleeble European user group meeting held in Delft in Netherlands on April 24-25, 2012 and presented there our ideas to metallurgists and material engineers. Representatives of the community 1 were invited to attend the ESS Science Symposium in Prague. **The ESS Science symposium** itself was then held on Thursday-Friday, November 15-16, 2012 in hotel Amarilis located in central Prague, Czech Republic with two satellite events - **CEED Expert Meeting** prior and **SPEED workshop** after the symposium.

3. CEED Expert Meeting prior the Symposium

The Expert meeting was held on Wednesday, November 14 in Rez near Prague (Appendix III). The main reason for organization of the CEED Expert meeting prior the symposium was to discuss separately the concept of the CEED diffractometer designed by the Czech team with the instrument scientists working at neutron engineering diffractometers at major large scale neutron sources. **Ke An** (VULCAN, SNS), **Stefanus Harjo** (TAKUMI, J-PARC), **Bjorn Clausen** (SMARTS, LANL), **Shu Yan Zhang** (ENGINE-X, ISIS), **Jiří Kulda** (ILL) who came to Prague to attend the ESS Science symposium attended this meeting. **Axel Steuwer** on behalf of ESS, Prof. **Yo Tomota** from Japan and 6 members of the Prague team joined this meeting.

After the morning special scientific talks by S. Harjo and B. Clausen, the attendees visited neutron diffractometers installed at the Řež research reactor LVR-15. The essential part of the meeting was the **3 hour roundtable discussion which followed the talk by Jan Šaroun on the Current concept of the design of the diffractometer CEED for ESS**. Details concerning issues discussed during the roundtable discussion and conclusions of the Expert meeting are covered by a special internal report.

4. Content of the Symposium

Two day program of the ESS symposium (Appendix II) consisted of 5 blocks of lectures in which invited participants presented 10-20 minutes long presentations.

1. ESS Update
Review on the progress of ESS construction.

2. Neutron and X-ray diffraction studies of engineering materials
Facilities, methods, experiments, results.

3. Metallurgy, testing and modelling of thermomechanically loaded engineering materials
Industrial demands, fabrication, processing, physical simulation, testing, microstructures, modelling.

4. In-situ neutron (X-ray) diffraction/imaging studies of engineering materials
*Approaches, methods, case studies***.**

5. Current status of planning of engineering diffractometers for ESS
Presentation on ESS engineering diffractometer and roundtable discussion.

After a brief update on the ESS construction by A. Steuwer and M. Strobl, instrument scientists from engineering diffractometers at LANSCE, ISIS, SNS, PSI and J-PARC gave excellent overview of the current state of art of the instrumentation used to perform in-situ engineering studies using neutron diffractometers and identified major challenges for such research at ESS. In the next block of lectures, Brian Alen from the DSI company described the state of art Gleeble simulators and D. Fabregue and G. Korpala introduced Physical Simulation methods and demonstrated the need for in-situ information on phase transition, stresses and microstructures in it. Majority of further speakers focused variety of in-situ neutron and X-ray diffraction studies on advanced engineering materials. Antonio Jose Ramirez Londono, from LNLS, Brasil shared his experiences with installation of the Gleeble simulator on the synchrotron at LNLS in Brazil. In the last block of lectures, the two merging CEED and SPEED concepts of the engineering diffractometer planned for ESS were briefly presented. The PPT slides the invited speakers used for their presentations well collected after the symposium.

5. SPEED workshop after the Symposium

Since the project for building engineering instrument for ESS proceeds in collaboration of Czech and German teams and practically all their members participated in the ESS Science Symposium on November 15-16 2012, it was decided to organize a special meeting of the two teams the day after the symposium on Saturday, November 17, which would be open to the other specialists who could stay one day more in Prague. Since the idea was originally proposed by the German team working on the design and development of the **Structured Pulse Engineering Diffractometer (SPEED)** the meeting was called simply **SPEED workshop.**

The program of the workshop (Appendix IV) started with discussion on the activities related with the planning for Engineering beamline at ESS coordinated by M. Strobl and A. Steuwer. S.-Y. Zwang from ENGIN-X (ISIS) and Ke An from VULCAN (SNS) reported on new activities at these prime neutron instruments. Following that, R. Kampmann introduced recent advance in the Design and expected potential of the **Structured Pulse Engineering Diffractometer (SPEED)** for ESS. H.-G. Brokmeier presented a very interesting talk concerning the advantages of neutron diffraction for texture studies and emphasized the industrial needs and interests in texture studies. P. Sittner briefly introduced ideas of the Prague team for environment to be installed at the engineering beamline at ESS that were mainly discussed in the afternoon discussion.

6. Conclusions from the event

The ESS Science symposium in Prague brought together for the first time members of community of engineers and material scientists who perform Physical simulations on Gleeble simulators with researchers involved in neutron and/or X-ray diffraction engineering studies of advanced engineering materials.

The symposium delivered a very good overview on the current status of the instrumentation used at engineering neutron diffractometers worldwide (diffractometer components and environment). The pointed out issues include:

1. Although the beam time request for strain scanning and texture studies remains high, demand for in-situ experiments has been steadily growing and it is expected to increase further. This contrasts with the prospect for strain scanning and texture studies which is expected to remain flat.
2. Advantages of the possibility of continuous data recording during in-situ studies with high intensity beam were emphasized (already common at high energy X-ray sources)
3. Main advantage of neutrons in the fierce competition with synchrotron X-rays in the material engineering field remains to be the possibility to have large gauge size for engineering materials with large grain sizes and ability to perform 3D scans through large bulk volumes.
4. The advantages of yet rarely used 2D detectors for in-situ experiments on engineering materials were emphasized
5. Benefits of the possibility to carry out some sort of imaging experiment on the same piece of sample was emphasized.
6. Benefits of the possibility to obtain at least partial information on texture evolution during in situ experiments was emphasized.
7. Benefits of maximized detector coverage of the engineering instruments were pointed out.
8. It was agreed that the currently used environment at engineering diffractometers does not allow to perform in-situ studies of true engineering processes due to the limits as sample size, heating/cooling rates, complex state of stress, long term experiments etc.
9. The range of environments used at modern engineering diffractometers (furnaces, cryostats, deformations rigs, scanning tables, robots, hexapod platforms, magnets, environmental chambers) is extremely wide and it is projected to grow significantly towards user defined environments motivated by industrial needs.
10. It was noted by some instrument scientists that, although it is important to cover wide area of material engineering problems, particularly if there is only one engineering beamline at the facility, there is a danger that, due to the shortage of financial and personnel resources, at some point, it will not be possible to perform all the work well. It was noted that there is a lesson from synchrotron beamlines, where they soon realized that, although they could do really great science, the results were not coming, since the instrument and environment were not user friendly.

It became obvious from the presentations of material engineers, that **the idea of the installation of Gleeble simulator on neutron beam at ESS is merely a projection of the current booming area of in-situ neutron and/or X-ray engineering studies** (most of the speakers presented results of such in-situ investigations) **to the industrially compatible scale and wide range of extreme conditions and loading histories.** Though the idea itself was generally welcome, many technical issues were raised. The pointed out issues include:

1. There exist relatively large and **well organized industrial/academic Physical Simulation community worldwide** represented by material engineers who are skillful in operating Gleeble simulators to simulate different kind of industrial processing i.e. welding, forging, melting, solidification etc.
2. Providing such physical simulation community with a world unique facility at ESS, where physical simulation studies could be combined with neutron engineering diffraction, would assure breakthrough in the material engineering field and bring industrial attention. Installing

Gleeble simulator at ESS would level up the current state of art in-situ engineering research at the large scale neutron sources to industrial scale.

3. Although high energy synchrotron X-ray diffraction is more appropriate for time resolved physical simulation, **neutron diffraction is more suitable for application to real industrial problems** due to the possibility to work with large component, to use larger gauge volumes and to study materials with larger grain sizes. Complementary X-ray and neutron diffraction investigations during physical simulations is obviously an ideal solution.
4. Since neutron diffraction methods used in strain scanning and texture measurements on one side and in-situ studies on the other side require slightly different neutron instruments, there will be two options – i) either to have one hybrid instrument and rebuild it frequently which is extremely time consuming or ii) to consider building of two slightly different engineering instruments in the long run. First instrument could be then optimized for angular resolution (strain scanning) while the second one for time resolution (physical simulation). If such two twin instruments are closely located, they will be able to share the expensive and space demanding environments and support labs. Given the envisioned increase of the beamtime demand, **the second option of two engineering instruments located aside is definitely a better solution for ESS.** Though the second option would be more expensive, it is definitely not twice expensive, due to large extent of the sharing.
5. There is **an urgent need for long term in-situ diffraction studies which would reveal evolution of material state** (internal stress, microstructure, texture) **during long term material testing** (creep, fatigue, corrosion etc.) In contrast to the current state of art consisting in performing such experiments in the lab and bringing either set of variously treated samples or bringing one sample periodically removed from the tester to the X-ray/neutron diffractometer, where it is loaded again, there is an alternative option to perform the long term experiment in a support lab (docking station for environment) next to the neutron beamline and periodically bring the tester together with the sample (multiple samples) to the neutron diffractometer for a short time measurement e.g. once a month.
6. It was mentioned that an increasing **demand for doing in-situ neutron diffraction experiments during thermo mechanical testing under magnetic or electrostatic fields** is very likely in near future.

APPENDIX I

List of Participants

First name	Last name	Country	Institution	E-mail
Brian	Allen	United States	Dynamic Systems Inc.	brian.allen@gleeble.com
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APPENDIX II

PROGRAM of the ESS Science Symposium

<table>
<tr><td></td><td colspan="4">PROGRAM of the ESS Science Symposium, Prague 2012</td></tr>
<tr><td></td><td>Wednesday
November 15</td><td>Thursday
November 15</td><td>Friday
November 16</td><td>Saturday
November 17</td></tr>
<tr><td>9:00</td><td rowspan="2"></td><td rowspan="2">Opening
Petr Lukáš</td><td rowspan="2">Klaus-Dieter Liss
ANSTO, Australia</td><td rowspan="21">SPEED satelite meeting</td></tr>
<tr><td>9:10</td></tr>
<tr><td>9:20</td><td rowspan="2"></td><td rowspan="2">Axel Steuwer
ESS</td></tr>
<tr><td>9:30</td><td rowspan="2">Helena Van Swygenhoven-Moens, PSI, Switzerland</td></tr>
<tr><td>9:40</td><td rowspan="2"></td><td rowspan="2">Oliver Kirstein
ESS</td></tr>
<tr><td>9:50</td><td rowspan="2">Ivan Lonardelli
University of Cambridge, UK</td></tr>
<tr><td>10:00</td><td rowspan="2"></td><td rowspan="2">Markus Strobl
ESS</td></tr>
<tr><td>10:10</td><td rowspan="2">Alexander Evans
ILL, France</td></tr>
<tr><td>10:20</td><td rowspan="2"></td><td rowspan="2">Coffee break</td></tr>
<tr><td>10:30</td><td rowspan="2">Coffee break</td></tr>
<tr><td>10:40</td><td rowspan="2"></td><td rowspan="2">Bjorn Clausen
SMARTS, LANSCE, USA</td></tr>
<tr><td>10:50</td><td rowspan="2">Antonio Jose Ramirez Londono,
LNLS, Brasil</td></tr>
<tr><td>11:00</td><td rowspan="2"></td><td rowspan="2">Shu Yan Zhang
ENGIN-X, ISIS, UK</td></tr>
<tr><td>11:10</td></tr>
<tr><td>11:20</td><td rowspan="2"></td><td rowspan="2">Ke An
VULCAN, SNS, USA</td><td rowspan="2">Steven Van Petegem
POLDI, PSI, Switzerland</td></tr>
<tr><td>11:30</td></tr>
<tr><td>11:40</td><td rowspan="2"></td><td rowspan="2">Steven Petermans
PSI, Switzerland</td><td rowspan="2">Yo Tomota
Ibaraki University, Japan</td></tr>
<tr><td>11:50</td></tr>
<tr><td>12:00</td><td rowspan="2"></td><td rowspan="2">Stefanus Harjo
TAKUMI, J-PARC, Japan</td><td rowspan="2"></td></tr>
<tr><td>12:30</td></tr>
<tr><td>13:00</td><td rowspan="4"></td><td rowspan="4">LUNCH</td><td rowspan="4">LUNCH</td></tr>
<tr><td>13:30</td></tr>
<tr><td>13:40</td></tr>
<tr><td>13:50</td></tr>
<tr><td>14:00</td><td rowspan="3"></td><td rowspan="3">Damien Fabreque
INSA, Lyon, France</td><td>Jan Šaroun,
NPI, Řež, Czech Republic</td></tr>
<tr><td>14:10</td></tr>
<tr><td>14:20</td><td rowspan="2">Jan Pilch
IP ASCR, Czech Republic</td></tr>
<tr><td>14:30</td><td rowspan="2"></td><td rowspan="2">Brian Allen
Dynamic Systems Inc., USA</td></tr>
<tr><td>14:40</td><td>Reinhard Kampmann</td></tr>
</table>

14:50			HZG, Germany	
15:00		**Grzegorz Korpała** TU Freiberg, Germany	**Peter Staron** HZG, Germany	
15:10				
15:20		**Thomas Kannengiesser** BAM, Germany	**Roundtable discussion** Axel Steuver, Petr Lukáš	
15:30				
15:40		***Coffee break***		
15:50				
16:00		**Alain Jacques** Inst. J. Lamour, Nancy,France	**Symposium closure** Farewell drink & refreshment	
16:10				
16:20		**Ondrej Muransky** ANSTO, Australia		
16:30				
16:40		**David Dye** Imperial College London, UK		
16:50				
17:00		**Debashishe Mukherji** TU Braunschweig, Germany		
17:10				
~				
19:00	**Welcome registration**	**SYMPOSIUM DINNER**		

APPENDIX III

Program and list of participants of the CEED Expert meeting

CEED Expert meeting *Saturday, Nov. 14, 2012*		
Stefanus Harjo	Japan	TAKUMI – Design Concept & Present Status
Bjørn Clausen	USA	Obtaining Material Parameters using Neutron Diffraction
		Tour the Řež research reactor LVR-15
		Lunch
Jan Šaroun	Czech Republic	Current concept of the CEED design
All		Roundtable discussion on the CEED concept

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APPENDIX IV

Program and list of participants of the SPEED workshop

Workshop on the Structured Pulse Engineering Diffractometer (SPEED) *Saturday, November 17 in Prague*		
09:00 - 10:00	**1. Welcome and overview of ESS and SPEED**	
09:00 - 09:05	Welcome	A. Schreyer
09:05 - 09:25	Overview engineering investigations at ESS	A. Steuwer
09:25 - 10:00	Design and expected potential of the Structured Pulse Engineering Diffractometer (SPEED) at ESS	R. Kampmann & M. Rouijaa
10:00 - 10:20	coffee	
10:20 – 12.30	**2. Needs, wishes and visions for engineering diffraction at ESS**	
10:20 - 11:00	Visions for engineering investigations at the ESS (invited)	P. Sittner & J. Pilch
11:00 - 11:20	Texture and strain investigations: Status and expected developments (tentative title, invited)	H.-G. Brokmeier
11:20 – 11:40	Celebration of 10 years of ENGIN-X (invited)	S.-Y. Zwang
11:40 – 12:00	Cutting edge engineering investigations at VULCAN (tentative title, invited)	A. Ke
12:00 - 12:30	**Discussion**	
12:30 - 14:00	Lunch	
14:00 - 15:00	**3. Discussion of requirements on SPEED**	

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APPENDIX V

Abstract book