

SIG14 D³:Diffuse, Disorder and Dynamics

Reported Period: 2019-2020

Report Date: April 2021

Reported by: Anders Østergaard Madsen (Chairman), Arkadiy Simonov (Secretary)

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1. Introduction.

SIG #14 brings together scientists working on dynamical properties, disorder and diffuse scattering. The main objectives are to enhance the exchange of information regarding recent progress in experiment and theory, to provide a platform for discussions, to promote use of diffraction and crystallographic tools in studying the physics and chemistry of materials which display some disorder.

2. SIG web site:

<https://ecanews.org/groups/sig-14-dynamics-disorder-diffuse-scattering/>

Researchgate page:

<https://www.researchgate.net/project/ECA-SIG14-D3-Dynamics-Disorder-Diffuse-Scattering>

**3. Number of ECA individual members registered with the SIG according to
(<http://www.xray.cz/eca/im-payment.htm>)**

Our SIG is not listed on the server.

4. Existence of a SIG mailing list: No

5. Approximate total number of researchers involved in the SIG (please indicate the basis for the estimate)

30 researchers signed up on the initial meeting in Oviedo.

6. List of MS organized by the SIG at the last ECM

MS27: Structural Dynamics, Disorder and Physical Properties

Chairs: Dmitry Chernyshov and Ruggero Frison

MS28: Dynamics and Disorder Probed by Diffuse Scattering

Chairs: Anders Ø. Madsen and Arkadiy Simonov

7. Prizes sponsored/coordinated

None

8. Past Activities other than Microsymposia at ECM

Title: **Correlated Disorder Workshop** Feb 25-26 2020. Herzberg near Aarau.

Number of Participants: 40

- ECA Individual Members registered with the SIG involved as lecturers

Two day workshop organized to discuss new physics and functionalities in systems with correlated disorder or structural frustration such as charge ices, or electronic or magnetic properties where disorder and/or frustration are important.

Title: **DISCUS Workshop on Diffuse Scattering and Structure Simulation**

March 30 – April 3, 2020. University of Erlangen-Nürnberg. **[Cancelled]**

Number of Participants: 30

- ECA Individual Members registered with the SIG involved in the organizing committee
- ECA Individual Members registered with the SIG involved as lecturers

In this workshop you will learn to interpret diffuse scattering and to simulate disordered crystal structures. Defects are quite common in crystals and are responsible for a number of properties like ionic conductivity, electronic properties of indirect semiconductors etc. In diffraction, defects manifest themselves by the presence of diffuse scattering. While its peak intensity usually is weak, the total scattering intensity will be an appreciable fraction of the Bragg intensities. Thus, the description of these structures is largely incomplete without proper interpretation of the diffuse scattering.

The workshop covers the techniques to simulate and to refine disordered structures for a wide range of defects, and the corresponding calculation of the diffraction pattern for single crystals and powder, as well as the calculation of the pair distribution function PDF.

Upgrades at ID28-diffuse and SNBL @ ESRF II

In August 2020, the ESRF opened its completely rebuilt x-ray source, ESRF-EBS (Extremely Brilliant Source), the world's first fourth-generation high-energy synchrotron. Diffuse scattering data collections can be done at many beamlines at ESRF, but there are two beamlines that are specifically focused on crystallography and disorder phenomena, BM01 (Swiss-Norwegian Beam Lines) and diffraction side-station at the inelastic scattering beamline ID28.

BM01 beamline, as well as other former bending magnet lines at ESRF, got a new source – 3 pole wiggler. Together with re-polished focusing mirrors and improved cooling system of the monochromator, the line delivers up to 5 times higher flux density on the sample position. Beamline offers a broad range of goniometry for single crystal, powder, and thin film experimentation as a function of temperature, gas flow, and electric field; many on-going experiments deal with disordered and dynamically evolving systems, and our goal is to provide highest quality Bragg and diffuse scattering data.

Ongoing evaluation of ID28 optics upgrade indicates that new source can provide the focal spot well below 10 μm , thus offering new range of applications, i.e. data collection under very high pressures and mapping on inhomogeneous samples. In present new options became accessible: clean diffuse data collection using closed-cycle cryostat; data collection under applied electric field;

high pressure experiments with diamond anvil cells; simultaneous collection of SAXS and WAXS data for mesocrystals.

Proposal: microsource 3D-PDF/tomography beamline μ 15 at Diamond-II

Diamond light source, the national UK synchrotron, is currently on the planning stage of a major upgrade to Diamond-II. The upgrade will include complete redesign of the machine and multiple beamlines. The members of SIG-14 have been involved in creating proposal for a new beamline μ 15 which is a complete redesign of the current high pressure I15 beamline. If approved, μ 15 will be a micro-source hard radiation beamline built for general applications but with particular focus on tomography (including PDF tomography) and single crystal diffuse scattering measurements.

9. Future/Programmed Activities

An Erice crystallography school on diffuse scattering has been planned for the year 2022.

10. Other matters.

11. Brief annual activity report

Members of the SIG14 were involved in the 'Correlated Disorder Workshop' and in the organization of the 'Discus workshop' as noted previously in the report. This last event was cancelled due to the covid19 situation. For the same reason, the steering committee of SIG14 has been communicating online, but have not have not been able to arrange physical meetings.

12. List SIG officers, name and e-mail, and specify their main function in the SIG:

Chair: Anders Østergaard Madsen (University of Copenhagen) <a.madsen@sund.ku.dk>
Vice chair: Bjorn Wehinger (Ca' Foscari University of Venice) <bjorn.wehinger@unive.it>
Secretary: Arkadiy Simonov (ETH Zurich) <arkadiy.simonov@mat.ethz.ch>
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