

SIG14 D³: Diffuse, Disorder and Dynamics

Reported Period: September 2022 – September 2023

Report Date: September 11, 2023

Reported by: Ella M. Schmidt (Chairman), Anna Hoser (Secretary)

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.

In the reporting period from September 2022 – September 2024 the members of the SIG have been involved in many different activities. Highlights include two prominent awards to SIG members (**Bragg prize** by the IUCr awarded to Prof. Dr. Arkadiy Simonov and the **Nardelli prize** by the Italian Crystallographic association awarded to Dr. Stefano Canossa), numerous teaching activities in schools and workshops and a scientific communication project by Dr. Stefano Canossa.

2. SIG website and Mailing list

SIG #14 currently has a small website at the ECA (<https://ecanews.org/groups/sig-14-dynamics-disorder-diffuse-scattering/>). In the future we plan to set up a small web page that will link teaching and scientific outreach resources, advertise workshops in the area of disorder, total scattering, dynamics and diffuse scattering and highlight publications of SIG members in the area.

Currently SIG #14 does not have an active mailing list. We have however a register of members (32 active members in September 2023) of the SIG and plan to setup a mailing list in the future that informs about the activities of the SIG, especially in the area of workshops and teaching – where we see a great potential to educate more researcher in the interest area of our SIG.

3. ECM organization

The SIG #14 representative in the organizing committee of ECM33 in Versailles 2022 was Anders Ø. Madsen. SIG #14 organized the following MS 26: “Quantum mechanical models for dynamics and diffuse scattering” and invited the keynote delivered by Reinhard Neder.

Ella M. Schmidt is the SIG #14 representative in the organizing committee of the ECM34 in Padova in 2024. Here, SIG #14 currently proposes two MS and two further joint MS with SIG #2 and SIG #7.

4. Scientific communication and outreach actives

SIG officer Stefano Canossa is putting together a list of teaching resources that cover Fourier transforms for teaching purposes. Furthermore as a science communication project he posts Fourier transforms of aperiodic patterns, fractals and mathematical tilings on Instagram (@specialdefects) and freely available on (<https://www.behance.net/specialdefects>).

5. Editorial activity of SIG members

- **Marc De Boissieu:** section editor of Acta Cryst B (IUCr)
- **Tatiana Gorelik:** co-editor of Acta Cryst A (IUCr)
- **Reinhard B. Neder:** co-editor of Acta Cryst B (IUCr)

6. Teaching activities of SIG members

6.1. Dedicated schools and workshops

In the reporting period SIG members (co-)organized 6 dedicated schools or workshops that promoted the special interests of the SIG as an overall theme or in dedicated parts of the workshop. In September 2023 two further workshops are planned.

List of the schools/workshops:

- Electron Crystallography School
 - SIG-Organizer: Tatiana Gorelik
 - Location: Caen, France
 - Dates: August 28 - September 1, 2022
 - Number of Participants: 47
 - Purpose: Diverse theoretical and practical aspects of 3D electron diffraction technique (3D ED / microED) and its application to structure determination of nano/microcrystalline materials of different classes – from inorganic, to organic and biological compounds.
- Analysis of Diffraction Data School and Conference
 - SIG-Organizers: Gavin Vaughan
 - Location: Grenoble, France
 - Dates: October 16 - 21, 2022
 - SIG Teaching lectures: Reinhard Neder, Wojciech Slawinski, Arkadiy Simonov
 - SIG Invited conference lectures: Andrew Goodwin, Ella Schmidt
 - Number of Participants: 124
 - Purpose: The ADD2022 School and Conference aim to deepen the understanding and to further the training of the various communities working on real-space data analysis for neutron and x-ray diffraction techniques. Fourier transformation of diffraction data into real-space, traditionally used for the structural determination of liquids and glasses, is now increasingly employed for partially-disordered crystalline powder samples, as well as for single-crystal samples exhibiting some local atomic disorder, and most recently for short-range spin-spin correlations in disordered or frustrated magnetic systems (in the case of neutron diffraction). The scientific scope of ADD2022 pertains to both x-ray and neutron diffraction techniques, and will again include single-crystal diffuse scattering as an integral part of the School and the Conference.
- Total Scattering Analysis School
 - SIG-Contributer: Reinhard Neder
 - Location: Oak Ridge National Laboratory
 - Dates: May 1- 5, 2023
- Workshop on 3D electron diffraction
 - SIG-Organizer: Tatiana Gorelik
 - Location: Antwerp, Belgium

- Dates: May 30 - 31, 2023
- Number of Participants: 38
- Purpose: Latest developments in electron diffraction, also including diffuse scattering analysis.
- DISCUS Workshop:
 - SIG-Organizer: Reinhard B. Neder
 - Location: Erlangen, Germany
 - Dates: July 24-27, 2023
 - Number of Participants: 21
 - Purpose: The attendees were given an introduction to the installation of the program, received lectures on disordered structures, diffuse scattering and PDF techniques. The main part of the workshop was devoted to cover the broad set of toolboxes in DISCUS to simulate disordered structures and to calculate the corresponding diffuse scattering, respectively the powder and single crystal PDF.
- SAXS Workshop
 - SIG-Organizer: Thomas Weber
 - Location: Zurich
 - Dates: September 9, 2023
 - Purpose: Introduction of SAXS with a series of lectures by experts from academia and industry and a tour of the X-ray platform at the Materials Science department at the ETH.
- Upcoming Workshops
 - Oak Ridge National Lab, Diffuse Scattering Workshop, September 21- 22, 2023, SIG-Organizer: Reinhard Neder, SIG Invited Speakers: Ella Schmidt, Nikolaj Roth
 - Oak Ridge National Lab, Diffuse Scattering Developers Workshop, September 25-28, 2023, SIG-Organizer: Reinhard Neder, SIG Invited Speakers, Ella Schmidt, Arkadiy Simonov

6.2. Teaching lectures

Apart from the schools and workshops listed above, the SIG members were very active in promoting the ideas and tools of disorder, dynamics and diffuse scattering analysis in various teaching settings. A list of 17 teaching lectures in the reporting period is provided:

- *"Single crystal diffuse scattering"*, ADD2022, October 17, 2022, **Reinhard Neder**
- *"RMCProfile: Local structure of crystalline to amorphous materials"*, ADD 2022, October 17, 2022, **Wojciech Slawinski**
- *"DISCUS: Simulation and refinement of disordered crystal structures"*, ADD2022, October 18, 2022, **Reinhard Neder**
- *"3D- Δ PDF: Pair distribution function analysis for single crystals"*, ADD2022, October 18, 2022, **Arkadiy Simonov**
- *"XRD experimental procedure and data reduction"*, ADD2022, October 18, 2022, **Gavin Vaughan**
- *"SCD experimental procedure and data reduction"*, ADD2022, October 18, 2022, **Reinhard Neder**
- *"PDF for pharmaceuticals"*, XRD-PDF (Pair Distribution Function) Workshop by Empa Academy and Malvern Panalytical, November 17, 2022, **Martin Schmidt**
- *"XRPD - challenging orange disordered structures"*, NanED Workshop II - Imperfect crystals, complementary with XPRD, December 7, 2022, **Martin Schmidt**
- *"Pair distribution function PDF"*, NanED Workshop II - Imperfect crystals, complementary with XPRD, December 8, 2022, **Reinhard Neder**

- *“Introduction to 3D-PDF”*, NanED Workshop II - Imperfect crystals, complementary with XPRD, December 8, 2022, **Ella Schmidt**
- *“Defect structures investigated with 3DED”*, NanED Workshop II - Imperfect crystals, complementary with XPRD, December 7, 2022, **Ute Kolb**
- *“Probing local order in ferroelectric thin films using high- energy X-rays and the 3D- Δ PDF method”*, DESY User Meeting, January 26, 2023, **Thomas Weber**
- *“Electron crystallography of 2D materials”*, IFW winter school, 1-3 February, 2023, **Tatiana Gorelik**
- *“Structure Determination”* and *“Scattering Theory and Correlation Functions”*, MATRAC 1 School on Application of Neutrons and Synchrotron Radiation in Engineering Materials Science, March, 13, 2023, **Ella Schmidt**
- *“Real Structure and Defects”*, MATRAC 1 School on Application of Neutrons and Synchrotron Radiation in Engineering Materials Science, March, 13, 2023, **Reinhard Neder**
- *“Structure analysis of organic compounds”* and *“Disorder quantification and 2 crystals”*, Electron Crystallography School, Pisa, 3-6 July 2023, **Tatiana Gorelik**
- *“Tiling art in Fourier space: creative crystallographic teaching using existing free software”*, IUCr Software Fayre, August 28, 2023, **Stefano Cannossa**

7. Invited lectures of individual SIG members

7.1. Plenary and Keynote lectures

- *“Analyzing single crystal diffuse scattering”*, ECM33, August 25, 2022, **Reinhard Neder**
- *“Electron crystallography - diverse facets of nanocrystalline materials”*, ECM33, August 27, 2022, **Tatiana Gorelik**
- *“Bragg prize lecture”*, IUCr Congress and General Assembly 2023, August 28, 2023, **Arkadiy Simonov**
- *“Beyond the average: A journey to the multiscale diversity of framework materials”*, 50th Meeting of the Italian Crystallographic Association, September, 5, 2024, **Nardelli prize lecture awarded to Stefano Canossa**

7.2 Other invited lectures

- *“Dynamic Quantum Crystallography”*, ECM33, August 25, 2022, **Anna Hoser**
- *“Thermal diffuse scattering and ab initio phonons in LaPdSb”*, ECM33, August 25, 2022, **Mathias Gutmann**
- *“Solution of single crystal diffuse scattering problem using 3D- Δ PDF deconvolution”*, ECM33, August 25, 2022, **Arkadiy Simonov**
- *“Multivariate frameworks and the eye of the beholder”*, ECM33, August 27, 2022, **Stefano Canossa**
- *“Using 3D- Δ PDFs from electron diffraction data to determine local structure”*, ECM33, August 27, 2022, **Ella Schmidt**
- *“PDF methods in materials chemistry”*, ADD2022, October 19, 2022, **Andrew Goodwin**
- *“3D- Δ PDF from electron diffraction data”*, ADD2022, October 20, 2022, **Ella Schmidt**
- *“Static and dynamic conformational freedom of ZIF-90 revealed by single crystal diffuse scattering”* Dynamic Materials, Crystals and Phenomena Conference, Fribourg, Switzerland, 22–24.03.2023, **Stefano Canossa**
- *“Dynamic Quantum Crystallography: Thermal motion in crystallography seen through a quantum-mechanical looking glass”*, Distinguished lectures in Quantum Crystallography and Complementary Fields, online lecture series, May 5, 2023, **Anders Madsen**

- "*Phonon vibrations probed using the electron microscope*", Distinguished lectures in Quantum Crystallography and Complementary Fields, online lecture series, May 5, 2023, **Rebecca Nicholls**
- "*Analysis of disordered crystal structures*", North Carolina State Symposium, May 8, 2023, **Reinhard Neder**
- "*Analyzing Single Crystal Diffuse Scattering*", Warsaw University, June 21, 2023, **Reinhard Neder**
- "*Functional disorder in crystals*", Danish Chemical Society Annual Meeting, August 17, 2023, **Nikolj Roth**
- "*Science Case*", IUCr Satellite Workshop: Next-generation atomistic-level structural modeling using combined powder and single-crystal scattering data, August 21, 2023, **Andrew Goodwin**
- "*Electron single crystal diffuse scattering*", IUCr Satellite Workshop: Next-generation atomistic-level structural modeling using combined powder and single-crystal scattering data, August 21, 2023, **Ella Schmidt**

8. List of SIG officers

Chair: Ella M. Schmidt – University of Bremen – ella.schmidt@uni-bremen.de

Vice Chair: Anders Ø. Madsen – University of Copenhagen - a.madsen@sund.ku.dk

Secretary: Anna Hoser - University of Warsaw - a.hoser@uw.edu.pl

Officers: Stefano Canossa, Dmitry Chernychov, Arkadiy Simonov, Wojciech Sławiński, Björn Wehinger