

EMRS SYMPOSIUM N

MONDAY 15 SEPTEMBER

Structure solution and refinement: Advances & perspectives, Chairs: Wladek Minor, Sven Lidin

09:00	Synchrotron SOLARIS, present status and future development M.J. Stankiewicz ^{1,2} , C. J. Bocchetta ¹ , R. Nietubyc ^{1,3} , K. Szamota-Leandersson ¹ , A. I. Wawrzyniak ^{1,2} and M. Zajac ¹ 1 National Synchrotron Radiation Centre SOLARIS, Jagiellonian Univ., 30-392 Krakow, Poland; 2 Inst. of Physics, Jagiellonian Univ. ul. Reymonta 4, 31-059 Krakow, Poland; 3 Narodowe Centrum Badań Jądrowych, 05-400 Otwock, Świerk, Poland
09:30	Recent advances in crystal structure solution by powder diffraction data Angela Altomare, Corrado Cuocci, Anna Molterni, Rosanna Rizzi, a a Institute of Crystallography CNR, via Amendola 122/o 70126 Bari, Italy
10:00	Beyond the Bragg peaks: Correlation function studies of the structure of materials Alex C. Hannon ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11, U.K.
10:30	Coffee break
	Nanocrystalline and nanoporous materials, Chairs: Jaroslaw Majewski, Michael Knapp
11:00	Crystallography of phase transitions in (Ti,Al)N nanocomposites controlled by microstructure defects David Rafaja Institute of Materials Science, TU Bergakademie Freiberg, Gustav-Zeuner-Str. 5, D-09599 Freiberg, Germany
11:30	Zeolitic materials Kenny Stahl Department of Chemistry Technical University of Denmark, 2800 Lyngby, Denmark
12:00	Small metal clusters in catalysis Zbigniew Kaszku ^r Institute of Physical Chemistry PAS, Warsaw, Poland
12:30	Insights into human dentine nanostructure by combined diffraction and phase contrast-enhanced tomography Paul Zaslansky, Jean-Baptiste Forien, Anke Maerten, Claudia Fleck Julius Wolff Inst. Charité - Universitätsmedizin Berlin: Fachgebiet Werkstofftechnik, Technische Univ Berlin, Germany
12:40	Lunch break
	Functional materials 1, Chairs: Zbigniew Kaszku, Krystyna Ławniczak-Jabłońska
14:00	In-situ synchrotron and neutron studies on Li-ion battery materials M. Knapp ¹ , N. Kiziltas-Yavuz ¹ , M. Yavuz ¹ , M. Muehlbauer ^{2,3} 1 Institute for Applied Materials- Energy Storage Systems (IAM-ESS), Karlsruhe Institute of Technology (KIT), Germany; 2. Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Technische Universität München, D-85748 Garching b. München, Germany; 3. Material Science, Technische Universität Darmstadt, D-64287 Darmstadt, Germany
14:30	In-situ and ex-situ neutron diffraction experiments on electrode materials for Li-ion batteries Matteo Bianchi _(a,b,c,d) , Emmanuelle Suard _(c) , Christian Masquelier _(a,d) and Laurence Croguennec _(b,d) (a) Lab. de Réactivité et de Chimie des Solides, CNRS-UMR#7314, Univ. de Picardie Jules Verne, F-80039 Amiens Cedex 1, France; (b) CNRS, Univ. Bordeaux, ICMCB, UPR 9048, F-33600 Pessac, France; (c) Inst. Laue-Langevin, 6 rue J. Horowitz, F-38000 Grenoble, France; (d) RS2E, Réseau Français sur le Stockage Electrochimique de l'Energie, FR CNRS#3459, F-80039 Amiens Cedex 1, France
15:00	In-situ XRD studies on the influence of stress on the low-temperature degradation of zirconia ceramics Klaus G. Nickel, Tobias Kiemele, Christoph Berhold, Mike Swain 1 to 3: University of Tübingen, Germany, Faculty of Science, Department of Geosciences, Applied Mineralogy; 4: University of Sydney, Faculty for Dentistry, Australia
15:10	Quantitative study of dislocation densities of friction stir processed in-situ particles reinforced TiB ₂ /AA6063 composites by X-ray line analysis T. Yan, Z. Chen, A. Borbely, G. Ji, S.Y. Zhong, V. Ji, H.W. Wang a State Key Laboratory of Metal Matrix Composites, Shanghai Jiao Tong University, Shanghai 200240, P.R. China b SMS Materials Center and CNRS UMR 5146, Ecole des mines de Saint Etienne, 158, cours Fauriel, 42023 Saint Etienne, France c Unité Matériaux et Transformations, CNRS UMR 8207, Université Lille 1, Villeneuve d'Ascq, 59655, France. d ICMMO/LEMHE, UMR CNRS 8182, Université Paris-Sud 11, Orsay Cedex, 91405, France
15:20	Crystallography orientation of Cu-Sn IMC in Cu/Sn-3.5Ag/Cu-xZn microbumps and Zn-doped solder joints Wei Tu, Hsiang-Ching Chang, Jenq-Gong Duh Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, Taiwan
15:30	Coffee break
	Crystallography at the turn of the millennium, Chairs: John Tse, Matteo Leoni
16:00	X-ray diffraction - toward the future of structural biology Wladek Minor ^{1,3,4,5,6} , A. Wlodawer ² , Heping Zheng ^{1,3,4,5} , Hou Jing ^{1,3,5,6} , M.D. Zimmerman ^{1,3,4,5,6} , Marek Grabowski ^{1,3,4,5,6} 1 University of Virginia, Charlottesville, VA 22903, USA; 2 National Cancer Institute, Frederick, MD 21702, USA; 3 Midwest Center for Structural Genomics, USA; 4 New York Structural Genomics Research Consortium, USA; 5 Center for Structural Genomics of Infectious Diseases, USA 6 Enzyme Function Initiative, USA

16:30	Aperiodic materials: Why and how? Sven Lidin Polymer and Materials Chemistry, Lund University, Box 124, SE-22100 Lund, Sweden
17:00	Quasicrystal structure analysis - goals and limits Walter Steurer Laboratory of Crystallography ETH Zurich Vladimir-Prelog-Weg 5 8093 Zurich, Switzerland
17:30	Ab Initio Random Structure Searching for phase prediction in niobites (ANbO ₃ , A=Li, Na, K, Rb). Anna Kimmel, Chris Pickard National Physical Laboratory, University College London, London, U.K.
17:40	Poster Session (in: Main Hall and Institute of Physics)
	TUESDAY 16 SEPTEMBER
	Diffraction and scattering tools for studies of materials structure, defects and properties, Chairs: Pierre Ruterana, Wiesław Lasocha
09:00	X-ray and neutron scattering studies of bio-relevant structures: From model lipid membranes to living cell cultures under flow stress Jaroslaw Majewski Los Alamos Neutron Scattering Center, H-805, Los Alamos National Laboratory, Los Alamos, NM, 87545, USA
09:30	Diffraction and phase contrast imaging of defects in crystals J.M Yi ¹ , T.S. Argunova ^{1,2} , and Jung Ho Je ¹ 1 X-ray Imaging Center, Department of Materials Science and Engineering, University of Science and Technology, Pohang, South Korea; 2 Ioffe Physico-Technical Institute, RAS, St Petersburg, Russian Federation
10:00	Synchrotron Mössbauer reflectometry: A tool for magnetic thin film analysis Dénes Lajos Nagy Wigner Research Centre for Physics of the Hungarian Academy of Sciences, Budapest, Hungary
10:30	Coffee break
	Structure and microstructure analysis using X-ray and electron diffraction, Chairs: Walter Steurer, Jung Ho Je
11:00	Progress in microstructure analysis by diffraction Matteo Leoni DICAM - University of Trento, via Mesiano, 77 - 38123 Trento, Italy
11:30	Structure solution of complex intermetallics using solely electron diffraction data Louisa Meshi, Shmuel Samaha 1) Department of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel 2) Ilse Katz Institute for Nanoscale Science and Technology, Ben Gurion university of the Negev, Beer-Sheva, Israel
12:00	Glancing incidence X-ray diffraction as an efficient tool to probe the structure and the microstructure of polycrystalline thin layers D Simeone ¹ , G. Baldinozzi ¹ , J-F Berar ² 1 CEA/DEN/DANS/DM2S/ LRC CARMEN CEN Saclay France & CNRS/ SPMS UMR8785 LRC CARMEN, Ecole Centrale de Paris, F92292, Chatenay Malabry. 2 Institut Neel, CNRS & Université Joseph Fourier, BP 166, Grenoble Cedex, France
12:10	XRPD study of crystal growth and phase transformations of nanocrystalline oxides Giora Kimmel, Dmitry Mogilyanski, Roni Z. Shneek, Jacob Zabicky Dept of Nucl. Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel; Characterization Lab. Center, Ilse Katz Institute for Nanoscale Science & Technology, Ben-Gurion Univ. of the Negev, Beer-Sheva, Israel; Dept of Materials Engineering, Ben-Gurion Univ. of the Negev, Beer-Sheva, Israel; Dept of Chemical Engineering, Ben-Gurion Univ. of the Negev, Beer-Sheva, Israel
12:20	Multiaxial diffraction analysis of highly textured materials: monoclinic HfO ₂ thin films A. Gómez-Núñez, J. Bassas, A. Vilà University of Barcelona, Department of Electronics, Martí i Franqués 1, E08028-Barcelona, Spain; University of Barcelona, Scientific and Technological Centers (CCITUB), E08028-Barcelona, Spain; University of Barcelona, Department of Electronics, Martí i Franqués 1, E08028-Barcelona, Spain
12:30	Orientation-sensitive growth of graphene on platinum thin films and thermal-assisted transfer of patterned graphene films Jae-Kyung Choi, Jinsung Kwak, Soon-Dong Park, Minbok Jung, Hyung Duk Yun, Seoktae Kang, Dong-Su Lee, Dong-Yeon Park, Suk-Kyung Hong, Sung Youb Kim, Hyung-Joon Shin, and Soon-Yong Kwon School of Materials Science and Engineering, Ulsan National Institute of Science and Technology (UNIST), Korea; School of Mechanical and Nuclear Engineering, Ulsan National Institute of Science and Technology (UNIST), Korea; Dept of Civil Engineering, Kyung Hee University, Korea; G-Mek Incorporation, Korea
12:40	Lunch break
	Electron microscopy as a fine crystallographic tool for semiconductors and other materials, Chairs: Manfred Burghammer, Magali Morales
14:00	Determination of growth polarity by Convergent Beam Electron Diffraction in III-V semiconductors Zuzanna Liliental-Weber Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.
14:30	The combined topological analysis, atomistic modeling and HRTEM of grain boundaries in wurtzite materials Pierre Ruterana CIMAP UMR 6252, ENSICAEN, 6 Bd Marechal Juin, 14050, Caen, France

15:00	Self-ordering on sapphire vicinal surfaces: A study by AFM and GISAXS measurements <u>Elsa Thune</u> 1, Caroline Matringe1, David Babonneau2, Ahmad Fakih1, René Guinebretière1 1. Laboratoire Science des Procédés Céramiques et de Traitement de Surface (SPCTS, UMR CNRS 7315), ENSCI, Centre Européen de la Céramique (CEC), 12 rue Atlantis, 87068 Limoges Cedex, France; 2. Institut PPRIME (UPR CNRS 3346), Université de Poitiers, SP2MI, Téléport 2, Boulevard Marie et Pierre Curie, BP 30179, 86962 Futuroscope Chasseneuil Cedex, France
15:10	Structure and crystallography of inclined GaN nanowires using TEM methods <u>A. Lotsari</u> 1, <u>G. P. Dimitrakopulos</u> 1, Th. Kehagias1, A. Adikianakis2, Ph. Komnina, A. Georgakilas2 1Physics Department, Aristotle University of Thessaloniki, GR 541 24, Thessaloniki, Greece; 2Microelectronics Research Group (MRG), IESL, FORTH, P.O. Box 1385, 71110 Heraklion Crete, Greece; and Physics Dept, Univ. of Crete, Heraklion Crete, Greece
15:20	X-ray and electron diffraction studies in ruby crystals <u>B.B.Nayak</u> , T.Dash, B.K. Mishra CSIR-IMMT, Bhubaneswar-751013, India
15:30	Coffee break
	Crystallography of novel and functional materials, Chairs: Alex Hannon, Bijanbihari Nayak
16:00	New hybrid organic-inorganic materials: Synthesis, structure, applications <u>Wiesław Łasocha</u> 1,2, Katarzyna Luberda-Durnaś2 1 Fac. of Chemistry, Jagiellonian Univ., Ingardena 3, 30-060 Krakow, Poland; 2 J. Haber Inst. of Catalysis, PAS, 30-239 Krakow, Poland
16:30	Applications of real time, high temperature diffraction at MCX@Elettra <u>Jasper Plaisier</u> , Mahmoud Abdellatif & Andrea Lauti Elettra – Sincrotrone Trieste, Strada Statale 14 – km 163,5, 34149 Basovizza, Trieste, Italy
17:00	Structural analysis of new titanium oxide material exhibiting functionality in the absence of light irradiation <u>Toshihiro Okajima</u> 1, <u>Toshio Irie</u> 2, <u>Hiroshi Shirasawa</u> 3, <u>Kenji Suzuki</u> 4 1 Kyushu Synchrotron Light Res.Ctrr, Saga 841-0005, Japan; 2 New Catalyst Res.Inst., Funabashi, Chiba 274-0825, Japan; 3 Graduated School of Medicine, Chiba Univ., Chiba, Chiba 263-8522, Japan; 4 Advanced Inst. of Materials Science, Sendai, Miyagi 982-0252, Japan.
17:10	Crystal structure peculiarities of the Zr(Ti)3Cr30 compounds and their hydrides <u>P. Lyuty</u> , V. Shtender, A. Riabov, I. Zavalny Karpenko Physico-Mechanical Institute of the NAS of Ukraine, 5 Naukova St., Lviv, 79601, Ukraine
17:20	Synthesis of magnetic doped kesterite single crystals <u>Maciej Bialogłowski</u> , Mohammad Fadaghı, Paulina Marek, Grzegorz Matyszczak, Michał Wrzecionek, Sławomir Podsiadło Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland
17:30	p-type and n-type polycrystalline silicon thin films formed by aluminium induced crystallization and solid phase epitaxy <u>Mehmet Karaman</u> , Özge Tüzün Özmen, Salar Habibpur Sedani, Rasit Turan GUNAM, Middle East Technical University , 06800 Ankara, Turkey: Department of Physics, Düzce University, 81620 Düzce, Turkey; GUNAM, Middle East Technical Univ. , 06800 Ankara, Turkey: Dept of Physics, Middle East Technical University, 06800 Ankara, Turkey
17:40	Poster Session (in: Main Hall and Institute of Physics)
	WEDNESDAY 17 SEPTEMBER
09:00	Plenary Session - Main Hall
12:30	Lunch break
	Materials Science - Advanced characterization - PART 1 (Joint with symposia H & J), Chairs: Jean Fompeyrine, Wojciech Paszkowicz, Thilo Glatzel
14:00	Reciprocal space meets real space - employing nano-beams for scanning diffraction T. Dane 1, E. Di Cola 1, L. Lardiere 1, C. Montero 2, C. Riekel 1, M. Sztucki 1, B. Weinhausen 1, and M. Burghammer 1,3 1 European Synchrotron Radiation Facility, Grenoble, France; 2 Université Montpellier 2, Laboratoire de Mécanique et Génie Civil , Montpellier, France; 3 Ghent University, Department of Analytical Chemistry, Ghent, Belgium
14:30	Combined refinement of GIXRF, XRR and XRD data in a global approach: analysis of textured In2O3/Ag/ In2O3/Si architectures and III-V based heterostructures <u>Magali Morales</u> (1), L. Lutterotti (2), Daniel Chateigner(2), Bérenger Caby(3), Emmanuel Nolot(3), Patrice Gergaud(3), G. Pepponi (4) (1) CIMAP – ENSICAEN, 6 bd Mar-I Juin, 14050 Caen Cedex 4 (2) CRISMAT ENSICAEN, 6 bd du Mar-I Juin, 14050 Caen Cedex 4 (3) CEA Grenoble, 17 rue des Martyrs, 38054 Grenoble Cedex 9 (4) Fondazione Bruno Kessler – Via S.Croce 77, 38122 Trento, Italia
15:00	Aberration-corrected atomic-resolution electron microscopy for advanced materials characterization Rolf Erni Electron Microscopy Center, Empa, Swiss Federal Labs for Materials Science and Technology, Dübendorf, Switzerland
15:30	Coffee break
	Materials Science - Advanced characterization - PART 2 (Joint with symposia H & J), Chairs: Jean Fompeyrine, Wojciech Paszkowicz, Thilo Glatzel
16:00	Local probing and writing with helium ions <u>E. van Veldhoven</u> 1, D. J. Maas1, G. Nanda2, P.F.A. Alkemade2 1 TNO, Nano-instrumentation, Delft, Netherlands 2 Delft Univ. Technol, Kavli Inst. of Nanoscience, Delft, The Netherlands
16:30	Investigation of photovoltaic and photo-catalytic materials by surface photovoltage techniques Thomas Dittrich Helmholtz Center Berlin for Materials and Energy, Hahn-Meitner-Platz 1, 14109 Berlin, Germany
17:00	Hall effect metrology for ultra-thin semiconducting layers Dirch H. Petersen, Henrik H. Henrichsen, Rong Lin, Peter F. Nielsen, Ole Hansen Department of Micro- and Nanotechnology, Technical University of Denmark, DTU Nanotech, Building 345E, DK-2800 Kongens Lyngby, Denmark : CAPRES A/S, Scion-DTU, Building 373, DK-2800 Kongens Lyngby, Denmark

17:30	Break
18:00	Best Presentation Awards Ceremony and Reception - Main Hall
THURSDAY 18 SEPTEMBER	
	Synchrotron tools: Present and future opportunities, Chairs: Izabela Sosnowska, Kenny Stahl
08:50	Characterizing nano-precipitates in steels using in-house SAXS and SANS <u>M. Ohnuma</u> 1, M. Furusaka 1, B.S. Seong 2, J. Suzuki 3, T. Ishida 1, R. Hashimoto 1 1 Hokkaido University, 5 Chome Kita 8 Jonishi, Kita Ward, Sapporo, Hokkaido 060-0808, Japan; 2 Korea Atomic Energy Research Institute., 989-111, Daedeokdaero, Yuseong-gu, Daejeon, 305-353, Rep. of Korea; 3 Comprehensive Res. Organization for Science and Society (CROSS), Tokai, Ibaraki 319-1106, Japan
09:00	Quantitative XRD analysis, a tool for the quality control of clinker and cements L. Leon-Reina(a), A. G. De la Torre(a) and M. A. G. Aranda(b) (a)Universidad de Málaga, Málaga, Spain; (b)CELLS-ALBA synchrotron, Barcelona, Spain
09:30	New facility for long duration experiments at Diamond synchrotron source Claire A. Murray, Paul Adamson, Sarah Day, Stephen P. Thompson, Jonathan Potter & Chiu C. Tang Diamond Light Source, Harwell Science and Innovation Campus, Didcot, Oxfordshire OX11 0DE, United Kingdom
10:00	100 years on. Farewell experimental crystallography? W I F David ISIS Facility, Rutherford Appleton Laboratory, OX11 0QX, UK; Inorganic Chemistry Lab., Univ. of Oxford, OX1 3QR, UK
10:30	Coffee break
	Functional materials 2, Chairs: Denes Nagy, Krzysztof Wozniak
11:00	Physical properties of complex metallic alloys in relation to crystal structures Janez Dolinsk J. Stefan Institute, University of Ljubljana, Jamova 39, SI-1000 Ljubljana, Slovenia
11:30	Crystallographic features and chemical bonding in thermoelectric materials Yuri Grin Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany
12:00	Growth of SnS2 single crystals for single-layer exfoliation Maciej Bialogłowski, Mohammad Fadaghı, Paulina Marek, Grzegorz Matyszczak, Michał Wrzecionek, Sławomir Podsiadło Warsaw Univ. of Technology, Noakowskiego 3, 00-664 Warsaw, Poland
12:10	The investigation of the structure of bulk metallic glasses before and after laser welding Wirkinia Pilarczyk Silesian University of Technology, The Faculty of Mechanical Engineering, Institute of Engineering Materials and Biomaterials, 18a Konarskiego Street, 44-100 Gliwice, Poland
12:20	Magnetic quantum dots formed in semiconductor – structural and magnetic properties as resulted from X-ray absorption study Krzystyna Lawniczak-Jablonska Institute of Physics, PAS, al. Lotników 32/46, 02 668 Warsaw, Poland
12:40	Lunch break
	Crystallography and physics of materials formed at high pressures, Chairs: Andre Authier, David Rafaja
14:00	Unexplored universe of high-pressure materials Andrzej Katrusiak Faculty of Chemistry, A.Mickiewicz Univ., Umultowska 89b, 61-614 Poznan, Poland
14:30	Structure and charge density in high pressure solids John S. Tse University of Saskatchewan, Saskatoon, Canada
15:00	Exploring the properties of materials using high-pressure x-ray diffraction: Recent advances and future challenges D. Errandonea Dept Fisica Aplicada, Universitat de València, 46100 Burjassot (Valencia), Spain
15:30	Coffee break
	Crystallography: Its past, present and future, Chairs: W.I.F. David, Angela Altomare
16:00	Fifty years of Time-of-Flight (TOF) neutron diffraction at pulsed neutron sources I.M. Sosnowska University of Warsaw, 00-691 Warsaw, Hoza 69, Poland
16:30	X-ray structural analysis century after the Braggs - success or failure? Krzysztof Wozniak Chemistry Department, University of Warsaw, Pasteura 1, 02-093 Warszawa, Poland
17:00-17:30	Early days of X-ray diffraction – first applications to material science André Authier Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Univ. P. & M. Curie, France