DanScatt Annual Meeting 2019

Department of Mathematics, Ny Munkegade 118, 8000 Aarhus C

Auditorium E (1533-103)

23rd – 24th May 2019, Aarhus University

AARHUS UNIVERSITET

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Contents

Practical information

The first part of the meeting will take place in Auditorium E at the Department of Mathematics, Ny Munkegade 118, 8000 Aarhus C. From Ny Munkegade, you can find Auditorium E by turning right after passing through the main entrance to the Department of Mathematics. Signs will guide you in the right direction. Registration will be in front of Auditorium E.

The poster session will be held at "Vandrehallen", Building 1530, 1st Floor.

WiFi

You can access Eduroam at the venue. If you do not have eduroam log on to AU-Guest and open a webbrowser and go to www.au.dk and follow the instructions. As guest you can sign in with Facebook, Google Drive, LinkedIn, SMS (Danish phone numbers) and Microsoft accounts.

Getting to the venue

City bus 2A (stop Kaserneboulevarden), city bus 22 (stop Aarhus Universitet/Kemisk Institut) or the Light Rail (Letbanen) L2 (stop Aarhus Universitet/Ringgaden are situated near the venue of Danscatt 2019.

Alternately, it takes about 30 minutes to walk from Aarhus train station to the department.

Parking

If you are going by car and have not registered for parking you can write an email to Marianne Sommer (sommer@chem.au.dk) with your license plate number. Parking can also be requested at the registration upon arrival. The map below shows where you can park if you have registered for parking.


5125
Edison
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Adorno
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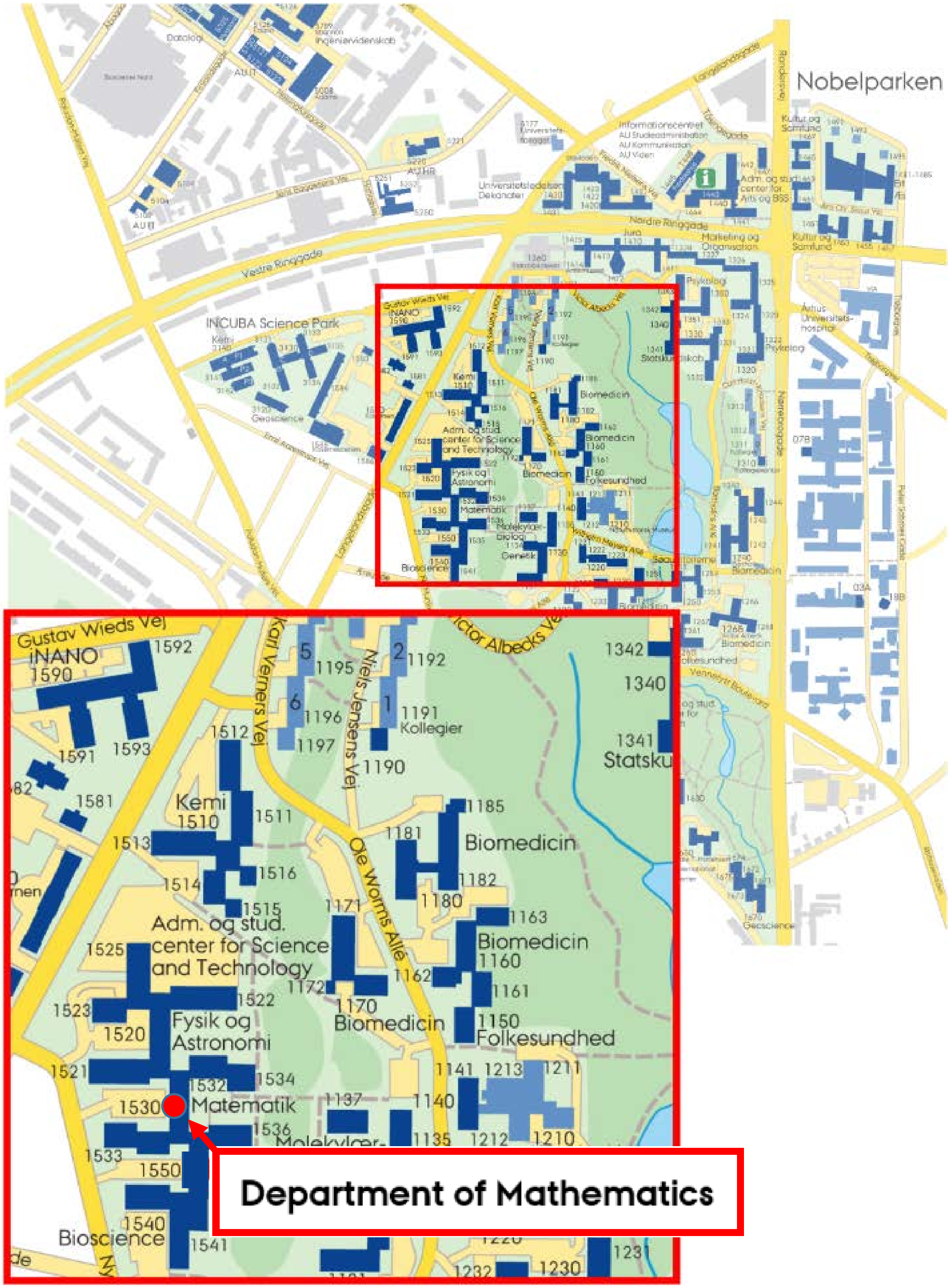
Map of Aarhus University Campus



Danscatt 2019 – Program

Aarhus University
Ny Munkegade 118, 8000 Aarhus C

	Thursday 23rd May
11.00 - 12.00	*Registration and sandwiches* *Vandrehallen, Building 1530-1st floor*
12.00 - 12.05	**Welcome** *Auditorium E, Mathematics, Building 1533-103*
	Chair: Henning Friis Poulsen
12.05 - 12.35	**Michel Kenzelmann:** The new possibilities at SINQ after the upgrade.
12.35 - 12.50	**Christian Kolle Christensen:** Electrochemically Driven Order-Disorder Transitions in $Li_xV_2O_5$ Bronzes
12.50 - 13.05	**Jacob Grinderslev:** Ammonium Borohydride: Investigation of Dynamics and Dihydrogen Bonding
13.05 - 13.20	**Jonathan Quinson:** Synthesis of surfactant-free Pt nanoparticles: solvent-dependent growth mechanisms probed by XAS, *in-situ* SAXS studies and PDF
13.20 - 13.35	**Lasse R. Jørgensen:** Probing the Structure of Thermoelectric Materials in Real-World Conditions: β-Zn_4Sb_3
13.35 - 13.50	*COFFEE BREAK* *Vandrehallen* ***(Posters to be displayed in Vandrehallen)***
	Chair: Søren S. Thirup
13.50 - 14.20	**Christoph Mueller-Dieckmann:** The MX beam lines after the ESRF upgrade.
14.20 - 14.35	**Julie W. Missel:** New structural insights into the regulation of aquaporins
14.35 - 14.50	**René L. Bærentsen:** Understanding the role of tripartite toxin-antitoxin systems in pathogenic *Escherichia coli*
14.50 - 15.20	**PhD prize**
15.20 - 15.45	*COFFEE BREAK* *Auditorium E, Mathematics, Building 1533-103*
	Chair: Mogens Christensen
15.45 - 16.15	**Johan Chang:** Physics and protein diffraction end station at the new SwissFEL
16.15 - 16.30	**Khadijeh Khalili:** Modeling of Time-Resolved X-ray Absorption Spectroscopy Probing Ultrafast Charge Carrier Dynamics in Organic Donor/Acceptor Compounds
16.30-16.45	**Thomas Boesen:** EMBION - the Danish National Cryo-EM Facility + guided tour at the EM facility during the poster session
16.45 - 17.00	**Henning Friis Poulsen:** Danscatt
17.00 - 18.45	**Poster Session sponsored by JJ-Xray** *Vandrehallen - Building 1530-1st floor*
19.00 – 22.30	*Dinner* *Mathematics Canteen*

	Friday 24th May
	Chair: Torben R. Jensen
9.00 - 9.30	**Jimmy Binderup & Martin Schmiele:** LINX - Neutrons at work
9.30 - 10.00	**Radovan Cerny:** Crystallography for rational design of novel ion conductors
10.00 - 10.15	*COFFEE BREAK* *Aud E, Mathematics, 1533, 103*
	Chair: Dorthe Posselt
10.15 - 10.45	**Sarah Koester:** Imaging biological cells by x-rays
10.45 - 11.00	**Helena Ø. Rasmussen:** Unfolding and Partial Refolding of an Industrial Cellulase from the SDS-Denatured State: From β-sheet to α-helix and back
11.00 - 11.15	**T. Hassenkam:** X-ray tomography of 3.7 billion year old remains of life
11.15 - 11.30	*COFFEE BREAK* *Aud E, Mathematics, 1533-103 (Remove posters from Vandrehallen)*
	Chair: Henrik Birkedal
11.30 - 12.00	**Kell Mortensen:** Structural Studies Of Block Copolymer Hydrogels
12.00 - 12.15	**Jette Oddershede:** Mapping Grain Morphology and Orientations in Polycrystalline Materials by Laboratory Diffraction Contrast Tomography
12.15 – 12.30	**Tiago Ramos:** Scanning X-ray Imaging Techniques for Characterization of Energy Materials
	Kirsten Marie Ørnsbjerg Jensen: Characterization of the formation of metal oxido clusters by complex modelling of PDF and SAXS
12.45	*Sandwiches and departure /All posters removed* *Auditorium E, Mathematics, Building 1533-103*
13:15-14:45	**DanMAX Consortium Meeting:** Discussion of DanMAX access strategy A status of the DanMAX project will be given by the DanMAX team. The DanMAX steering committee will present a suggestion for user access, which we wish to discuss with the user consortium. *Auditorium 1, Building 1514-213 (Chemistry)*

The new possibilities at SINQ after the upgrade

Michel Kenzelmann*

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I will give an overview of the opportunities at Swiss Neutron Spallation Source SINQ operated at the Paul Scherrer Institut in Switzerland. We have recently upgraded a number of instruments, and are in midst of a major facility upgrade until June 2020.

The SINQ upgrade includes a complete renewal of all neutron guides, and 4 new or strongly redesigned instruments. The new neutron guides are designed to increase the neutron flux at the sample position with less background scattering. This will allow the study of smaller samples or samples in complex sample environments. Novel instrument concepts will allow more efficient scattering experiments by orders of magnitude.

I will also present some recent science highlights performed at SINQ, taken from the wide spectrum of areas of interest to SINQ users. This includes studies addressing grand challenges in engineering, health, energy, food, and quantum technologies.

Electrochemically Driven Order-Disorder Transitions in $Li_xV_2O_5$ Bronzes

Christian K. Christensen, Daniel R. Sørensen, Jeanette Hvam, Dorthe B. Ravnsbæk*

Dept. of Physics, Chemistry and Pharmacy, SDU, Campusvej 55, 5230 Odense M, Denmark

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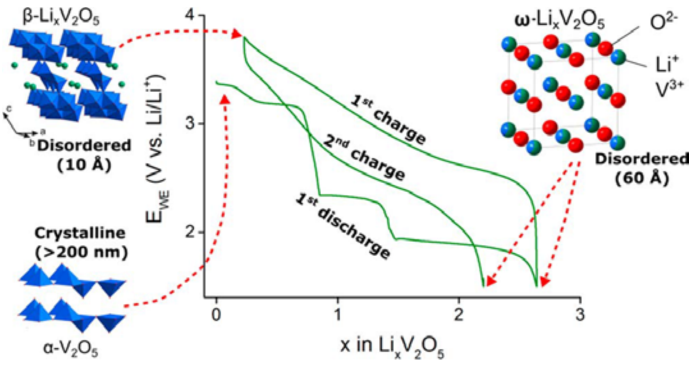
Some materials for rechargeable electrodes undergo an irreversible loss of crystallinity during battery operation. An example of such a material is orthorhombic V_2O_5, which loses long range order upon intercalation of >2 Li.[1] Very little is presently known about the mechanism of either disordering or ion-storage in this material during subsequent charge-discharge cycles. This is in spite of several studies showing that disordered $Li_xV_2O_5$ can provide ~310 mAh/g stable reversible capacity when cycled between 1.5 and 3.8 V, which exceeds the capacity of, videly used $LiCoO_2$ and even "Li-rich $LiNi_xCo_yMn_{1-x-y}O_2$ (NMC)" (240 and 280 mAh/g,[2] respectively).



We have investigated the structural evolution during Li-insertion and -extraction and the associated disordering process in deep discharged V_2O_5 electrodes by means of combined ex situ and operando powder X-ray diffraction and total scattering (i.e. pair distribution function analysis).[3] We find that, the crystalline domain size decreased drastically from >2000 Å to ~60 Å when three Li is inserted to form the ω-$Li_3V_2O_5$ phase. From detailed PDF analysis it was revealed that the resulting disordered rock salt structure has a local dispersed cation ordering within the ccp oxygen lattice. The domain size of this cation ordering is estimated to 10-15 Å. The charged phase has very short range order, 10-15 Å, and the structure is best described as the β-$Li_xV_2O_5$ built on edge and corner sharing $[VO_6]$ octahedra linked by corner sharing $[VO_5]$ square pyramids.

Our results suggest that this material may hold potential as cheap electrode materials despite the fact that they lose long range order. Also our methodology opens for investigating a wide range of order-disorder phenomena in electrochemically driven phase transitions.

References:
1. Delmas, C. *et al.*, *Solid State Ionics* **69** (1994) 257-264.
2. Rozier, P. and Tarascon, J. M., *J. Electrochem. Soc.*, **162** (2015) A2490−A2499.
3. Christensen, C.K., Sørensen, D.R., Hvam, J. and Ravnsbæk, D.B., *Chem. Mater.*, **31** (2019) 512-520

Ammonium Borohydride: Investigation of Dynamics and Dihydrogen Bonding

Jakob B. Grinderslev[1], Mikael S. Andersson[2], Stanislav Filippov[3], Jeff A. Armstrong[4], Maths Karlsson[2], Sergei I. Simak[3], Ulrich Haussermann,[5] Torben R. Jensen[1]

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Energy dense materials may be considered as corner stones in a society based on renewable energy sources. Ammonium borohydride, NH_4BH_4, has one of the highest gravimetric (24.5 wt % H_2) and volumetric hydrogen content (157.3 g·H_2/L) among known compounds and 75 % of the H_2 is released in three distinct exothermic reactions below 160 °C.

The crystal structure of NH_4BH_4 consist of the tetrahedral complex ions, NH_4^+ and BH_4^-, arranged as in the fcc NaCl type structure, with disordered H-positions.[1] Strong intermolecular bonds, dihydrogen bonds, arise from the presence of partially positively charged $H^{\delta+}$ on NH_4^+ and partially negatively charged $H^{\delta-}$ on BH_4^-, which introduces an inherent instability towards H_2-release. At room temperature, NH_4BH_4 decays over a few hours, while it can be stored indefinitely at temperature below -40 °C. Molecular dynamics simulations and NMR measurements reveal the presence of dynamic disorder in the temperature range 100-250 K, caused by a rapid reorientation of the two complex ions.[2]

NH_4BH_4 is an unique model system for the fundamental study of dihydrogen bonding in solid materials. Furthermore, structural changes occur at low temperatures (< 100 K), which causes changes in the crystal structure and the dynamics of the complex ions. Here, NH_4BH_4 is investigated by thermal analysis (TG-DSC-MS), *in situ* synchrotron powder X-ray diffraction (SR-PXD), inelastic neutron scattering (INS) and quasi-elastic neutron scattering (QENS).

In situ SR PXD show no polymorphic transition in the temperature range 100 to 330 K, after which NH_4BH_4 decomposes. In contrast, INS measurements clearly reveal a polymorphic transition at lower temperature, at 45 to 50 K, likely due to altered reorientational dynamics of NH_4^+ and/or BH_4^-. Above 50 K, B-H bending modes and one of the N-H bending modes are observed in the wavenumber range 1000 – 1500 cm^{-1}. Libration and translation bands are apparent in the range 80 – 300 cm^{-1}, which are clearly altered during the polymorphic transition. At 5 K, bending modes from BH_4^- show weak signs of splitting, suggesting that the ion has become immobile.

QENS results reveal three distinct relaxation regimes; a frozen regime below 50 K, and two dynamic regimes in the range 50 to 125 K and 125 to 240 K, respectively. The former is attributed to the dynamics of NH_4^+, while the latter is attributed to BH_4^-. The onset temperature of BH_4^- dynamics is similar to that of the isostructural KBH_4 and $RbBH_4$. QENS results indicate preferred NH_4^+ orientations related to the orientation of the more frozen BH_4^- (at $T < 125$ K).

References

1. A. J. Karkamkar *et al.*, *Chem. Mater.*, 2009, **21**, 4356.
2. R. Flacau *et al.*, *Chem. Comm.* 2010, **46**, 9164-9166.

Synthesis of surfactant-free Pt nanoparticles: solvent-dependent growth mechanisms probed by XAS, *in-situ* SAXS studies and PDF

Jonathan Quinson,*,[a] Jette K. Mathiensen,[a] Alessandro Zana,[b] Jacob J. K. Kirkensgaard,[c]
Mehtap Oezaslan,[d] Kirsten M. Ø. Jensen*,[a] and Matthias Arenz*,[b]

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The Co4Cat^{TM} (colloids for catalysts) synthesis is a new method to obtain colloidal dispersions of surfactant-free precious metal nanoparticles (NPs) in alkaline mono-alcohols [1]. This technology leads to NPs with superior catalytic performances versus industrial benchmarks. To optimize the synthesis and the catalytic properties, a detailed understanding of the NP growth mechanism is gained using X-ray absorption spectroscopy (XAS) [2] but also transmission electron microscopy (TEM) and *in-situ* small angle X-ray scattering (SAXS) [3]. The growth mechanism is strongly solvent–dependent: in methanol a fast nucleation and moderate growth is achieved whereas in ethanol the nucleation is followed by a continuous growth, Figure 1. Together with infra-red spectroscopy (IR) studies, these results are explained by the *in-situ* formation of CO adsorbed on the NP surface formed by oxidation of the solvent (or absence of these species due to poor oxidation properties) while the original Pt^{IV} precursor is reduced to Pt^{II} and Pt^{0} during the synthesis. This knowledge leads to optimized syntheses, e.g. to achieve a fast synthesis at room temperature [4] and propose different strategies to achieve NP size control. Pair distribution function analyses recently performed suggests that an important factor to control further the NPs synthesis in methanol is the formation of Pt-hydroxy or/and methoxy complexes serving as 'seeds' in the nucleation process.

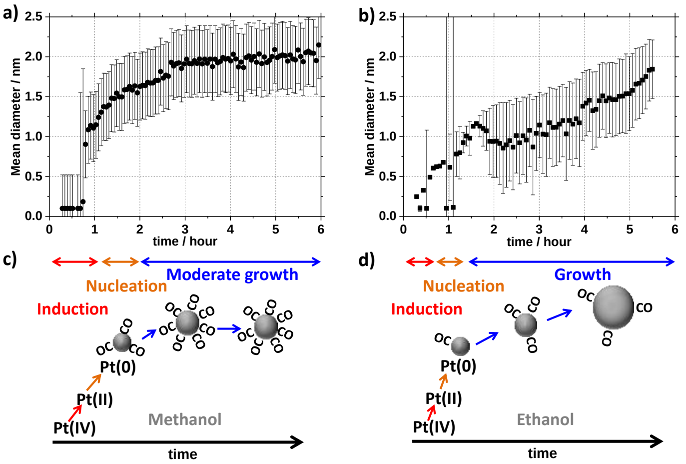

Figure 1. (a,b) In-situ SAXS study of Pt NP formation and (c,d) model accounting for the different grwoth mechanisms in differen solvent

[1] Quinson et al. Angew. Chem. **2018**, 57, 12338
[2] Quinson et al. ChemSusChem **2019**, 12, 1229.
[3] Quinson et al. In preparation.
[4] Quinson et at. Submitted.

Probing the Structure of Thermoelectric Materials in Real-World Conditions: β-Zn_4Sb_3

Lasse Rabøl Jørgensen(1), Christian Moselund Zeuthen(1), Nils Lau Nyborg Broge(1), Kasper Borup(1), Martin Roelsgaard(1), Bo Brummerstedt Iversen(1),*
(1)*Aarhus University, Center for Materials Crystallography, Aarhus, Denmark*
* Corresponding Author: bo@chem.au.dk

The lacking structural integrity of thermoelectric (TE) materials in operation environments is a major limiting factor in the commercialization process. In a TE module, the materials are exposed to both a thermal gradient, which induces significant mechanical stress on the material in the direction of the gradient, along with a direct current, which has also been shown to influence the composition of well-known TE materials [1,2]. Current literature focusing on the stability aspect of TE materials only includes variable temperature powder X-ray diffraction [2,3], which is an experimental setting that does not resemble the environment of an operating module. In the present study, a custom build TE operando setup is presented as seen in Figure 1. It is built to be compatible with the synchrotron beamline of P02.1 at DESY in Hamburg and offers the possibility of simultaneously inducing a current and thermal gradient through a bulk TE material, while monitoring the electrical resistance and the atomic structure. The first trial run scrutinized β-Zn_4Sb_3, where Zn-ions are known to be mobile from theoretical calculations and ex-situ characterization methods [1,2,5]. By measuring conventional X-ray diffraction and total scattering data, it was possible to track the decomposition of the β-Zn_4Sb_3 phase into the ZnSb phase while varying the applied current. In general, the effect of current on TE materials is yet to be deduced despite it constituting a major part of the operation environment. Investigating thermoelectric materials in realistic operation settings yields the best prerequisites for ultimately tailoring stable and reliable TE materials.

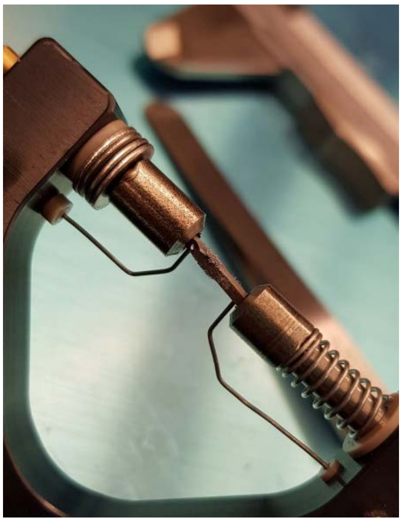

Figure 1 – First version of the Thermoelectric Operando Setup

[1] Yin et al., *Appl. Phys. Lett.*, 2012, **101**, 043901
[2] Yin et al., *ACS Appl. Mater. Interfaces*, 2014, **6** (13), 10542–10548
[3] Jørgensen et al., *J. Mater. Chem. A*, 2018, **6**, 17171-17176
[4] Jørgensen et al., *J. Phys. Chem. C*, 2018, **122** (10), 5317–5324
[5] Løvvik et al., *Comput. Mater. Sci.*, 2011, **9**, 2663-2665

Structural Biology at the ESRF-EBS

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European Synchrotron Radiation Facility

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Abstract text

The European Synchrotron Radiation Facility (ESRF) is currently undergoing a complete replacement of the machine. This upgrade will greatly improve the brightness of the X-ray source by decreasing the horizontal emittance and divergence of the storage ring. The restart of users' operation is foreseen for late August 2020.

This presentation will give an overview of the Structural Biology beamlines and its ancillary technique facilities as they were and which improvements will be available after the machine upgrade. The new ID29 beamline, dedicated to synchrotron serial crystallography experiments will be presented as well an overview given on the services available during the shutdown period.

New structural insights into the regulation of aquaporins

Julie Winkel Missel[1], Kamil Gotfryd[1], Andreia Filipa Mósca[2], Sigurd Friis Truelsen[3], Kaituo Wang[1], Mariana Spulber[4], Simon Krabbe[5], Claus Hélix-Nielsen[3,4], Graça Soveral[2], Per Amstrup Pedersen[5] & Pontus Gourdon[1,6]

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Obesity is a major threat to global health and metabolically associated with glycerol homeostasis. Glycerol flux across plasma membranes, a key component for maintenance of body glycerol levels, is facilitated by aquaglyceroporins. Here we present the first crystal structure of a human aquaglyceroporin (AQP10) determined at 2.3 Å resolution. The structure reveals an unusually wide selectivity (ar/R) filter, and a unique cytoplasmic gate formed by pore-lining residues and a loop. *In vitro* and *in vivo* functional data disclose a glycerol-specific pH-dependence and pinpoint a pH sensor of the glycerol facilitator, corroborating with the structural findings. Molecular dynamics simulations indicate how gate opening is achieved at low pH inducing local structural rearrangements widening the channel. These findings display a novel type of aquaporin regulation important for controlling adipocyte volume and body fat mass. Thus, targeting the novel gate to simulate constitutive glycerol release may open up a novel avenue to treat obesity and related metabolic diseases.

Understanding the role of tripartite toxin-antitoxin systems in pathogenic *Escherichia coli*

René L. Bærentsen[1], Stine V. Nielsen[2], Francesco Bisiak[1], Kenn Gerdes[2], Ditlev E. Brodersen[1]

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Type II toxin-antitoxin systems are small bacterial operons that express a toxin component reducing bacterial growth, and an antitoxin component that neutralizes the effect of the toxin through direct protein-protein interaction. *hipBA* is one of the most well-characterized modules, and its activity has been linked to increased formation of dormant cells able to survive antibiotic treatment.

A novel *hipBA* homolog has been found in the uropathogenic *E. coli* strain O127:H6. This system, named *hipBST,* is unique since it contains three open reading frames, and protein sequence alignments suggest that whereas *hipB* has retained its DNA-binding motif, *hipS* and *hipT* align to the N- and C-terminal parts of *hipA*, suggesting an evolutionary split into two distinct proteins.

We have determined the three-dimensional crystal structure at a resolution of 2.4 Å of this novel protein-complex as found in an antibiotic resistant pathogenic strain of *E. coli*. This represents the first structure of a three-component toxin-antitoxin module, and will help us understand the driving force behind the evolution of tripartite systems, and possibly reveal novel drug strategies towards the emerging threat of multiresistant pathogens.

X-ray Diffraction under Extreme Conditions –

Status on the SwissFEL cristallina beamline

Johan Chang

University of Zurich

With the emergence of two European free electron lasers (XFEL and SwissFEL), prospects for novel x-ray diffraction experiments are promising. This talk discusses plans for the Cristallina beamline at the Swiss Free Electron Laser (SwissFEL). Diffraction instruments, for both “soft” and “hard” condensed matter, are foreseen and example science cases in bio-physics, earth science and quantum matter research will be presented to illustrate future potential and directions. Methodology for efficient use of the pulsed x-ray structure, so-called parasite modes, will be presented together with requirements for sample environment. In this fashion, the talk is inclined towards x-ray diffraction under extreme conditions. Specifically, extremities in magnetic fields and pressure is going to be discussed.

Modeling of Time-Resolved X-ray Absorption Spectroscopy Probing Ultrafast Charge Carrier Dynamics in Organic Donor/Acceptor Compounds

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[3] *The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany*

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In order to develop and improve new types of organic photovoltaic (OPV) devices and reach higher levels of conversion efficiency of solar energy to electric current, it is essential to have a deep understanding of the photoinduced processes in such devices. We investigate the charge transfer dynamics of a donor-acceptor pair, which is widely used as a building block in low band-gap block copolymers for organic photovoltaics. We simulate dynamics of the benzothiadiazole-thiophene molecule (BT-1T) upon interaction with a vacuum ultraviolet (VUV) pulse and study the potential of probing the subsequent charge dynamics with time-resolved X-ray absorption spectroscopy (TRXAS). TRXAS allows detecting the local geometric structure of the system under study and, at the same time, the underlying electronic structure changes that drive the structural dynamics. The photoinduced dynamics in BT-1T are calculated using on-the-fly non-adiabatic molecular dynamics simulations based on Tully's Fewest Switches Surface Hopping approach via XMOLECULE electronic structure toolkit [1]. For snapshots at various time-delays, the sulphur *K*-edge absorption lines in the time-resolved X-ray absorption spectrum reflect the ultrafast charge dynamics in the molecule. We show how our simulations demonstrate the perspective for ultrafast time resolved X-ray experiments at X-ray free electron lasers namely in addressing charge transfer dynamics in organic molecules.

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[1] Y. Hao, L. Inhester, K. Hanasaki, S. K. Son, and R. Santra, “Efficient electronic structure calculation for molecular ionization dynamics at high x-ray intensity,” Struct Dyn. 2, 041707 (2015).

Crystal Chemistry Design of Metal Hydrides as Solid-State Electrolytes

Radovan Černý

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Quai Ernest-Ansermet 24, CH-1211 Geneva, Switzerland

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Complex hydrides based on light hydro- borate anions such as borohydride BH_4^- or *closo*-borate anion $B_{12}H_{12}^{2-}$ find their place as solid stores for hydrogen, and since recently, also as solid electrolytes in Li- and Na-ion batteries. The mobility of the cations depends on the pathways available in the anion packing, chemical interaction of cations with anions and on the anion thermal motion such as tumbling or rotation. While the latter two require important experimental and theoretical effort, the first parameter can be easily analysed and quantified from the crystal structure data obtained by X-ray powder diffraction. A thorough crystal chemistry analysis of observed crystal structures, allows us to find the structural aristotypes and to draw conclusions about the bonding and building principles in this important category of materials as it was done recently for the borohydrides.[1]

Among others, the modification of $Na_2B_{12}H_{12}$, promising Na-ion conductor, by anion modification and anion mixing will be shown (Figure 1).[2-4] The role of packing of the *poly*-anions and structural relations between various solid Li- and Na-electrolytes will be at centre of the presentation.

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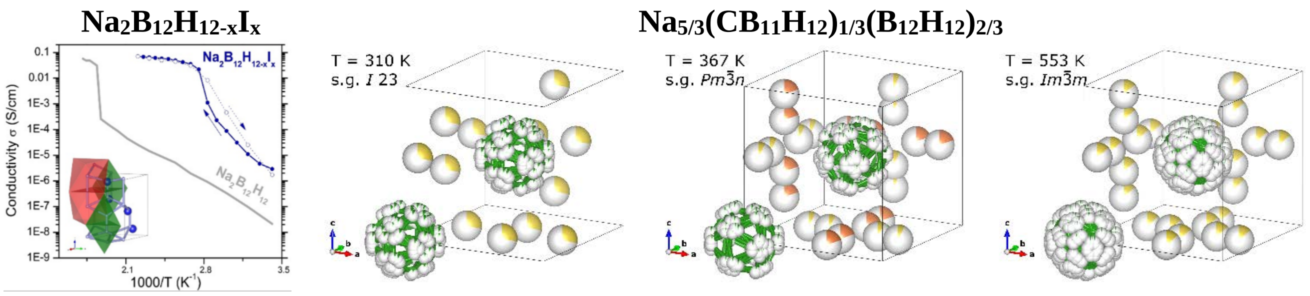
$Na_2B_{12}H_{12-x}I_x$

$Na_{5/3}(CB_{11}H_{12})_{1/3}(B_{12}H_{12})_{2/3}$

Figure 1: **(left)** Ionic conductivity of a sample containing 52 wt% $Na_2B_{12}H_{12-x}I_x$ and 48 wt% NaI. The conductivity of the precursor $Na_2B_{12}H_{12}$ is shown for comparison. Na-ion conduction channels in *hcp* sublattice with face-sharing T and O interstices sites in *h*-$Na_2B_{12}H_{12-x}I_x$. In blue the static Na positions as optimized by DFT. **(right)** Evolution of anionic and cationic disorder in $Na_{5/3}(CB_{11}H_{12})_{1/3}(B_{12}H_{12})_{2/3}$. Green and yellow spheres represent boron and sodium atoms respectively. Orange spheres indicates a different Wyckoff site for Na (only in *Pm*-3*n*). The colour partial filling indicates the partial site occupation.

Imaging biological cells by x-rays

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X-rays provide high resolution due to their small wavelength and high penetration power, allowing for imaging of comparatively large, three-dimensional objects. For these reasons, X-rays have been established as complementary probes for bio-imaging, in addition to well-established methods such as visible light fluorescence microscopy and electron microscopy (EM). Scanning small angle X-ray scattering (SAXS), in particular, is well suited for systems with some degree of order, such as bundles of parallel filaments, or high-density aggregates. The method exploits two unique features of X-ray imaging: not only are highly focused beams used to spatially resolve different constituents of biological cells, but each individual scattering pattern contains a wealth of information about the internal structure on molecular length scales.

I will present scanning SAXS experiments that were performed at dedicated synchrotron beamlines, which provide a small beam between 100 nm and 2 µm in diameter, high flux, high-end pixel detectors and a sample environment suitable for cell samples, e.g. ID13 at the European Synchrotron Radiation Facility (ESRF), P10 at Deutsches Elektronen-Synchrotron (DESY) or cSAXS at Swiss Light Source (SLS). I will summarize the most important results we recently obtained on different biological systems, such as components of the cytoskeleton and the DNA in the nucleus.

Unfolding and Partial Refolding of an Industrial Cellulase from the SDS-Denatured State: From β-sheet to α-helix and back

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Enzymes are used in many applications including food manufacturing, cosmetics, medication, and detergent formulations. Detergent formulations also contain ionic and nonionic surfactants as essential ingredient. It is well known that ionic surfactants such as sodium dodecyl sulfate (SDS) can denature proteins. Furthermore, it has earlier been shown that the nonionic surfactant octaethylene glycol monododecyl ether ($C_{12}E_8$) can refold certain globular proteins, which have been unfolded by SDS [1]. In this study, the cellulase Cel7b from *Humicola insolens* used in the detergent industry, which mostly contains β-sheet secondary structure, was studied. The unfolding using SDS and subsequent refolding using $C_{12}E_8$ and α-cyclo dextrin (α-CD) was investigated using near- and far-UV circular dichroism (CD), small-angle X-ray scattering (SAXS), isothermal titration calorimetry (ITC), and activity measurements. The results show that at low SDS concentrations Cel7b forms large aggregates due to neutralization of the protein charge by the anionic SDS molecules. CD shows that the protein adopts a-helical secondary structure, in the complexes with SDS. Cel7b could be partially refolded using $C_{12}E_8$; the secondary structure was almost completely restored to mainly β-sheet structure, whereas the tertiary structure was partially restored. Activity measurements show that enzymatic activity is partially restored at high concentrations of $C_{12}E_8$. However, SAXS measurements reveal that upon addition of $C_{12}E_8$, the sample becomes aggregated as is observed for samples with low amounts of SDS. This suggests that SDS and $C_{12}E_8$ form free mixed micelles, but as the system approaches charge neutralization the electrostatic interactions of Cel7b cannot be compensated for by the mixing entropy of SDS and $C_{12}E_8$ in mixed micelles. Attempts to refold using α-CD also resulted in aggregation at high amounts of α-CD.

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Abstract Danscatt

X-ray tomography of 3.7 billion year old remains of life

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Metasedimentary rocks from Isua, West Greenland (> 3,700 million years old) contain metamorphic mineral assemblage with garnet and quartz intergrowths that contains layers of carbonaceous inclusions of biogenic origin[1-3]. We studied this material trapped in inclusions within quartz grains by non-destructive ptychographic X-ray nanotomography (PXCT). The 3D electron density maps generated by PXCT were correlated with maps from X-ray fluorescence tomography and micro-Raman spectroscopy. We found that the material trapped inside inclusions in the quartz grains consist of nano-graphitic material encasing domains of iron-rich carbonaceous material. These results corroborates earlier claims[1-3] for biogenic origins and are compatible with relics of metamorphosed biological material originally containing high iron /carbon ratios, similar to organisms using iron in their metabolic functions. Therefore, we present the potentially oldest direct evidence in Earths geological record for life relying on iron metabolism.

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STRUCTURAL STUDIES OF BLOCK COPOLYMER HYDROGELS

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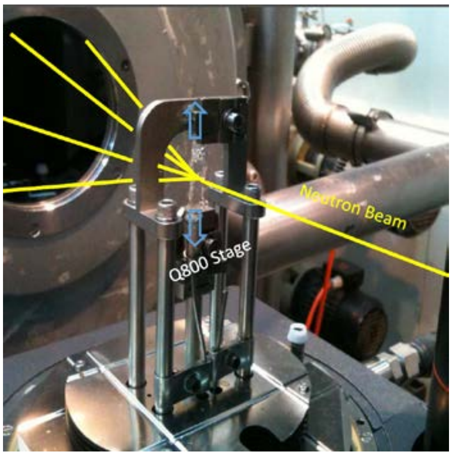
Polymer hydrogels are polymer networks swollen in water. These gels have particular interests in context with biomedical applications toward materials such as lenses and artificial muscle, cartilage, and tendons. The properties of hydrogels are significantly affected by the network structure. We have made a large variety of studies based on PEO-PPO type of amphiphilic block copolymers that lead to networks and gels of various kind, depending on specific molecular architecture.



In situ SANS and stress measurements. The sample is a crosslinked hydrogel based on four-armed PEO-PPO block copolymers.

We review structural study of aqueous suspensions of both linear PEO-PPO type of block copolymers [1] and 4-armed PEO−PPO block copolymer star with the PPO block near the center [2]. Furthermore, we present recent studies on crosslinked star molecules, consisting of blends of respectively, tetra amine (TAT) and tetra-N-hydroxysuccinimide (TNT) terminated star molecules [2,3]. The structural properties of the cross-linked stars have characteristics that are rather similar to the simple linear PEO−PPO type of copolymers: at low temperatures, the measured structure is dominated by the characteristics of individual molecules, while at higher temperatures hydrophobic effects of the PPO domains cause self-assembly into spherical or rod-like micelles. These micelles form ordered meso-phases, in which the texture can be controlled by simple shear. The structure of the crosslinked 1:1 TAT−TNT system is basically organized into two-dimensional network sheets. The cross-linked network is elastic and can be stretched. Both neutron and X-ray scattering show a consistent response to uniaxial strain, with no changes in characteristic molecular dimensions, likely related to the layer-dominated structure.

Acknowledgements

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Mapping Grain Morphology and Orientations in Polycrystalline Materials by Laboratory Diffraction Contrast Tomography

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Recent developments of the Laboratory Diffraction Contrast Tomography (LabDCT) technique have extended its capabilities to include full reconstruction of the 3D grain structure, including both grain morphology and crystallographic orientation. With both the grain morphology and orientation, it is possible to extract the full five parameters describing the grain boundary characteristics, which opens new possibilities for statistical studies of grain boundary properties as illustrated in Figure 1.

LabDCT makes use of high-resolution diffraction images acquired on a ZEISS Xradia 520 Versa X-ray microscope. The 3D crystallographic imaging capabilities of LabDCT complements the structural data simultaneously obtained by traditional absorption-contrast tomography (ACT, e.g. cracks, voids and inclusions), and together the combination of ACT and LabDCT provide unprecedented insight into materials structure.

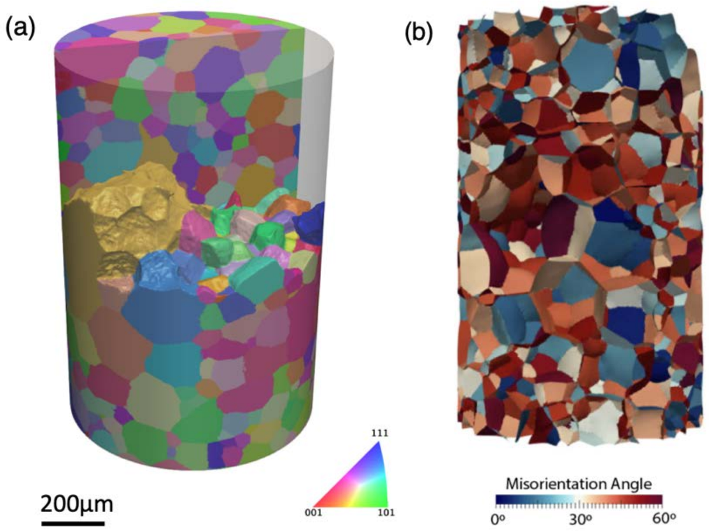

Figure 1 (a) 3D rendering of an iron sample characterized by LabDCT, with IPF coloring. (b) 3D rendering of the grain boundaries in the same sample volume, colored by misorientation angle.

We will present a selection of LabDCT results with particularly emphasis on its non-destructive operation to demonstrate how the technique can be used to gain a better understanding of materials structure evolution in 3D. In addition, wse will discuss boundary conditions of the current implementation, compare with related characterization techniques and point to the future of the technique

Scanning X-ray Imaging Techniques for Characterization of Energy Materials

Tiago C. Ramos (Tiago João Ayres Pereira da Cunha Ramos)

As X-ray coherent diffraction imaging expands into new scientific areas, *in situ,* and *operando* studies, faster acquisition times are becoming a decisive factor for the success of an experiment.

So far, scanning coherent diffraction imaging (ptychography) rely on a series of overlapping measurements, from different scanning positions, to reconstruct two-dimensional absorption and phase-contrast projection images that can be further used with tomographic algorithms to reconstruct three-dimensional representations of the sample's refractive indices. In this work, we present an alternative numerical reconstruction algorithm for direct tomographic reconstruction of a sample's complex refractive indices from the measured intensities of its far-field coherent diffraction patterns. The well-known phase-retrieval problem in ptychography is formulated in a tomographic framework which allows for simultaneous reconstruction of the illumination function and the sample's refractive indices in three dimensions. The combination of all measured diffraction data into a single reconstruction algorithm relaxes the current measurement oversampling conditions which decreases the overall data acquisition time and dose impinging on the sample.

Our implementation allows a flexible description of the tomographic setup, where diffraction patterns may be collected from any given sample spatial orientation. Our iterative reconstruction algorithm is based on the Levenberg-Marquardt algorithm and the performance of our proposed method is demonstrated with simulated and real datasets.

Characterization of the formation of metal oxido clusters by complex modelling of PDF and SAXS

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Metal oxides of bismuth and its oxido clusters in solution have attracted much attention with potential applications ranging from antibacterial agents to photocatalysis. In order to improve the photocatalytic activity of β-Bi_2O_3, it has been shown that easily accessible $\{Bi_{38}O_{45}\}$-based clusters represent well suited molecular precursors [1]. However, the chemical processes involved in the cluster formation are not well understood: While the molecular structures of various clusters have been solved by single crystal diffraction, it is much more challenging to study structures of such clusters directly in solution [2]. Bismuth oxido clusters exist in a range of sizes, most of them built up by simple or edge-sharing octahedral $\{Bi_6O_X\}$ units, but studies on their conversion processes are restricted to electrospray mass spectrometry [2]. Here, we use *in situ* X-ray total scattering with PDF analysis to study the formation of a $\{Bi_{38}O_{45}\}$ cluster starting from $[Bi_6O_5(OH)_3(NO_3)_5]\cdot(H_2O)_3$ crystals dissolved in DMSO. The PDF analysis gives unique insight into the structural rearrangements on the atomic scale. By combining with Small Angle X-ray Scattering, SAXS, we furthermore investigate the size, morphology and size dispersion of the clusters taking place in the process. These two techniques complement each other, allowing us to follow the cluster chemistry as it takes place.

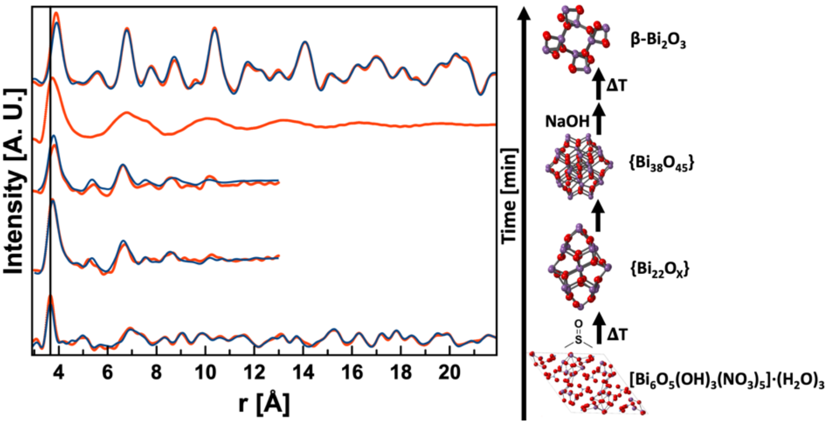

Figure 1: The chemical process from $[Bi_6O_5(OH)_3(NO_3)_5]\cdot(H_2O)_3$ crystals dissolved in DMSO through an bismuth oxido growth process and an amorphous phase, before nucleation of β-Bi_2O_3 crystals**.** A line about r = 3.8 Å is inserted to guide the eye to observe increasing Bi – Bi distances.

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