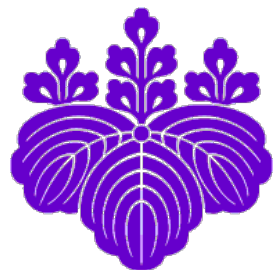


オーフス大CMCでの構造科学研究

笠井 秀隆

[1] Division of Physics, Faculty of Pure and Applied Sciences,
Tsukuba Research Center for Interdisciplinary Materials Science (TIMS) & Center for Integrated
Research in Fundamental Science and Engineering (CiRfSE), University of Tsukuba.

[2] Center for Materials Crystallography (CMC), Department of Chemistry, Aarhus University

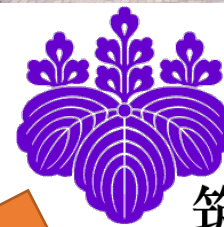
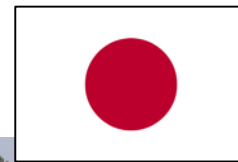


Outline

1. Center for Materials Crystallography (CMC), Aarhus University
2. Collaborative Research
 - 3-1. Development of New Vacuum Diffractometer
 - 3-2. Core Deformation in α -Boron
 - 3-3. Van der Waals interaction in TiS_2 , MoS_2
3. Prospect

International Tenure-Track

For International collaborative works



1/Apr/2015

筑波大学
University of Tsukuba



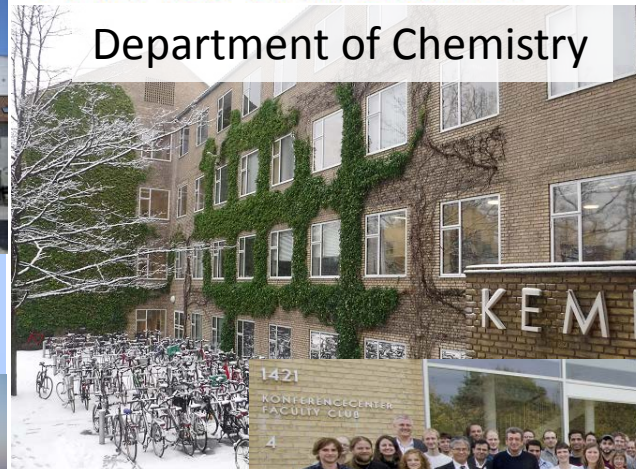
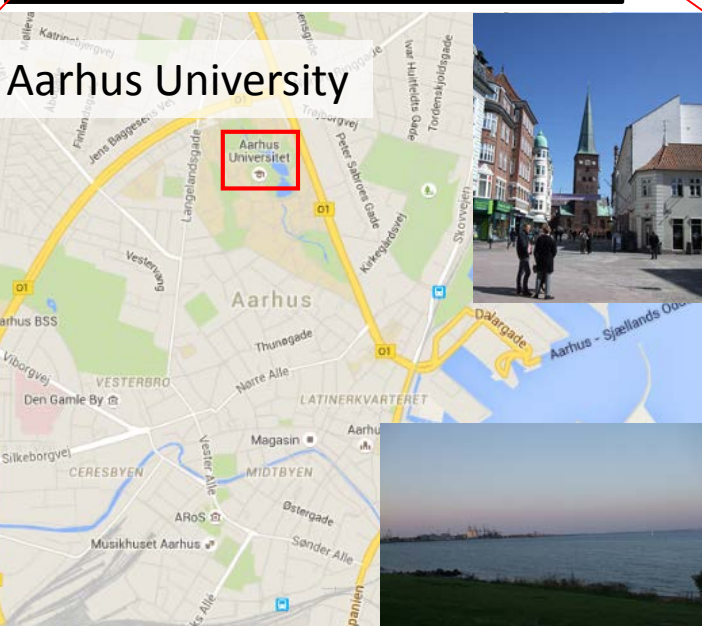
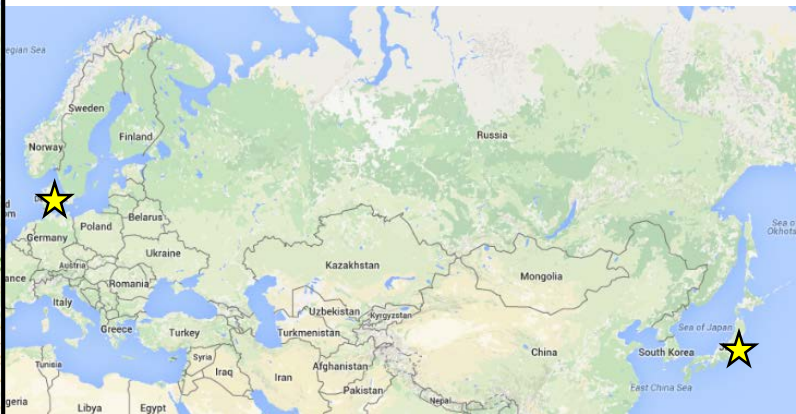
17/Apr/2015 –

AARHUS UNIVERSITET

Department of Chemistry



Prof. Bo B. Iversen

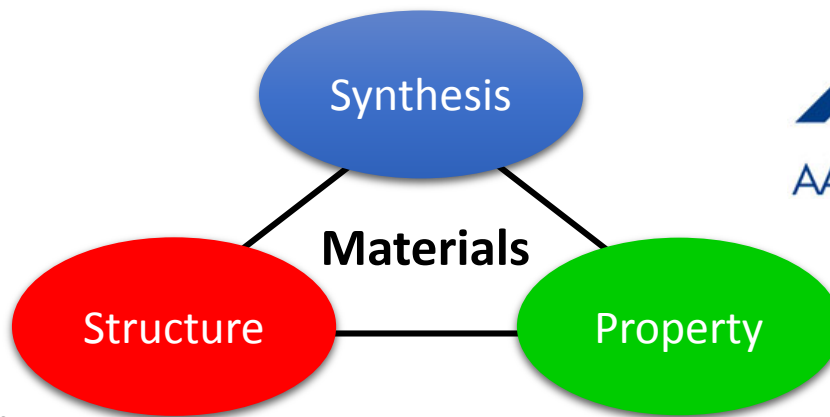


Center for Materials Crystallography (CMC)

CMC Leader



Prof. Bo B. Iversen



Materials Science based on Crystallography
using the most advanced Synchrotron and Neutron facility

The University of Milan



Established in Jan. 2010



PETRA-III, Germany



SPring-8, Japan



SNS, USA



Interdisciplinary Nanoscience Center
Aarhus University

6 countries and 100 research members

Research at CMC, Aarhus Univ.

CMC Leader



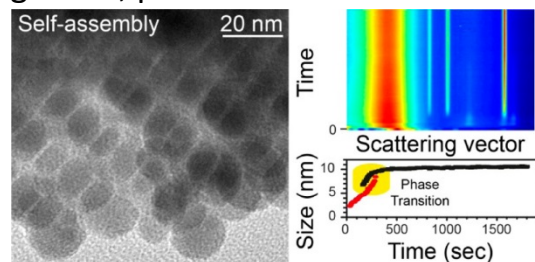
Prof. Bo B. Iversen



Dr. Jacob Overgaard
(Senior Scientist)

Nanoparticles

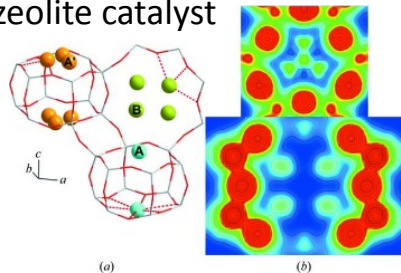
In situ study of nanoparticle formation, growth, phase transition



P. Nørby et al., *ACS Nano*. **8**, 4295 (2014).

Catalyst

Complete structure of active zeolite catalyst



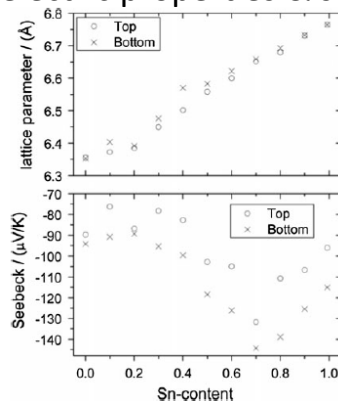
C. W. Andersen et al., *IUCr-J.* **1**, 382 (2014).

Energy materials

Ion battery materials

Thermoelectric materials

Thermoelectric properties & structure



M. Søndergaard et al., *J. Electron. Mater.* **42**, 1417 (2012).

Materials Crystallography

Magnetic materials



Assoc. Prof.
Mogens Christensen

High pressure study



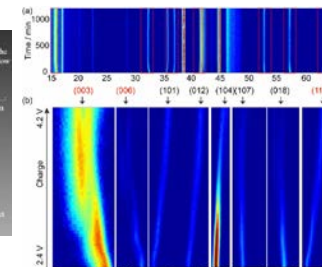
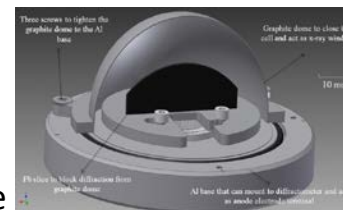
Assistant Prof.
Martin Bremholm

Hydrogen storage materials



Assoc. Prof.
Torben R. Jensen

In operando study of Li/Na batteries



Y. Shen et al., *Rev. Sci. Instrum.* **85**, 104103 (2014).

M. Søndergaard et al., *J. Electron. Mater.* **42**, 1417 (2012).

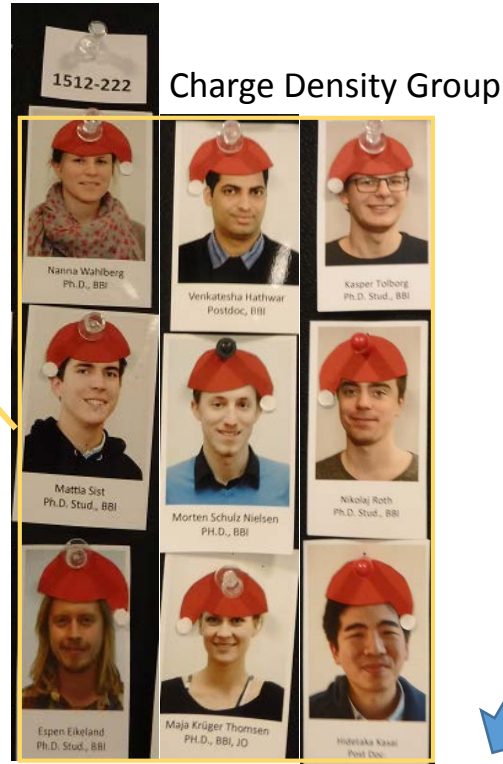
Beamline development at new Neutron and Synchrotron facility, ESS & MAX IV (Lund, Sweden)



<http://www.alp.edu.pl/max-iv-and-ess/>

Research Life at CMC

CMC members in Aarhus Univ.



Assoc. Prof. Mogens Christensen
Summer Lecture at Univ. Tsukuba (July 2015)



Assistant Prof.
Martin Bremholm



Discussion on
Samples

Prof. Bo B. Iversen



Discussion

Previous: Jan.14
Next: Jan. 27



Advise for
Analysis

Dr. Jacob Overgaard
(Senior Scientist)



Meetings in CMC, Aarhus Univ.

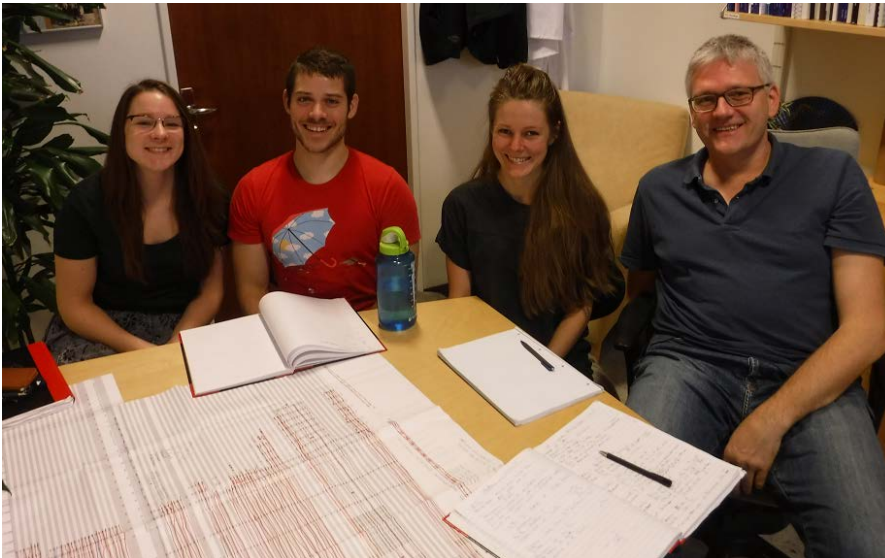
Group Meeting (Tuesday morning)



Study Group (Tuesday & Friday)



Synchrotron X-ray Experiment Meeting
(Before & After Beamtime)



Postdoc & PhD Meeting
(~1 time/month)



Experiments in Synchrotron Radiation Facilities

Spring-8, Japan

- (1) 2 beamtimes for Single Crystal Diffraction
- (2) 3 beamtimes for Powder Diffraction



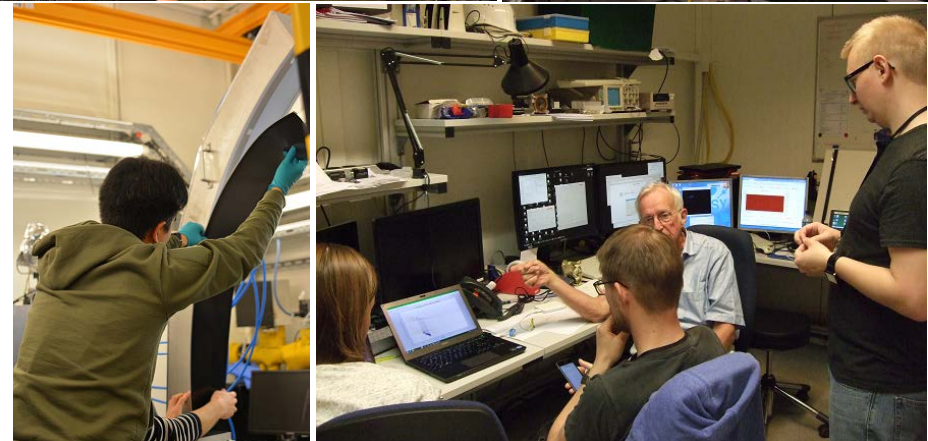
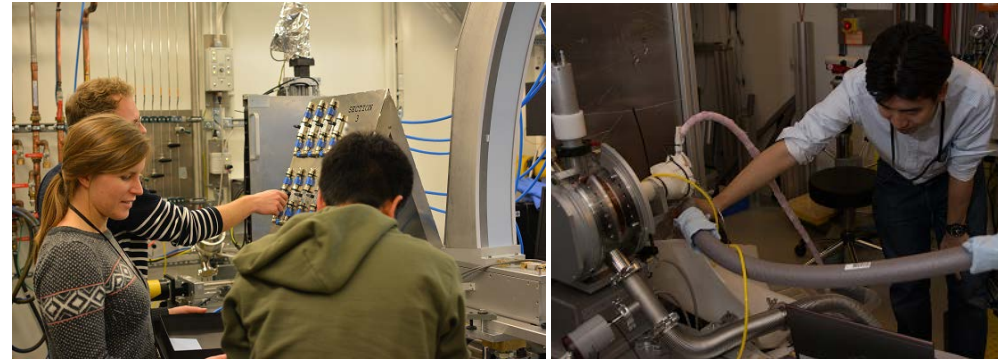
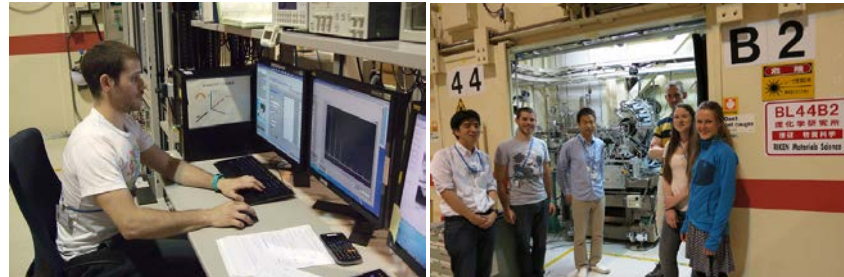
PETRA-III, Germany

- (1) 2 beamtimes for Powder Diffraction



“the most brilliant Storage ring light source in the world”

<http://photon-science.desy.de/>

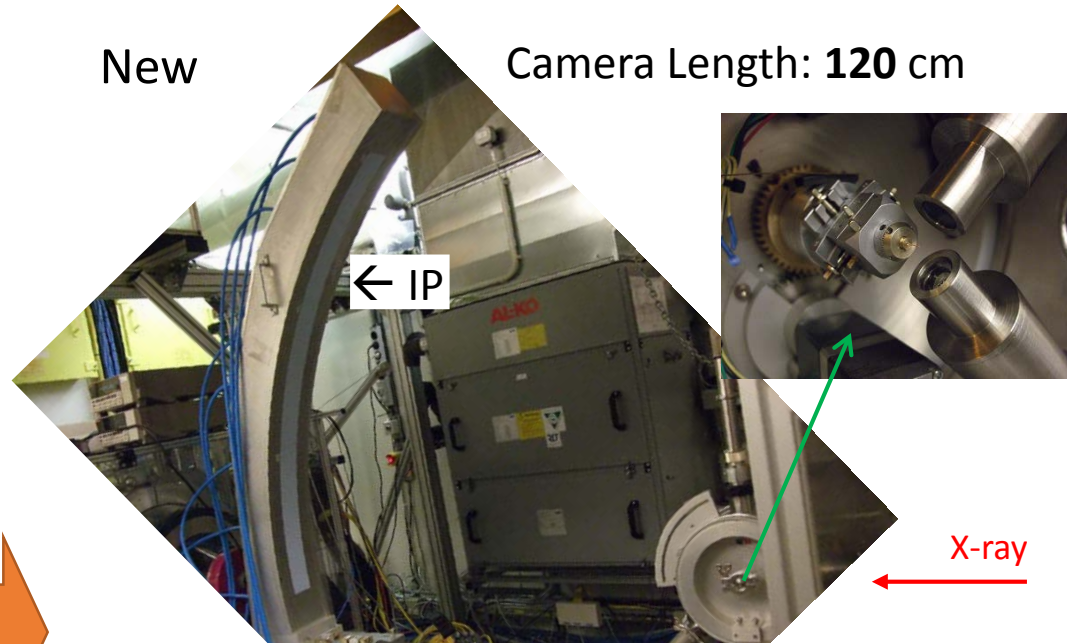
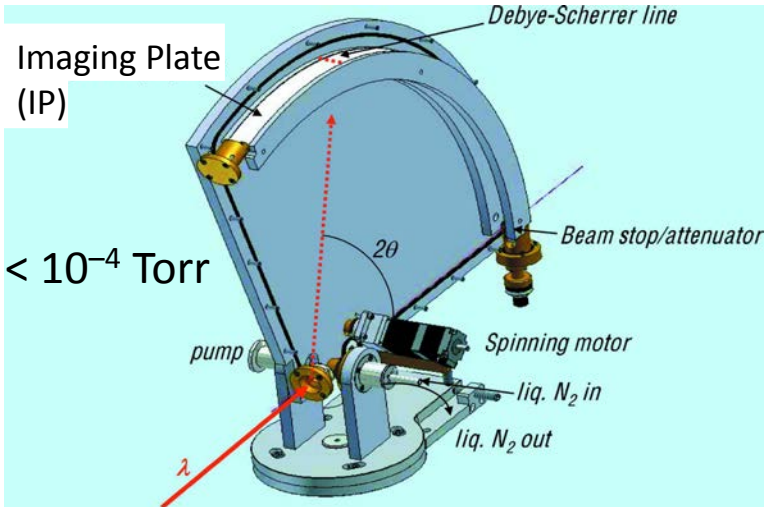


Development of New Vacuum Diffractometer

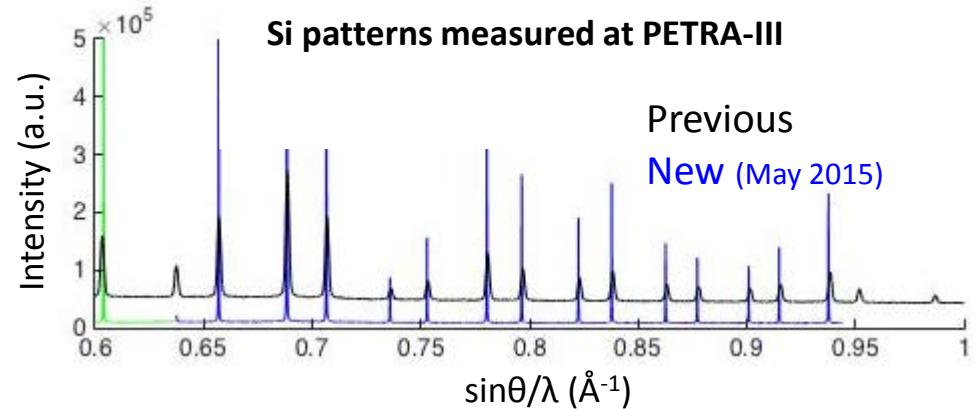
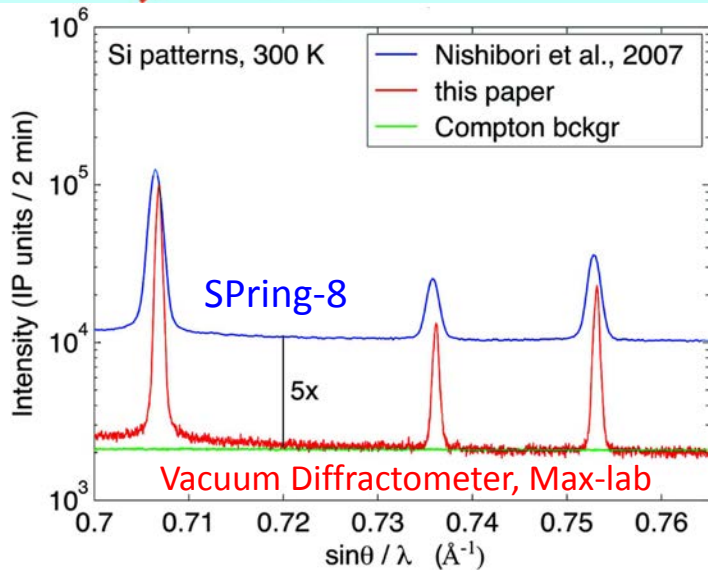
Previous
Camera Length: 30 cm

New

Camera Length: 120 cm



Decrease of Compton Background



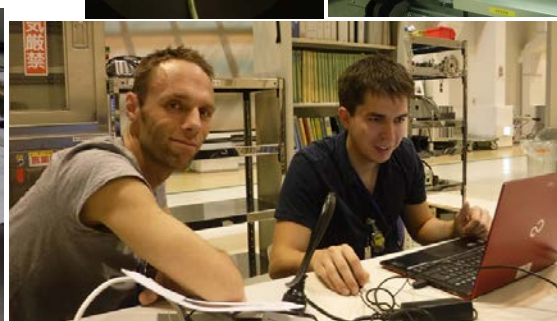
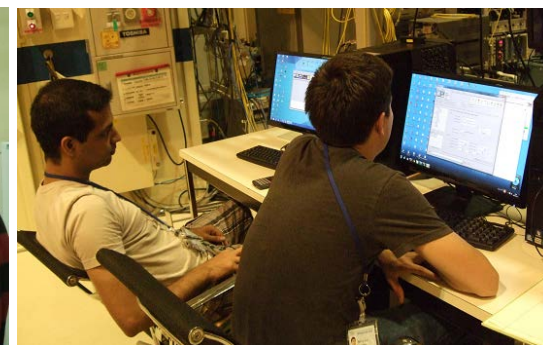
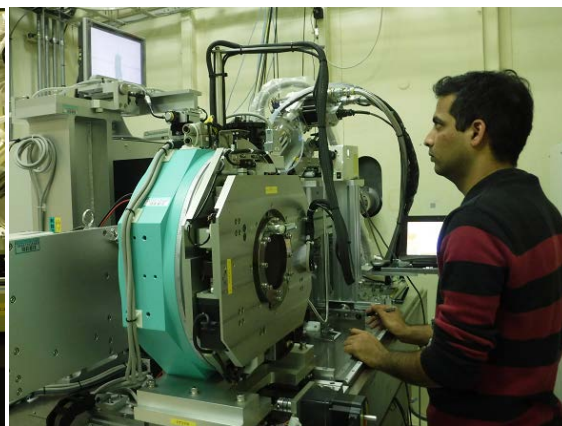
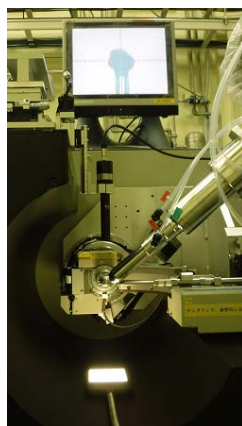
S/N was improved, but the intensities were wrong.
Data acquisition from IP causes the problem.

Experiments at SPring-8

Test using Lab X-ray in CMC

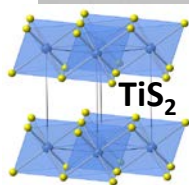


Synchrotron X-ray single crystal diffraction at BL02B1 of SPring-8



TiS₂ (July 2015), MoS₂ (Nov. 2015)

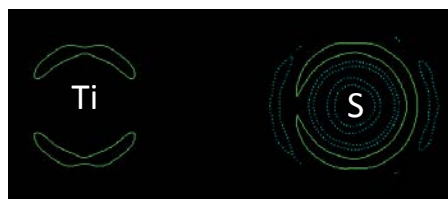
$\lambda = 0.25 \text{ \AA}$, (Resolution: $d > 0.3 \text{ \AA}$)
20 K



Extended Hansen-Coppens multipole model

$$\rho(\mathbf{r}) = \underbrace{P_c \kappa_c^3 \rho_{\text{core}}(\kappa_c r)}_{\text{Core}} + \underbrace{P_v \kappa_v^3 \rho_{\text{valence}}(\kappa_v r) + \sum_{l=0}^{l_{\text{max}}} \kappa_l'^3 R_l(\kappa_l' r) \sum_{m=0}^l P_{lm\pm} d_{lm\pm}(\theta, \phi)}_{\text{Valence}}$$

Residual density (step: 0.1 e\AA^{-3})



Theory



Experiment

Looking for the best model

Prospect

1. New Vacuum Diffractometer

We are trying to fix the problem regarding data acquisition using Imaging Plate.

Next beamtime for PETRA-III: June 29 – July 5, 2016

2. Core Electron Density Deformation in α -Boron

We will measure high resolution powder diffraction data ($d > 0.25 \text{ \AA}$) at PETRA-III using 60 keV synchrotron X-ray with the new vacuum diffractometer.

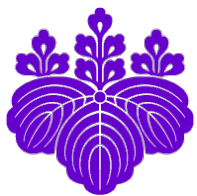
Next beamtime for PETRA-III: June 29 – July 5, 2016

3. Van der Waals Interaction in TiS_2 , MoS_2

We measured single crystal diffraction data ($d > 0.3 \text{ \AA}$) at SPring-8.

I'm working on modelling using the Hansen-Coppens multipole model.

After the final modelling, we'll discuss van der Waals interaction from electron density.

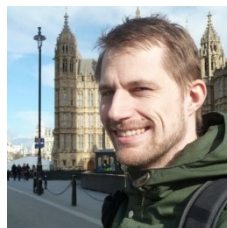


Acknowledgements

Prof. Eiji Nishibori & Prof. Bo Brummerstedt Iversen



Powder Diffraction using New Diffractometer



Mads R. V. Jørgensen Nanna Wahlberg
Jacob Becker

Niels Bindzus

Single Crystal Diffraction & Multipole Analysis



Mattia Sist

Jacob Overgaard

Venkatesha R. Hathwar

Simone Cenedese

Samples



Mette Ø. Filsø

Martin Bremholm

Simone Søndergaard-Pedersen



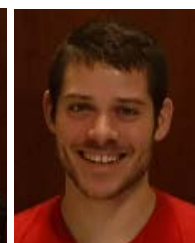
Kasper Tolborg

Ann-Christin Dippel

Sebastian Christensen

Jens Als-Nielsen

Spring-8 Powder Diffraction



Casper W. Andersen

Anders B. Blichfeld

Hazel Reardon

Sanna Sommer

