AXAA

Australian X-ray Analytical Association

Newsletter Issue 1 2021

President's Address

Dear AXAA members,

The development and wide-scale delivery of not just one, but multiple vaccines for a novel virus within a year of its emergence is nothing short of extraordinary, and a reminder of the tangible value of science and technology to our society. X-ray techniques have been particularly instrumental in revealing the structure of the virus and identifying targets for vaccine development and treatments. Here at the synchrotron I was lucky to see first-hand how many X-ray techniques were employed to contribute to the challenge. Protein crystallography of course was essential (see below for some ways that the MX beamline at the Australian Synchrotron has been contributing to global COVID research), but X-ray absorption spectroscopy was also used in efforts to locally produce magnetic nanoparticles for test kits.

2021 has been a little stop-start that's for sure, but with vaccine deployment already rolling out, there is hope that border closures will become less frequent and we might continue our slow return to normal life. This uncertainty has meant we (AXAA) were a little quiet in the first part of this year, but fear not, we have plans to increase our activities going forward and make up for lost time. Stay tuned for AXAA events popping up in the coming months, with details to be communicated soon.

A topical subject on our minds recently has been improving workplace culture to be safe and inclusive, and from the AXAA committee, we would like to reaffirm our commitment to continuous improvement in this space. Our community is diverse and intersectional, and it is growing (we just reached a milestone of 500 followers on Twitter!). We commit to providing events and resources that are inclusive and accessible, and represent the diversity and intersectionality of our community. We want AXAA to be a catalyst for participation in X-ray and neutron science, and to actively lower barriers wherever we find them. We also challenge you, as a community, to not only hold us to account, but also to champion these values in your workplaces.

Jessica Hamilton

AXAA President

Understanding COVID-19 through Synchrotron Radiation

Rachel Williamson and Alan Riboldi-Tunnicliffe

Principal Scientists, MX, Australian Synchrotron

The importance of maintaining access to synchrotron radiation to drive structural biology-related research into SARS-CoV-2 led to an early decision in February 2020 by ANSTO/Australian Synchrotron to reach out and support the efforts of our user community working in this field.

In early March 2020 a special rapid access mode was offered for researchers undertaking COVID-19 research on the Macromolecular Crystallography (MX) beamlines. This was later expanded to include all beamlines, with the usual processes for proposal submission, review and user access fast-tracked to ensure that our scientific community could make the most of this rapid access mode. A number of Australian researchers responded to the COVID-19 outbreak quickly, rapidly transitioning into new areas of research. When, following Australian Government guidelines, the Australian Synchrotron moved to essential operations mode on Monday 23 March, cancelling all user experiments, there was already a highly focused cohort of Australian researchers accessing the Microfocus Crystallography Beamline (MX2) for structural biology research on COVID-19 related proteins.

Researchers accessing MX2 for COVID-19 related research have been investigating the structure and function of proteins from the SARS-CoV-2 virus alone, as well as interactions between these viral proteins and human proteins that may be involved in the cycle of infection and replication within the human body. Knowledge of the roles that proteins play in this cycle is vital for the development of effective therapeutics for COVID-19.

Dr Dene Littler, working within the laboratory of Prof. Rossjohn (https://rossjohnlab.com), from Monash University was one of the first researchers to access MX2 for COVID-19 related research. Dr Littler and his colleagues published the first SARS-CoV-2-related protein structure solved at the ANSTO/Australian Synchrotron, making the resulting structure publicly available via the Protein Data Bank (PDB) in April 2020. The speed of turnaround between data collection in February to structure deposition and publication of the initial structural report in June in iScience (Littler *et al.,* iScience *23*, 101258) was remarkable.

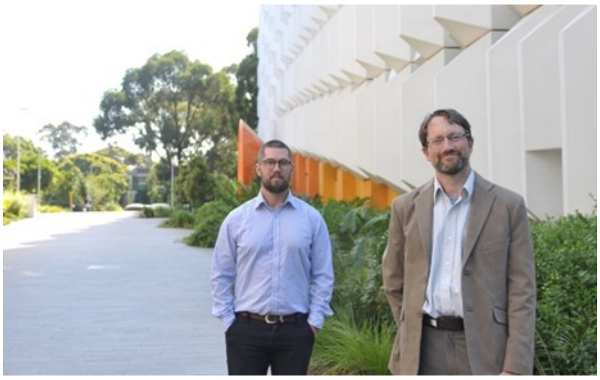

Figure 1. *Dr Ben Gully and Dr Dene Littler (Biomedicine Discovery Institute, Monash University)*

Dr Littler's protein of interest was SARS-CoV-2 Non-structural protein 9 (Nsp9), a small conserved viral protein thought to be involved in RNA-binding and shown to be essential to viral replication. This makes Nsp9 a good target for developing drugs against COVID-19. Dr Littler and his colleagues have since identified a possible protein binding site within NSP9 and have published structures of Nsp9 alone and bound to a peptide (**Figure 2**). They are continuing to work to better understand its significance.

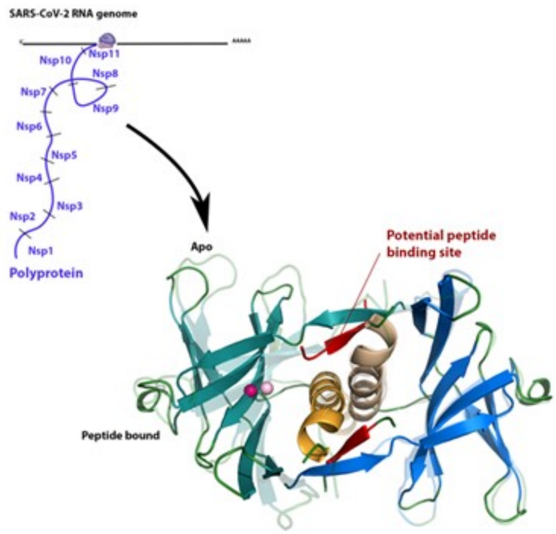

Figure 2. *The structure of Nsp9 (Littler et al. iScience 2020)*

Another research group that has made great use of the Australian Synchrotron for their COVID-19 research is that of Assoc. Prof Wai-Hong Tham at the Walter and Eliza Institute (WEHI). Prof Tham and her team are interested in disrupting the interaction between the now-famous spike protein of SARS-CoV-2 and the human protein ACE2 (a receptor for the viral spike protein), the mechanism by which the virus enters human cells. The high-affinity interaction with ACE2 is mediated by the receptor-binding domain (RBD) of the spike protein.

The WEHI team's strategy is to disrupt viral entry into host cells by using nanobodies. Nanobodies are camelid-derived single domain antibodies and represent the smallest naturally derived antigen-binding fragment (approximately 15 kDa in size). Their small size along with high antigen-binding affinity, solubility, increased stability and ease of recombinant production (compared with traditional antibodies) make them attractive as potential therapeutics. These properties also allow the potential for the development of inhaled bio-therapies.

To generate nanobodies, alpacas are immunized with virus spike and RBD proteins, the nanobodies from isolated plasma cells are then cloned, and antigen-specific nanobodies are screened and selected for from these libraries. The WEHI team will screen for nanobodies that inhibit the interaction of virus spike proteins with human ACE2, hence stopping virus entry and preventing SARS-CoV-2 infection.

Conclusion

Throughout the Victorian lockdowns of 2020, the Australian Synchrotron continued to shine, providing vital research infrastructure and supporting the contributions of Australian scientists during one of the greatest public health and societal challenges of our time. The Microfocus Crystallography beamline (MX2) continues to be one of several beamlines actively involved in SARS-CoV-2 and COVID-19 research and continues to be used by both Australian and international research teams to determine the structures of proteins from the SARS-CoV-2 virus, and/or related to our body's response to COVID-19.

Access requests for researchers undertaking SARS-CoV2/COVID-19 can be submitted via the COVID-19 access round (https://portal.synchrotron.org.au) and selecting MX1: Macromolecular Crystallography as the equipment set ID, and then Special Rapid Access COVID-19 (for the round).

Dr Dene Littler
(works within the laboratory of Prof. Rossjohn, Monash University (https://rossjohnlab.com))
Please cite Dene's article as: Littler, D.R., Gully, B.S., Colson, R.N., Rossjohn, J., Crystal structure of the SARS-CoV-2 non-structural protein 9, Nsp9, ISCIENCE (2020), doi: https://doi.org/10.1016/j.isci.2020.101258.

Assoc. Prof Wai-hong Tham, Dr Melanie Dietrich, Dr Phillip Pymm
Assoc. Prof Wai-hong Tham group at The Walter and Eliza Hall Institute (WEHI), Melbourne https://www.wehi.edu.au/people/wai-hong-tham)

A New IAEA Database of XRF laboratories worldwide goes online

Roman Padilla Álvarez

IAEA

Nowadays, it is estimated that X-Ray Fluorescence (XRF) facilities are present in almost every country, but in many occasions their capabilities are not yet well known by the wide community of end-users that might benefit from the advantages of this powerful analytical technique. Although several national and regional societies and networks pursue the exchange of information and to strengthen the cooperation among the XRF communities, there has not been a repository of information on facilities available worldwide so far that might increase their visibility. The latter is of utmost relevance to end-users that might need to identify a potential partner for interdisciplinary research projects or a provider of analytical services.

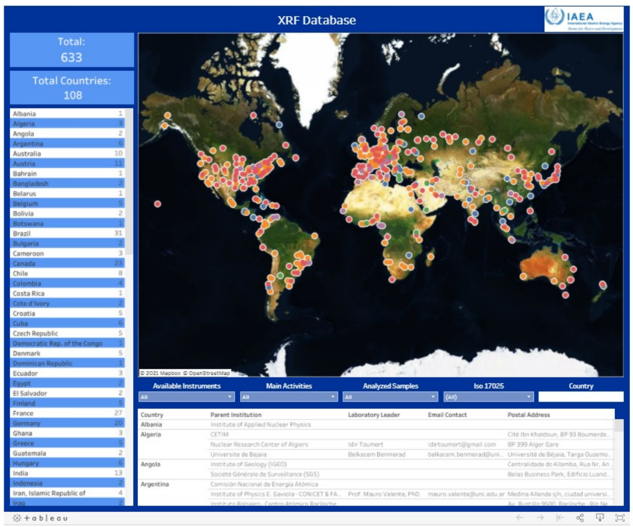

Figure 1*. The interactive worldwide map of XRF facilities from IAEA*

At the IAEA Nuclear Science and Instrumentation Laboratory (NSIL) , Physics Section, Division of Nuclear Applications in Physics and Chemistry, we have created several databases and Interactive Maps depicting different nuclear research and instrumentation facilities operating worldwide. The youngest of these databases is the worldwide Interactive Map of XRF Laboratories, which offers information on more than 460 XRF facilities available in close to 90 countries. This database intends to provide a broad overview of laboratories employing XRF techniques for fundamental or applied research, analytical services as well as for education & training purposes. The collected information is compiled either directly from the organizations operating these facilities by using an online registration form, or it is gathered from different publicly accessible sources.

More information and requests for updates could be made by contacting us via NSIL at iaea.org.

The Macquarie Deformation-DIA facility at the Australian Synchrotron: a tool for high-pressure, high-temperature experiments with synchrotron radiation

Nicholas Farmer[1], Tracy Rushmer[1], Jeremy Wykes[2]

[1]*Macquarie University,* [2]*ANSTO Australian Synchrotron*

Introduction

Experiments simulating the high pressure, high temperature conditions of the deep Earth play a crucial role in our understanding of processes such as the formation of the Earth's crust and the structure and composition of the Earth's mantle. Combining a multi-anvil apparatus which can subject samples to these conditions with a Synchrotron radiation source allows us to observe these processes in situ, which is especially important for samples that change during the process of recovering them to ambient conditions.

The Macquarie D-DIA press is a multi-anvil press in which six tungsten carbide anvils act on a solid assembly which can be either cubic or cuboidal. In addition to the main hydraulic ram that applies pressure equally through all six anvils, this press is equipped with two extra rams that can optionally be used to apply deviatoric stress to a sample, which can be used to investigate the deformation of rocks and minerals under extreme conditions. An especially unusual and useful feature of this apparatus is that is mounted on castor wheels, which allows it to be installed at any beamline with sufficient space in the experimental hutch, or even used away from a beamline as a conventional 'offline' multi-anvil apparatus. The press is also mounted on a series of motorized stages which allow the sample to move along three axes and rotate around the vertical axis; this allows the sample to be positioned in the beam path.

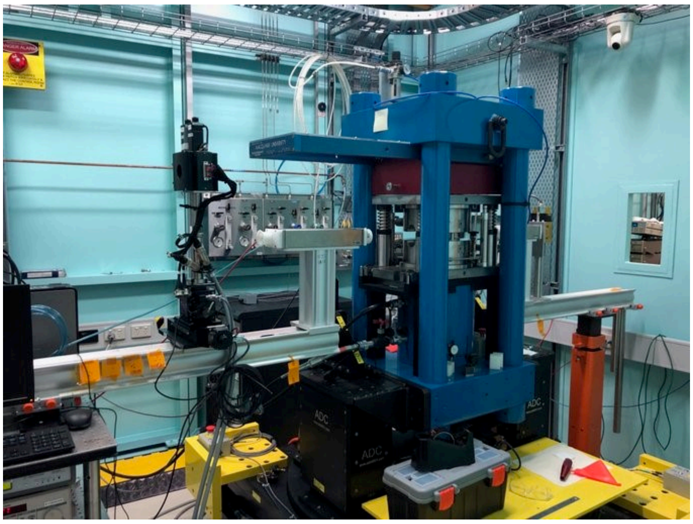

Figure 1. *The D-DIA press installed in Hutch C of the XAS beamline of the Australian Synchrotron.*

The sample is placed inside a graphite tube which acts as a resistive heater, in a 7 mm cube made from a mixture of boron and epoxy. We have developed this assembly to allow pressures of up to 6 GPa and temperatures of up to 1500 °C to be attained, equivalent to a depth within the Earth of ~150 km, while also being reasonably transparent to X-rays. The pressure generation and sample heating control systems have been integrated into the EPICS control system used at the XAS beamline, and the pressure and electric current supplied to the sample can be controlled precisely and automatically maintained at the desired conditions. Further details can be found in our recent article [1].

Optical and detector setup

The incident X-ray beam at the XAS beamline is monochromatic, with energies of ~4-34 keV accessible using the collimating and refocusing mirrors. The beam can be focused to a size of ~250 µm at the sample, with flux at the focal spot in the order of 10^{12} photons/second. Using this X-ray source and the detector setup we have developed, we can make both transmission-mode X-ray absorption spectroscopy and energy-dispersive X-ray diffraction measurements.

To make XAS measurements, we measured X-ray intensity up- and downstream of the press using ion chambers, with the beam focused ~50 cm behind the press, so that the beam is converging through the sample. A set of slits is used upstream of the press to control the size of the incident beam. These measurements can be made readily at energies > 13 keV, where transmission through the sample and assembly is >10^{-4}, and with increasing difficulty at lower energies as transmission decreases precipitously.

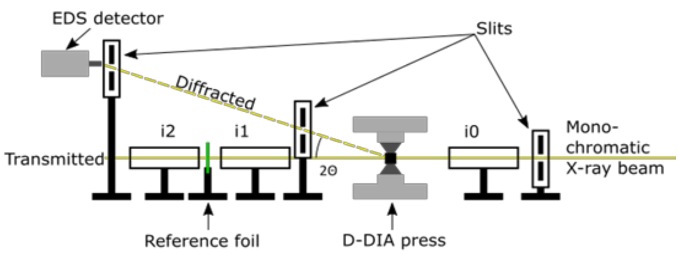

Figure 2. *Schematic diagram of the experimental setup for in situ XAS and XRD measurements in Hutch C*

X-ray diffraction measurements are made using an energy scanning XRD setup inspired by the approach of Filipponi et al. [2], using the XAS configuration with the addition of two sets of slits downstream from the detector and an X-ray detector (here a single element Vortex X-ray detector measuring X-ray intensity) at a fixed angle to the incident beam (i.e., fixed 2Θ). XRD measurements are made by varying incident X-ray energy using the monochromator to scan the energy range corresponding to a diffraction peak. This method possesses high incident energy resolution but does not allow multiple diffraction peaks to be measured in parallel, and is limited to the energy range accessible using the monochromator.

Results and discussion

Pressure and temperature calibration

We conducted a calibration of press load to sample pressure by in situ XRD of a NaCl pressure standard. A pellet of NaCl, Au and hexagonal BN (5:1:5 by mass) was loaded into the central sample chamber of a 7 mm assembly. This assembly was loaded into the press and the NaCl 200 and Au 111 peaks were located in order to calibrate 2Θ. The press load was increased steadily to 80 US tons over a period of 4.5 hours using the automated control system. During this time, diffraction patterns of the NaCl 200 and Au 111 peaks were collected every 30 minutes. When the load of 80 US tons was reached the electrical circuit for heating was connected, and power was applied to the heater in 25 W increments, while automatically maintaining press load using the EPICS control system. Diffraction patterns of the NaCl 200 and Au 111 peaks were collected at each power increment. In the ambient-temperature compression series, pressure was calculated by fitting the unit cell dimensions measured for NaCl to its equation of state, and increases linearly with press load up to 80 US tons.

To calibrate the relationship between heater power and temperature, and to measure the effect of heating the sample on pressure, the volumes of both NaCl and Au collected at each increment of heater power were simultaneously fit to equations of state. The pressure and temperature conditions at which a material has a particular volume define a line in pressure-temperature space (i.e., an isochore). When two or more materials are considered the intersection of these isochores defines the pressure and temperature of the experiment. The relationship between heater power and temperature is approximately linear up to 600 °C. This result is consistent with an offline experiment we conducted in which we synthesised a temperature-sensitive mineral assemblage (orthopyroxene + clinopyroxene).

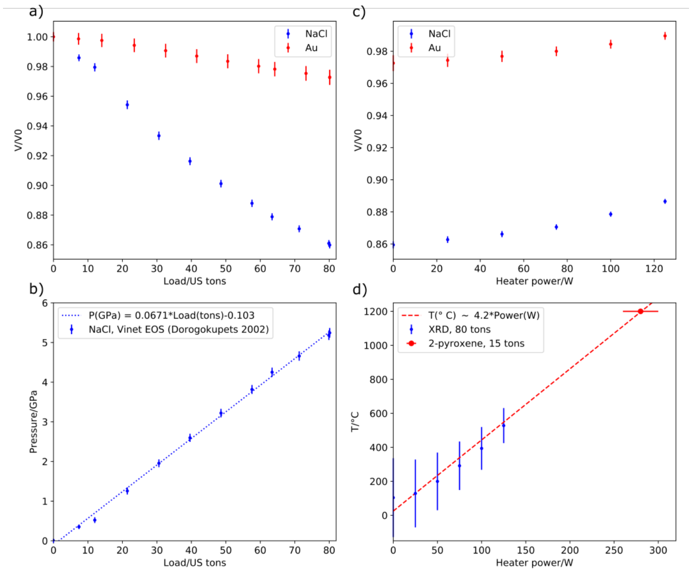

Figure 3. *a: Volume measured at different values of load for NaCl and Au. b: Calibrated load/pressure relationship from NaCl. c: Measured volume of NaCl and Au at 80 tons with different values of heater power. d: Calibrated heater power/temperature relationship, uncertainties calculated using Markov chain Monte Carlo method.*

XAS measurements

This pressure and temperature calibration is particularly important for experiments on silicate liquids; without a well-defined pressure and temperature calibration it is difficult to ensure that experiments are conducted above the solidus of our samples. We have conducted experiments measuring X-ray absorption near-edge spectra (XANES) of Zr dissolved as a minor component (3 wt.%) in silicate melt.

XANES spectra were collected at ~1470 °C, at pressures of 1.25, 2.56, 3.92 and 5.26 GPa, and show a distinctive trend of the one of the peaks of the white line increasing in magnitude with pressure, which has been linked to increasing coordination number in Zr [3]. This difference is greatest between 2.56 and 3.92 GPa, corresponding to the upper mantle. This implies a coordination change in Zr at mantle conditions; as the chemical behaviour of Zr in silicate melts has been linked to its coordination environment [4], these results indicate a previously unexplored change in the geochemical behaviour of Zr in the mantle.

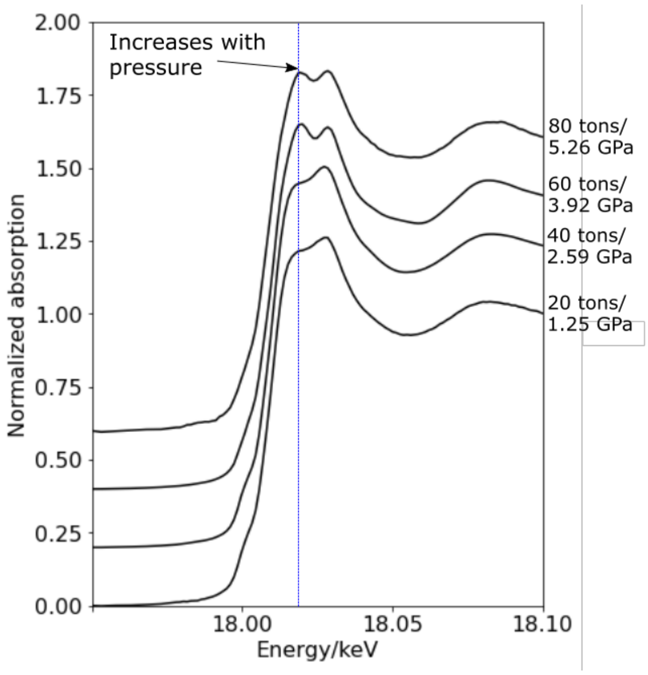

Figure 4. *K-edge x-ray absorption spectra of Zr showing variation with pressure.*

Conclusion

The Macquarie D-DIA apparatus provides high pressure, high temperature experimental capabilities at the Australian Synchrotron. To date, we have used X-ray diffraction methods to establish a pressure and temperature calibration particular to our assembly, which is a vital precondition for further work offline or at beamlines where in situ XRD is impossible. We have demonstrated that high quality in situ XANES measurements are possible with this apparatus, and we are working on applying this to trace elements important for geological processes.

References

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[4] F. Farges, C.W. Ponander, G.E. Brown Jr. *Geochimica et Cosmochimica Acta* 1991, 55 (6), 1563-74

Crystallisation of chocolate observed by simultaneous XRD-DSC measurement

Rigaku Applications Library

Introduction

Chocolate gets its mild taste, flavor, and meltable texture through tempering. The tempering process deliberately changes the crystallisation temperature, thereby controlling the crystal phase efficiently. Cocoa butter has several polymorphs that show different sub-lattice structures. Among them, type V is known as the best for chocolate production because of its stability and high melting point. Its formation is controlled by the tempering speed. Here we study the crystal structure and crystallisation temperature of chocolate obtained under several tempering speeds by simultaneous XRD-DSC measurement.

Experimental Method

These experiments used a Rigaku 9kW SmartLab X-ray diffractometer equipped with an in situ DSC (Differential Scanning Calorimeter) mounted to the goniometer. This experimental setup allows the user to simultaneously observe changes in crystal structure and thermal changes.

The SmartLab XRD used a micro-area measurement optic (CBO-f) and HyPix-3000 Hybrid Photon Counting (HPC) detector in 2D mode. Still scans were performed from 11 to 28° 2-theta. The detector was placed at 20° 2-theta, and each scan took 1 minute.

Simultaneous DSC runs were performed using a consistent heat up rate of 0.5°C/hr to approximately 38°C and then cooling at rates of 5, 2, 1 and 0.5°C/min.

Analyses were performed using the integrated X-ray analysis software Smartlab Studio II with XRD, DSC and Data Visualisation plugins.

Measurements and Results

After melting type V chocolates at 38 °C, the crystallisation processes were studied under different cooling rates. Table 1 shows the onset and peak temperatures of the exothermic peaks,

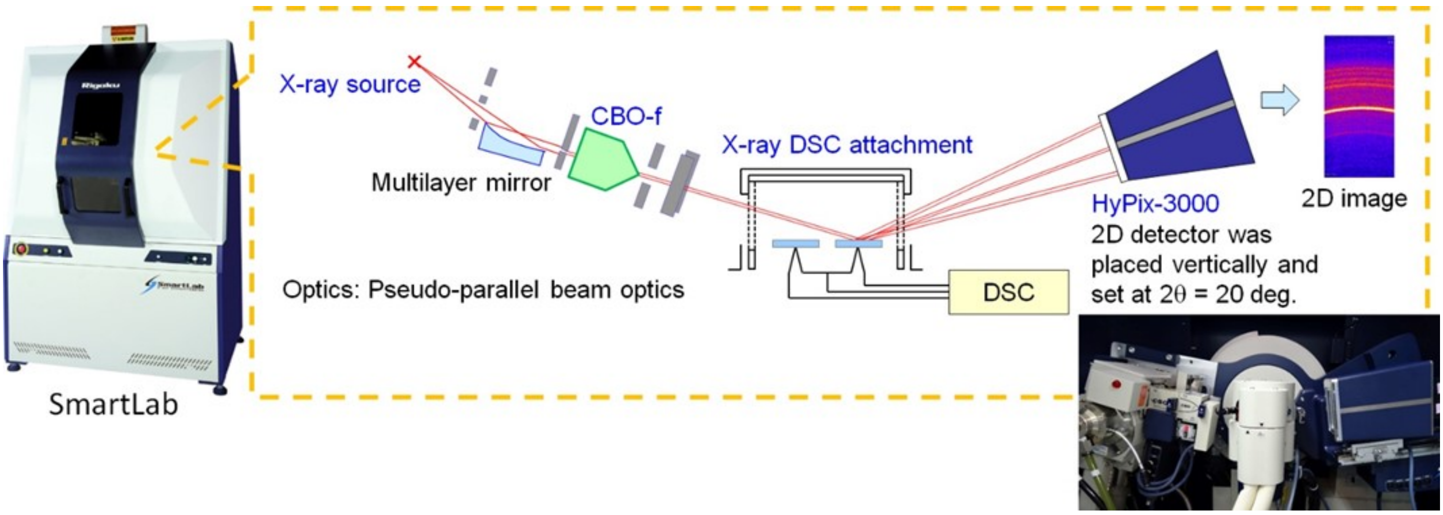

Figure 1. *Schematic of the Rigaku 9 kW SmartLab X-ray Diffractometer with in situ DSC*

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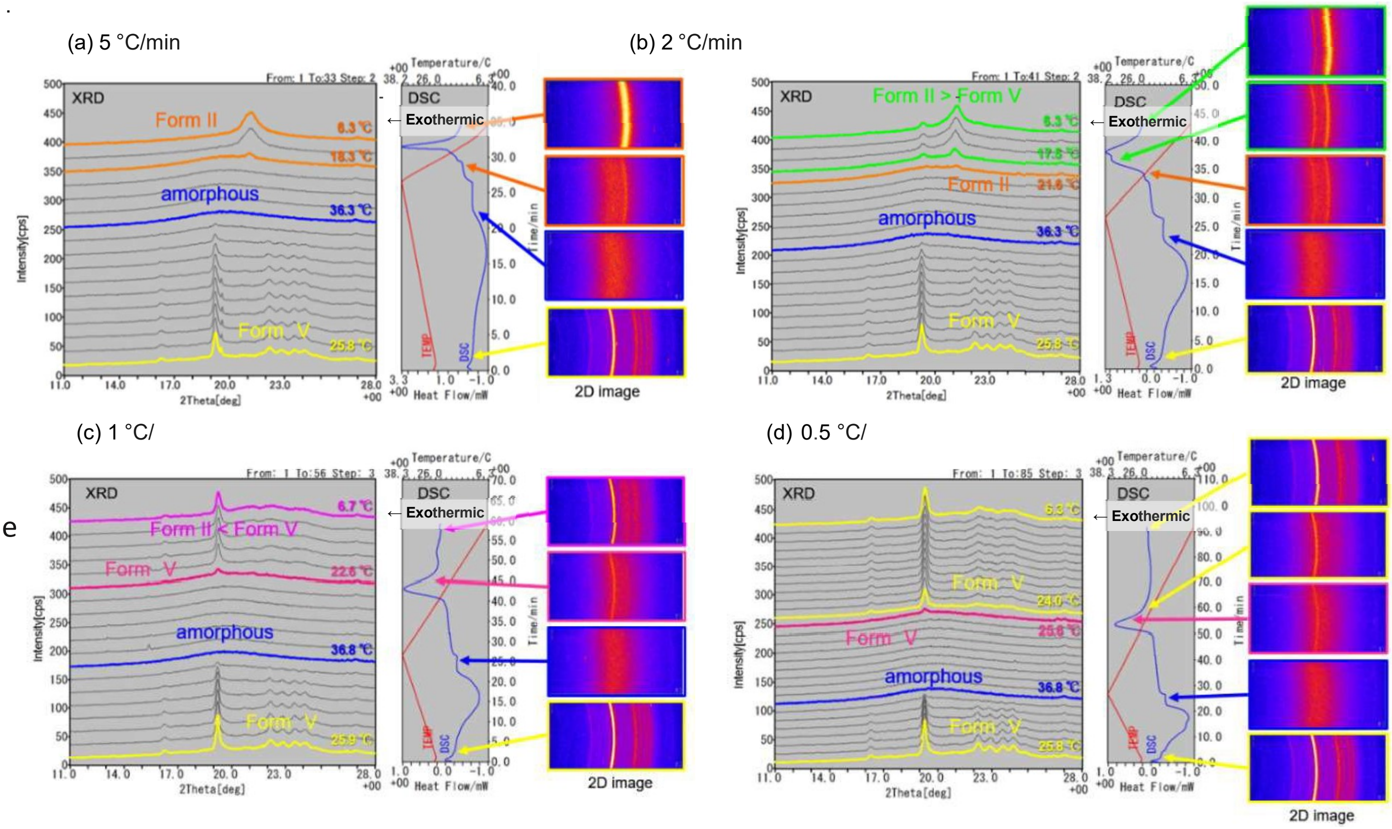

__Figure 2.__ Results of simultaneous XRD-DSC measurements by different cooling rates

Cooling rate(°C/ min)	Exothermic peak of DSC			X-ray diffraction	
	Onset temperature (°C)	Temperature of peak (°C)		Temperature of early stage (°C)	Crys-tal phase
		First peak	Second peak		
5	21.6	15.2	-	17	II
2	22.3	17.4	15.1	20	II>>V
1	23.2	20.9		23	V>II
0.5	25.3	23.9		24	V

__Table 1.__ The onset and peak temperatures of exothermic peaks of DSC curves, and early-stage temperature where the observation of X-ray diffraction peak begins, and the crystal phases

early-stage temperature where the observation of the X-ray diffraction peak begins, and the crystal phases. The onset temperature at which crystallisation begins shifts to the high- temperature side by controlling the cooling rate from 5 to 0.5 °C/min. The temperature interval between the onset and the peak temperature at which crystal growth is almost complete decreases as the cooling rate is slowed. The X-ray diffraction profiles show the phase transition from type II to type V. These results indicate that the nucleation of stable phase, type V, is sufficiently formed at high temperatures by a slow cooling rate, and crystal growth is rapidly achieved.

This study revealed that heating to 38° and slow cooling are essential to obtain Form V, the delicious chocolate phase.

Conclusions

Simultaneous XRD- DSC measurements facilitate the study of the onset-temperature of crystallisation, something that is difficult to observe in X-ray diffraction data alone. In addition, changes to the X-ray diffraction profile give information on whether the endothermic peak observed from DSC measurement is caused by melting or a structural phase transition.

Broadcast live from Bruker's YouTube channel the first Thursday of every month at 9:00 AM CT, our **Live from the Lab** streaming series explores X-ray Diffraction, X-ray Microscopy, and Elemental Analysis topics, with advice from applications experts who also answer questions that come in during the show.

Upcoming:
S1 E9 (Mar 12, 2021): When Would You Use 0D, 1D and 2D X-ray Diffraction?
S1 E10 (Apr 1, 2021): TBA

On Demand:
S1 E8: X-ray Sources for XRD
S1 E7: Features & Benefits of Powerful Benchtop WDXRF System
S1 E6: What is Combustion/Fusion Analysis?

AINSE THE AUSTRALIAN INSTITUTE OF NUCLEAR SCIENCE AND ENGINEERING

The Annual AINSE Winter School will be held on line 5—9 July 2021. This is an excellent opportunity for senior undergraduates to meet future collaborators and go hands-on with ANSTO's landmark facilities. Nominations will be accepted until 28 May 2021.

For more information visit **https://www.ainse.edu.au/winter-school/**

XAFS2021 Virtual
Sydney, Australia
11-13 July 2021

Due to the ongoing COVID-19 pandemic, the Local and International Organising Committees have made the decision to postpone the in-person XAFS2021 conference to July 2022.

A virtual event is now scheduled for 11-13 July 2021, to prelude the in-person July 2022 conference. The aim of this virtual conference is to provide a platform for the international XAFS community to remain connected leading into 2022. Students and early career researchers are the focus of this event with a programme of workshops, sessions on up-to-date developments in synchrotron radiation science and, above all, the opportunity for students and early career researchers to connect with the XAFS community and showcase their research.

The call for abstracts is open now!
https://xafs2021.org/call-for-abstracts.php

Featured Training Courses

Malvern Panalytical is offering two intensive training courses in XRF data collection and analysis.

XRF in the Workplace

Serving to provide high-quality training for industry and research professionals, this 5-day course will focus on most facets of XRF spectrometry. This course is suitable for all users of XRF, regardless of the brand of your instrumentation. Register here: 17th – 21st May | 8th - 12th November

Super Q Hands-on Training (For WDXRF users)

The SuperQ Software Training course is aimed at personnel interested in learning the step-by-step procedure of using the software for various aspects of running their XRF system. It is a 3-day course, with hands-on experience in using the software. Register here: 4th – 6th May | 13th – 15th October

Featured webinars

Malvern Panalytical is offering a series of free XRD webinars geared towards researchers interested in expanding their knowledge in X-ray diffraction.

Introduction to powder XRD
Watch on demand

XRD phase quantification
28 Apr, 2pm PER: .Register here

Transmission vs reflection measurements: practical tips for your XRD experiment and analysis
6 May, 2pm PER: Register here

Special Announcement: Virtual DXC

This year the Denver X-ray Conference will celebrate 70 years as the leading annual forum on general X-ray analysis, including both X-ray fluorescence and X-ray diffraction. The DXC will be held virtually from 2 – 6 August 2021. All Conference content will be housed on the Whova event app, accessible beginning 2 – 6 August and through 1 October for on-demand viewing, on mobile and desktop.

Key dates
15th April: Abstract submission
1st June: Jerome B. Cohen Student Award Deadline
1st June: Robert L. Snyder Student Award Deadline
15th July: Pre-registration Discount Deadline
30th September: Submission of Manuscripts Deadline

Find out more: https://www.dxcicdd.com/register-dxc/

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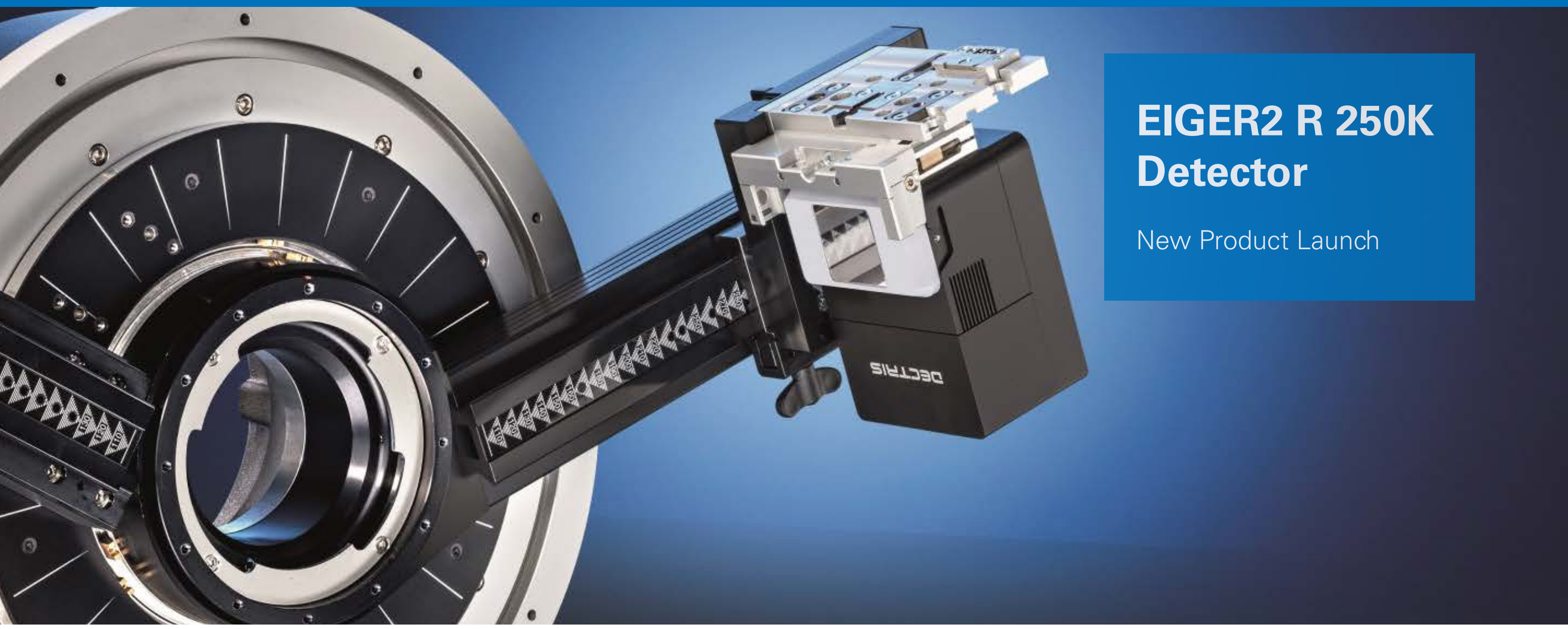

EIGER2 R 250K Detector

New Product Launch

Good Things Come in Smaller(er) Packages

Christina Drathen, Bruker AXS GmbH, Germany

Meet the EIGER2 R 250K detector, the newest addition to Bruker's detector family for X-ray diffraction.

Developed by DECTRIS, the technology leader for Hybrid Photon Counting (HPC) detectors, the EIGER2 R 250K boasts a large square sensor, over 250,000 pixels, and incorporates the latest technological enhancements of the EIGER2 R family, like the doubled dynamic range and the expanded energy and threshold range.

At Bruker, we integrated the EIGER2 R seamlessly into our DIFFRAC.SUITE software, and designed a detector mount and dedicated beam-path accessories. D8 ADVANCE and D8 DISCOVER diffractometers with the EIGER2 R detector enable fast and reliable optimization of the instrument geometry and efficient data collection for many XRD applications.

The EIGER2 R 500K has been the premiere XRD detector solution since 2017. So why are we now offering a smaller version – the EIGER2 R 250K? Users across academia and industry appreciate the intuitive operation and excellent results they get with our D8 diffraction solutions equipped with EIGER2 R 500K detector. In talking with those users, we found that many applications do not require the panoramic sensor size of the 500K. With the EIGER2 R 250K, we are now offering the same perfect pixel size, near limitless dynamic range and solution level integration, just in a smaller size.

Watch our launch video introducing the EIGER2 R 250K for D8 diffractometers and learn from our application scientists why they like the EIGER2 R for thin film analysis and powder diffraction applications: bit.ly/EIGER2R250K

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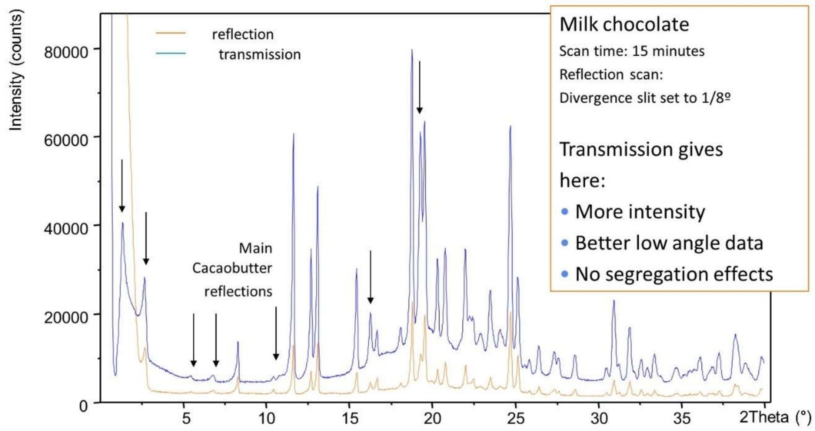
TRANSMISSION VS REFLECTION GEOMETRY

Tips & tricks plus practical considerations for your XRD experiments

Blog by Dr Martijn Fransen
XRD Scientist and Director of Malvern Panalytical's Digital Solutions

In almost every powder diffractometer, the reflection geometry is used. This is where the detector is on the same side of the sample surface. This geometry works very well for inorganic materials that can be prepared as flat samples with randomly oriented crystallites. However, it is very difficult to measure reflections below 5 degrees 2Theta accurately using reflection geometry. For instance, special care is needed to keep the background to a reasonable level. And the peak position is very sensitive to any error in sample preparation. This is especially inherent in reflection geometry and cannot be overcome.

Transmission geometry on the other hand is easy and straight forward for measuring reflections at low angles. Moreover, transmission measurements let you minimize preferred orientation effects. They are an especially great match for low-absorbing organic materials such as those used in the pharmaceutical industry.I learned about this years ago when I started to work with this method, and one of my contacts, **Prof. Henk Schenk from the University of Amsterdam**, suggested that I use chocolate as a test sample. This works best with thin chocolate slabs (e.g. a few mm thickness) as they immediately fit in a standard sample holder after biting off the edges (!). The results were surprising to me.



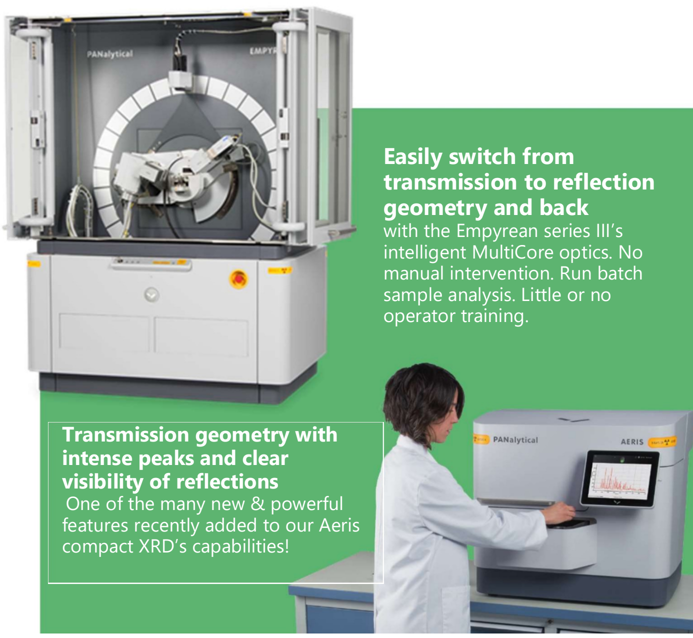
As you can see in the scan, transmission geometry gave much more intense peaks, and a clear visibility of reflections at 2.3 and 2.5 degrees 2Theta, respectively. I used a 1/8 degrees divergence slit in the reflection geometry, knowing that I would get better low angle data by going to smaller divergence slit sizes. This would, however, negatively impact the intensity difference even further, over 10x!

Of course, the transmission geometry only works if the samples are sufficiently transparent to X-rays. If this is not the case, one can easily switch to reflection geometry and back with Malvern Panalytical's recently introduced **MultiCore optics** in our new Empyrean series 3. Thanks to this intelligent XRD, easily switch between experimental set ups, run batch samples without any manual intervention. This reduces operator training and operator error. Plus it comes in handy for busy or central laboratories.

Having said that, more and more samples can be analyzed in transmission geometry because of recent developments in X-ray optics: one can now analyze even cell phone **batteries** by using much higher-energetic radiation, like Mo and Ag radiation. Pharmaceutical substances can better be done well be done with the more common Cu radiation. Our **pharma** PXRD customers using transmission geometry praise the massive improvement in data quality over reflection geometry and use the transmission geometry in their drug development and scale-up processes. Even advanced analyses like non-ambient studies under varying temperature and/or relative humidity are possible in transmission geometry, with the same benefits.

Join our Ask an XRD Expert webinar series:

- Watch on demand: Introduction to powder XRD. Register **here**
- 28 Apr, 2pm PER: XRD phase quantification. Register **here**
- 6 May, 2pm PER: Transmission vs reflection measurements: practical tips for your XRD experiment and analysis. Register **here**



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Candidates should send the membership form from the AXAA website, and a short statement about how they intend to contribute to the organisation, to the National Council Secretary Anita D'Angelo.

AXAA Resource Centre

There are a range of resources available on the AXAA website, including video recordings of the two Public Lectures at AXAA-2017, tips for Rietveld Analysis, Clay Analysis, XRF tips, and more. We welcome further contributions to our Resource Centre.

Next AXAA Newsletter

The next issue of the AXAA Newsletter will be distributed in August 2021. Please feel free to send contributions for the newsletter to Valerie Mitchell at *ausxray@gmail.com*. Any comments or feedback about the Newsletter are welcome.

A Day in the Life of an X-ray / Neutron Scientist

We are seeking posts for our 'Day in the Life' series. If you'd like to contribute, or know someone who might be interested, please contact National Council