SIG No 4 "Electron Crystallography"

Reported Period: ***2019-2020-2021***
Report Date: 31.01.2021
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1. Introduction. (50 words max.)

The aim of SIG4 is to raise the awareness and acceptance of Electron Crystallography to a rank comparable to X-ray crystallography. Since the last few years have seen the emergence of many methods of electron crystallography, SIG4 officers now intend to bring all these methods together under a single terminology for greater clarity and visibility: **3D Electron Diffraction** (acronym 3D ED).

2. SIG web site:

SIG 4 url: https://ecaelectronsig.wordpress.com/

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

4. Existence of a SIG mailing list: Yes

Address of the mailing list: ecaelectronsig@iucr.org
Number of members in the SIG mailing list: 45

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

45 researchers (mailing list)

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

7. Prizes sponsored/coordinated

ECM32 (2019, Vienna): NanoMEGAS poster prize

8. Past Activities other than Microsymposia at ECM

8.1. WORKSHOPS, CONGRESSES, CONFERENCES

Title: 2nd Workshop on Advanced Diffraction Techniques for Biology
Grenoble, 19-22 November 2019
https://www2.ccp4.ac.uk/?mxnew=adtb-2019/
- Level of involvement of SIG in the activity:
  - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: The course covered X-rays, neutrons and electrons diffraction by crystals of biological macromolecules. Various techniques were investigated: Macromolecular crystal growth, In situ (in plate) X-ray diffraction, Serial X-ray crystallography, Time resolved X-ray crystallography, Neutron diffraction, Electron diffraction of nano-crystals with the aim of solving de novo structures, searching ligands, elucidating reaction mechanisms...This 4 days course combined theoretical lectures and practicals on ESRF beamlines and other EPN instruments. It was dedicated to researchers (advanced PhD, PostDoc, Scientist) interested in macromolecular structural studies at atomic resolution using crystallographic approaches.

Title: 3D electron diffraction across nanocrystallography, GE3C online Congress

20 January 2020 (Webinar)
- Number of Participants: >100
-Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
- Description: Invited plenary lecture at the GE3C on line Congress.

Title: 3rd Junior Colloquium of the French Society of Microscopies (online)
18-20 November 2020
- Number of Participants: about 50
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: This colloquium is mainly aimed at doctoral and post-doctoral students, with the possibility of presenting their work in the form of an oral presentation or a poster. During this conference, invited industrialists who work with microscopy were present to share their experience and explain what place microscopy has within their company.

Title: Christmas (online) workshop on electron crystallography
17 December 2020
- Number of Participants (planned): registered ~600, actually present ~300
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
    - ✓ Endorsed (SIG logo on the web page/leaflets)
- Description: The workshop was organized in order to fill the information gap due to the cancellation / rescheduling of the major crystallographic events. One-day online event comprised a collection of reports from the most prominent European research groups related to 3D electron diffraction.

Title: The 39th Ad Hoc Workshop on program Jana – electron diffraction (online)
14-15 January 2021
- Number of Participants: 30
-Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Lectures and tutorial introducing structure analysis from 3D electron diffraction data using programs PETS2 and Jana2020.

8.2. WEBINARS, SEMINARS, LECTURES

Title: Webinar on Advance TEM Tools
13 May 2020
- Number of Participants: 230
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Introduction and application examples in Orientation and Phase mapping analysis by ASTAR technique in Transmission Electron Microscope. ASTAR can provide sample properties details in nm scale for variant materials like alloys, metals, ceramics, nanoparticles, etc. Webinar organized by NanoMEGAS.

Title: Introduction to Precession Electron Diffraction Mapping with TEM
2 June 2020 (Webinar)
- Number of Participants: 248

- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Orientation and Phase mapping, and stain analysis method can be applied in TEM by scanning the sample with a smallest possible probe towards the best possible spatial resolution collecting series of electron diffraction patterns. Webinar organized by NanoMEGAS.

Title: Introduction to Precession Electron Diffraction Mapping with TEM
16 June 2020 (Webinar)
- Number of Participants: 220
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Pair distribution function using electron diffraction data by TEM, provides useful information and can characterize amorphous or nanocrystalline materials. The PDF diagram gives information for the interatomic distance for the amorphous or nanocrystalline materials, leading to material characterization. Webinar organized by NanoMEGAS.

Title: Webinar on Advance Characterization Techniques in TEM by Precession Electron Diffraction
18 June 2020
- Number of Participants: 280
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Precession electron diffraction (PED) method is a well know technique to enhance diffraction quality data in Transmission Microscope (TEM). PED is applied in several advance techniques in TEM leading to improved results. Automated Crystal Orientation mapping in TEM, and 3D electron diffraction by Precession Electron Diffraction Tomography method, are some of the methods that were described in this webinar. Webinar organized by NanoMEGAS.

Title: From inorganic nanoparticles to protein nanocrystals
30 June 2020 (Webinar)
- Number of Participants: >100 (estimated)
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: A webinar organized by Amsterdam Scientific Instruments to promote 3D electron diffraction.

Title: The Nano-Crystallography Revolution: 3D Electron Diffraction from Inorganic Nanocrystals to Macromolecules
7 July 2020 (Seminar and Webinar)
- Number of Participants: 70
-Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Seminar organized by the University of Basel in the Switzerland Innovation Park of Basel about 3D electron diffraction and the most recent development of the technique.

Title: Advanced TEM Applications in Material Science using ASTAR and PED
17 July 2020 (Webinar)
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Precession-enhanced Orientation and Phase mapping method can be further applied in situ, to determine material properties in different conditions and study dynamical phenomena. In this webinar, Automated Crystal Orientation Mapping combined with Cross-correlative Microscopy and in situ studies was shown. Webinar organized by NanoMEGAS.

Title: Concept, instrumentation and practical aspects of applications of 3D Electron Diffraction
10 November 2020 (Webinar)
- Number of Participants: >100
-Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Seminar organized by Eldico Scientific.

Title: ASTAR: Phase & Orientation mapping at nm scale by 4D - SPED in TEM.
2 December 2020 (Webinar)
- Number of Participants: 180
- Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Method introduction and applications in several materials, and precession benefits are described during this webinar. In situ examples by heating, or in liquid in TEM are also shown, to determine dynamical properties of the materials. Webinar organized by NanoMEGAS.

Title: XRD and 3D ED partners in structure solution and refinement.
3 December 2020 (Webinar)
- Number of Participants: >100
-Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Seminar organized by STOE for discussing the possible synergy between 3D electron diffraction and powder x-ray diffraction.

Title: The Nanocrystallography Revolution
9 December 2020 (Webinar)
- Number of Participants: >100
-Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Seminar organized by Eldico Scientific to discuss the actual state of development of 3D electron diffraction.

Title: ASTAR: Novel features and advanced results applied to a variety of challenging materials.
9 December 2020 (Webinar)
Number of Participants: 150
- Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Advance tools of ASTAR software dedicated for ACOM analysis, provides further details of the sample properties, like grain boundary maps and size measurement, grain size distribution, twins identification, texture analysis, grains overlapping, dislocations, etc. Those advanced tools and applications in several materials are discussed in detail in this webinar. Webinar organized by NanoMEGAS.

Title: Specialized Electron Crystallography Sample Holder (StartIP Matching day)
18 December 2020
https://www.inits.at/en/startip_portfolio/specialized-electron-crystallography-sample-holder/
- Number of Participants: 80
- Level of involvement of SIG in the activity:
✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: A 5' talk about the concept of the holder with the purpose to find a company to build a goniometer / holder for 3D ED. Crystallography is a chemistry technique for characterizing compounds.

Standard crystallography uses X-ray technology, but this is limited because crystals must be a certain size. Only about a third of crystalline compounds make large crystals. Alternatively, transmission electron microscopes can be used for the same technique. Here, there is no lower size limitation, but these machines are designed for imaging, not crystallography. This technology is a sample holder for these microscopes but specialized for crystallography, with the aim of removing one of the current bottlenecks of this technique. START:IP supports the commercialization of exciting research results by connecting providers of cutting-edge technologies from academic or industrial research with interested founders, corporations and investors.

Title: Demanding crystallographic problems of inorganics solved by 3D-ED - Benefits of STEM-ADT
13 January 2021 (Webinar)
- Number of Participants: 100
-Level of involvement of SIG in the activity:
    ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Seminar organized by Eldico Scientific.

Title: Low-dose electron crystallography: fast, easy and powerful
15 January 2021 (Webinar)
- Number of Participants: 50
-Level of involvement of SIG in the activity:
    ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Presentation of a 3D electron diffraction method for beam sensitive materials. Webinar organized by the Institute of Structural Biology (Grenoble, France).

Title: Kay Diederichs Course on Crystallography
Konstanz, 2 February 2021
- Level of involvement of SIG in the activity:
    ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Lecture on 3D Electron Diffraction.

9. Future/Programmed Activities.

Title: Electron Nanocrystallography (NanED) – ITN project funded by EU (grant n° 956099)
- Number of Participants: 10 PI's + 15 PhD students + several researchers
- Level of involvement of SIG in the activity: All the PI's involved are members of the SIG4
    ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    ✓ Endorsed (SIG logo on the web page/leaflets) at the moment no but we think to involve the SIG4 during the project
- Description: NanED aims to form a new generation of electron crystallographers, able to master and develop 3D electron diffraction techniques in an interdisciplinary and interconnected network, where competences and know-how of usually distant scientific sectors are shared and merged.
NanED includes several European scientists hitherto active in the development of electron diffraction methods for structural crystallography and a pool of large and small companies interested in instruments development and materials or pharmaceuticals production and analysis. Ten different countries are represented:
Italy, Czech Republic, France, Sweden, Belgium, the Netherlands, Switzerland, Germany and United Kingdom. NanED will organize in the next four years several training open workshops in order to train young scientists on 3D electron diffraction.

Title: 1st CCP4 Crystallographic School in South Africa – Data Collection to Structure Refinement and Beyond

22 February – 5 March 2021, Online
https://www.ccp4.ac.uk/?workshop=ccp4-crystallographic-school-in-south-africa/
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: The workshop will cover all aspects of protein structure solution by X-ray crystallography, including the fundamental concepts of protein crystallography, crystallographic data collection, processing of diffraction data, phasing, structure refinement, validation and deposition in the PDB, as well as an introduction to CryoEM and Electron Diffraction.

Title: The 40th Ad Hoc Workshop on program Jana – electron diffraction
March 2021 (Webinar, exact date to be established)
- Number of Participants: 50 (estimated)
-Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Member registered with the SIG involved as lecturer
- Description: Lectures and tutorial introducing structure analysis from 3D electron diffraction data using programs PETS2 and Jana2020.

Title: A four half-day introductory course on Three-Dimensional Electron Diffraction
12-15 April 2021 (Online)
https://register.gotowebinar.com/register/19403493398252302
- Number of Participants: >200 (estimated)
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
    - ✓ Endorsed (SIG logo on the web page/leaflets)
- Description: 3D electron diffraction is a powerful method for structure determination of nano- and submicron-sized crystals. It overcomes the fundamental drawback of single crystal X-ray diffraction, where large crystals are indispensable. Here, we offer the course where you can learn details about how to collect, process and use 3D electron diffraction data for structure elucidation.

Title: 25th IUCr Congress – postponed to 2021
Prague, 14-22 August 2021 (Hybrid congress)
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
- List of MS proposed by the Commission of Electron Crystallography
    - CryoEM for macromolecules – from single particles to microcrystals
    - Combination of X-ray and electrons for structure characterization
    - Application of electron crystallography to functional materials
    - Analysis of the fine structure in electron diffraction data
    - In-situ and time resolved electron crystallography
    - Crystal structures of pharmaceutical and organic compounds from electron diffraction
    - Recent advances in electron crystallography techniques
- List of MS proposed by another commission but supported by the Commission of Electron Crystallography
    - Validation of cryoEM structures and maps
    - Energy materials
    - Ab initio powder structure analysis for polymorphism and phase transformation studies with pharmaceutical applications
    - Ptychography: present and near future
    - Disordered materials: spectroscopic and scattering techniques

Title: ePDF workshop – satellite to IUCr meeting – postponed to 2021
- Number of Participants (planned): 60
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
    - ✓ Endorsed (SIG logo on the web page/leaflets)
- Description: The workshop is organized as a satellite event to IUCr congress in Prague. The topical focus is devoted to electron scattering phenomena beyond Bragg diffraction, calculation of pair distribution function from electron diffraction data (ePDF), interpretation of the data and the strength and limitation of the method. The workshop will be rescheduled and organized in online format.

Title: Electron Crystallography School - 3D Electron Diffraction/MicroED Bridging Small Molecule and Macromolecular Crystallography – satellite to IUCr meeting– postponed to 2021
August 11-14, 2021, Tabor, South Bohemia, Czech Republic (or Virtual school)
https://www.xray.cz/iucr/workshops/tabor/default.htm
- Number of Participants: >100
-Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
    - ✓Endorsed (SIG logo on the web page/leaflets): No, it was sponsored by IUCr
- Description: School on 3D electron diffraction/MicroED techniques and how to apply them for structure determination of nano/microcrystals too small for X-ray diffraction. The topics will cover inorganic compounds, pharmaceutics and proteins. It includes both lectures and practical sessions.
Topics:
- The development of various 3D electron diffraction/MicroED techniques – a historical perspective
- Introduction to transmission electron microscopy and electron diffraction
- 3D electron diffraction/MicroED (SAED, PED, EDT) and space group determination
- Sample preparation for both materials and life sciences
- 3D ED/MicroED Data collection
- Radiation damage
- 3D ED Data Processing and data merging including practical demo labs
- Methods for phasing diffraction data – small molecules and macromolecules
- Practical demo labs for structure solution and refinement with 3D ED/MicroED data – two groups for small molecules and macromolecules, respectively
- Dynamical refinement
- New developments in 3D electron crystallography

Title: European Microscopy Congress 2020 (EMC2020), session: Diffraction techniques and structural analysis - postponed to 2024
Copenhagen, 2024
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Members registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
- Description: Diffraction techniques and structural analysis. Structural analysis and nanoscale crystallography using electron diffraction and related methods has undergone a renaissance in recent years. There have been a series of major developments in recent years that have transformed the field, including: the advent of remarkably sensitive, almost noise-free, cameras and detectors; the introduction of automated data collection and big data processing (e.g. machine learning); and the availability of dedicated software that enables robust and reliable structure determination from electron data. This has led to an explosion of interest across a wide range of materials and life sciences in using these techniques to (i) solve crystal structures not amenable to more conventional x-ray

diffraction and (ii) to use the high spatial resolution of the microscopes to reveal hitherto unseen micro- and nano-structure using 4D scanning methods, acquiring diffraction patterns at every real space probe position.
This session highlights the progress made in this area using both scanning electron microscopy (with techniques such as EBSD (2D and 3D), ECCI, TKD and (scanning) transmission electron microscopy such as 4D-STEM, SED, SPED, PED, CBED, SCBED, HRTEM, time-resolved diffraction and ptychography. We would also encourage submission of papers from complementary fields such as atom probe tomography and scanning transmission x-ray microscopy.

Title: Congress of the French Crystallographic Association
29 June – 2 July 2021 (Online)
- Level of involvement of SIG in the activity:
    - ✓ ECA Individual Member registered with the SIG involved in the organizing committee
    - ✓ ECA Individual Members registered with the SIG involved as lecturers
- Description: Congress on crystallography in materials science, biology and mineralogy.

10. Other matters. (50 words max.)

The SIG4 website was enriched with 11 presentations on recent results in 3D electron diffraction.

11. Brief annual activity report (100 words max.)

The one-day online workshop organized by SIG4 was a great success, with about 300 participants simultaneously connected.

SIG4 still takes an active part in the program committee of the 15th IUCr meeting in Prague (2021). And a member of SIG4 is involved in the organization of the next European Microscopy Congress (Copenhagen, 2024).

Despite the pandemic, SIG4 members remain very active in presenting the most recent developments in 3D electron diffraction at webinars, with usually more than 100 attendees.

The number of participants to the SIG4 events clearly evidences the interest of the scientific community for 3D electron diffraction developments. SIG4 would therefore insist to get large rooms for microsymposia involving 3D electron diffraction at the next ECM congresses.

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

Stéphanie KODJIKIAN, Stephanie.kodjikian@neel.cnrs.fr, chair
Mauro GEMMI, Mauro.Gemmi@iit.it, co-chair
Lukas PALATINUS, palat@fzu.cz, secretary
Jérôme PACAUD, jerome.pacaud@univ-poitiers.fr, moderator of the mailing list