AXAA

Australian X-ray Analytical Association

Newsletter Issue 1 2026

Chairperson's Address

Dear AXAA members,

I am excited to announce that the official website for **Crystal36–AXAA2026 Workshop, Conference and Exhibition** is now live:

Website: www.crystal36axaa2026.org*

Venue: Adelaide Hills Convention Centre, SouthAustralia

Dates: 29 November – 2 December 2026

I am also happy to announce the **call for nominations** for the AXAA Madsen-Gore Award, recognising an influential AXAA analyst, and the AXAA Award for an Outstanding Early Career Scientist. Both nominations will be closed on 30th September 2026. The recipients of these prestigious AXAA awards will be celebrated and announced during the **Crystal36–AXAA2026** Conference.

The conference also provides up to five **Rising Star awards** for excellent abstracts from students and early career postdocs and will be giving oral presentation opportunities in a dedicated session. This application will be open till 17th August 2026.

This conference represents an unprecedented collaboration between the Single Crystal and Polycrystalline X-ray Analysis communities through the combined efforts of SCANZ and AXAA. Bringing together workshops, conference sessions, and an industry exhibition under one banner, Crystal36–AXAA2026 is set to become not only the **largest** X-ray analysis conference held in Australasia in recent years, but also one of the **most accessible** conferences for students, who will be entitled to **half-price registration** and partial **student travel bursaries** supported by AXAA. This reflects our longstanding commitment to directing all association income towards supporting students, conferences, and exhibitions.

I sincerely thank the dedicated conference committee members from both SCANZ and AXAA for their outstanding collaborative planning and hard work over the past year, as well as ASN Events for their professional management and coordination of the conference infrastructure. Many innovations in analytical technologies are driven by our valued sponsors and instrument manufacturers. I am confident that the exhibition will provide attendees with exciting opportunities to discover the latest instruments, software solutions, and technological developments shaping the future of X-ray analysis.

The conference will feature internationally recognised experts and leading Australian specialists delivering plenary and keynote presentations across a broad range of cutting-edge topics. Five major presentation themes have been developed for abstract submissions:

- X-ray, Neutron and Electron Diffraction, X-ray Fluorescence, Microscale methods and Imaging techniques
- Structural biology, including Cryo-electron microscopy, Pharmaceuticals, Soft matter and the use of AI systems like Alphafold
- Metals, Alloys, Energy Storage, Materials and Structural chemistry
- Applications in the Environment, Geology and Mining, Industrial materials, Archaeology, Heritage and Cultural materials
- New instrumentation, In-situ and Operando experiments, and Advanced data analysis methods

*eduroam or a private network may be required to access the website, as it is not available on some government networks (e.g. CSIRO, ANSTO)

Pre-Conference Workshops

The pre-conference workshop program will include:

AXAA Basic XRD/XRF Workshops

ICDD Database and Software Workshops

These workshops are generously subsidised by AXAA and ICDD, enabling very affordable registration fees for students.

Post-Conference Workshops

Following the conference, advanced specialist workshops will be hosted at the University of Adelaide by sponsoring vendors, focusing on powerful and advanced capabilities within modern analytical software platforms.

I warmly invite researchers, industry professionals, students, instrument scientists, and practitioners across all fields of diffraction and X-ray analysis to join us in Adelaide for what promises to be an outstanding scientific gathering.

I look forward to welcoming you to Crystal36–AXAA2026!

Best regards!

Dr. Tony Wang
Chairperson, Australian X-ray Analytical Association
Senior Research Infrastructure Specialist (XRD), QUT
Active Member, Non-ambient Subcommittee, International Centre for Diffraction Data

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Critical elements tellurium and cobalt in surface environments: insights from X-ray fluorescence microscopy and X-ray absorption spectroscopy experiments

Owen P. Missen, owen.missen@utas.edu.au, ORCID: 0000-0002-2121-9971
Lecturer in Environmental Geology, Centre for Ore Deposit and Earth Sciences, University of Tasmania, TAS, PO Box 807, Sandy Bay 7006, Australia

Preamble

Understanding processes that drive natural cycling of under-studied critical elements such as cobalt and tellurium is important as humanity continues to use a larger range of commodities in greater amounts to drive the green energy transition. In this article, I outline the use of Synchrotron X-ray techniques to study cycling of tellurium and cobalt in surface environments.

Methods

Soil samples were collected from surface environments, typically aiming for saprolith at 10-20 cm depth, and regolith samples if saprolith was not present. Tellurium-rich soil samples were collected from epithermal Moctezuma mine, Sonora, Mexico (Missen et al. 2022a), while Co-rich samples were collected from sites across Australia encompassing a range of Co-hosting deposit types (Cu-Co, Co-As, carbonate-hosted and pyrite-hosted). The soils were mixed with epoxy in 0.7 mm plastic vials, hardened then cut and remounted using epoxy into a 2.5 cm diameter mount. We found that mounting priority samples from different sites into one overall mount resulted in more productive Synchrotron sessions, with less sample changes required.

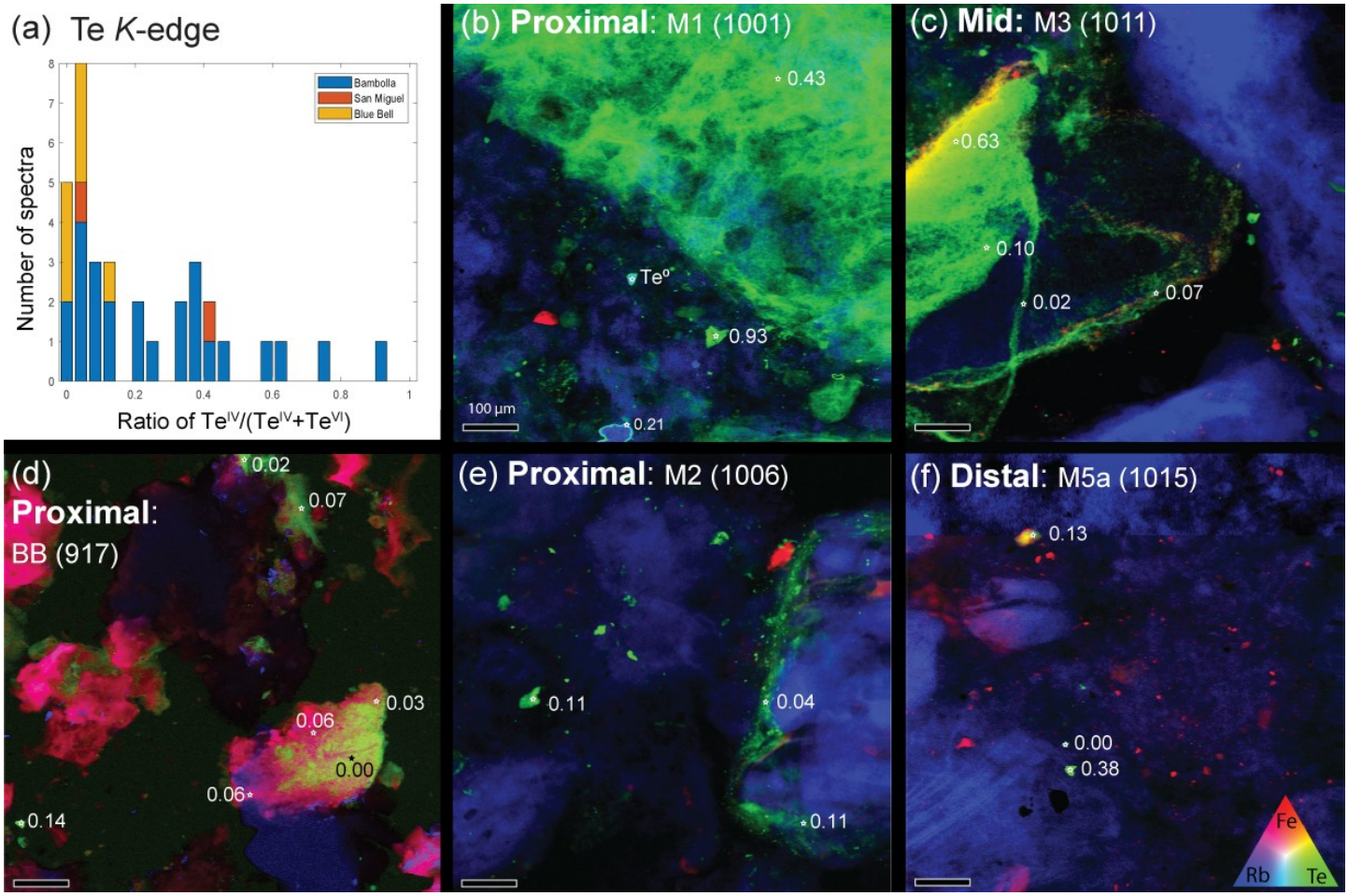

Figure 1: *Histogram showing distribution of TeIV/(TeIV+TeVI) ratios in analysed soil samples, determined at the K-edge. (b-f) RGB images of X-ray fluorescence (XRF) maps at Spring-8. TeIV/(TeIV+TeVI) ratios at specific micro-XANES points are shown next to stars indicating analysis points. All scale bars are 100 µm, reproduced from Missen et al. (2022b) by CC 4.0.*

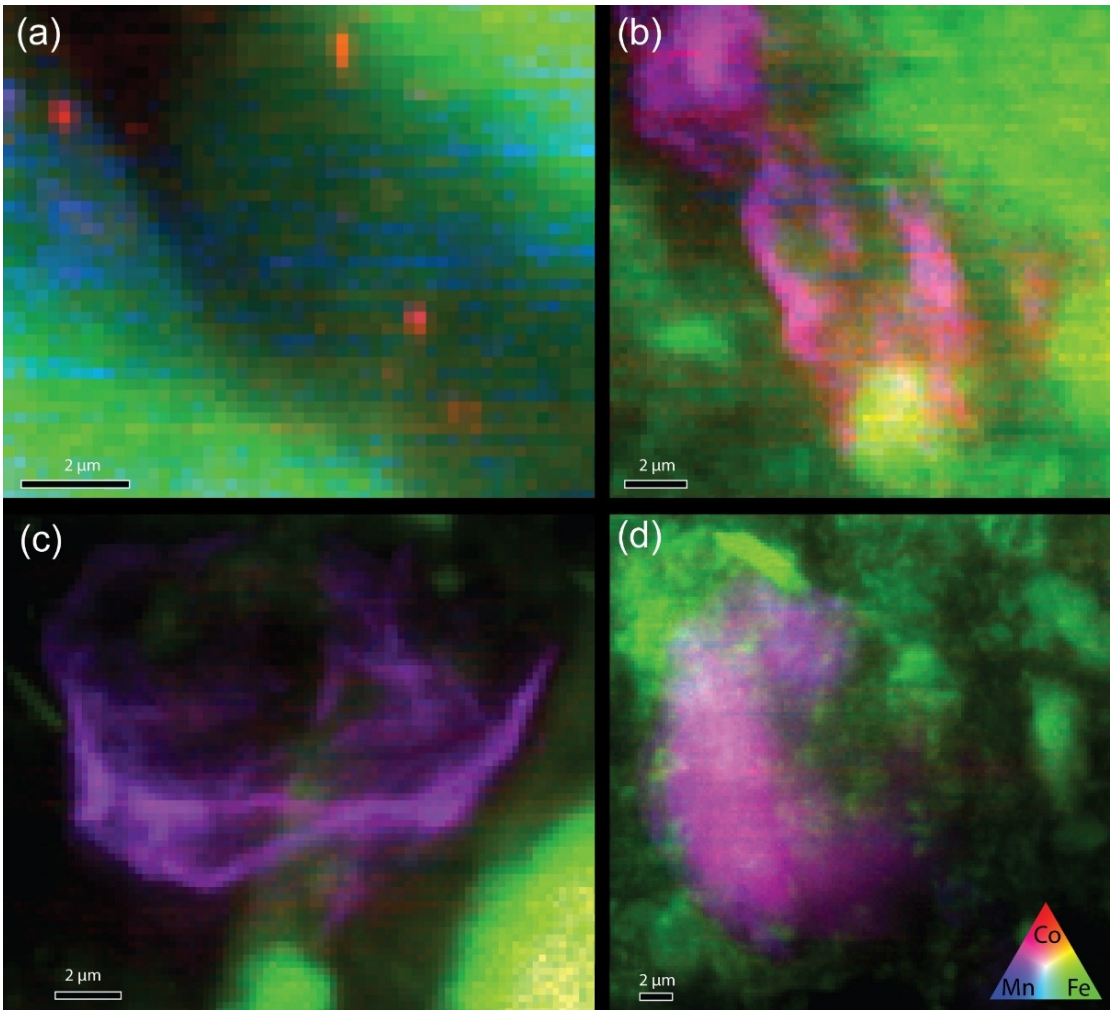

Figure 2: *Co-Mn-Fe XRF maps showing Co-Mn oxide nanoparticle clusters (purple overlap of red Co and blue Mn) collected at ID21, reproduced from Missen et al. (2024) by CC 4.0.*

Samples were analysed at two Synchrotron beamlines (von der Heyden, 2020), beamline BL37XU at Spring8, Japan for Te K edge (Missen et al. 2022b) and beamline ID21 at ESRF, Grenoble, France for Te L_3 edge (Missen et al. 2022b) and Co K edge (Missen et al. 2024). A combination of X-ray fluorescence microscopy (XFM) to map the high-resolution trace element geochemistry and X-ray Absorption Near Edge Spectroscopy (XANES) to trace oxidation state of the element of interest was used. Both tellurium and cobalt are redox-active elements in surface environments meaning that XANES is an ideal technique to use for their analysis.

Results

Tellurium exhibited three different oxidation states in Moctezuma surface environments, Te^0 (native tellurium), Te^{4+} and Te^{6+}. Linear combination fitting (LCF) was used to quantify the variation in Te^{4+} and Te^{6+} which have different peak positions in XANES spectra by comparing with Te oxidation state standards. The energy difference between Te^{4+} and Te^{6+} is larger at the Te K edge which made it more suitable for LCF of Te oxidation states than the Te L_3 edge.

Co exhibited all of the Co^{2+}, Co^{3+} or mixture of Co^{2+}/Co^{3+} oxidation states across the analysed sites, though not all sites had all three scenarios. LCF using the Orange software was used to identify clusters of spectra due to the larger number of spectra generated by the ID21 beamline spot XANES compared to the longer Te K edge scans at Spring-8.

Discussion

Cobalt and tellurium both appear to be more mobile in surface environments than might be expected based on evidence of nanoparticle cycling, demonstrating the importance of (1) analysing for nanoparticulate phases in terrestrial environments and (2) not assuming oxidation state homogeneity in soils.

Our understanding of (bio)geochemical cycling for many elements remains limited. Critical elements are nonetheless found in many deposit types, usually as minor elements. Their behaviour in outcropping zones of deposits – and in surface environments more generally – requires more detailed micro- and nano-studies using new combinations of techniques including X-ray based analyses to track their environmental behaviour. Using new combinations of techniques such as synchrotron X-ray techniques (X-ray fluorescence microscopy and X-ray absorption spectroscopy) coupled with single particle inductively coupled plasma–mass spectrometry (SP ICP-MS) provides detail to submicron resolution on oxidation state and size of nanoparticulate phases.

The value of this type of research will likely become increasingly important through the 21st Century as humanity uses critical elements in ever increasing amounts. The studies described here focused on surface outcrops of deposits. Other areas where such studies will be relevant is around recycling facilities or landfills where processing of critical element-containing products occurs. The benefits of such work include management of critical element stockpiles, and also potentially in providing new pathways for converting one compound into another (e.g. converting oxidised tellurium into native tellurium nanoparticles).

Acknowledgements

Thank you to all my coauthors for contributing to the papers briefly described in this newsletter piece, especially Dr Stuart Mills for sourcing the cobalt work funding. I gratefully acknowledge Glenda and Greg Lewin AM and the Geological Society of Australia (GSA) for funding to support the cobalt work described in this article through Museums Victoria. I also acknowledge support from the project "Building Capacity in Regional Australia to Enhance Australia's Economy through Research, Training, and Environmentally Sustainable Production of Critical Metals", a Regional Research Collaboration (RRC) initiative funded by the Australian Government Department of Education which has allowed me to continue researching critical metals in mine wastes and surface environments.

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X-ray Absorption Spectroscopy setup on a laboratory X-ray powder diffractometer

Olga Narygina[1]*, Milen Gateshki[2], Charalampos Zarkadas[2], and Detlef Beckers[2]

[1]Malvern Panalytical B.V., 7602 EA Almelo, The Netherlands;

[2]Malvern Panalytical Pty Ltd., 2170 NSW Sydney, Australia

*Correspondence:
olga.narygina@malvernpanalytical.com

Introduction

X-ray absorption spectroscopy (XAS) is a powerful technique for studying a material's structure. It analyses the behaviour of the absorption coefficient near an element's absorption edge. XAS spectrum is typically divided into two regions. XANES (X-ray absorption near edge structure) part extends up to 50–100 eV above the edge and is sensitive to the oxidation state, electronic structure, and local environment of an atom. The higher-energy part of the spectrum is called EXAFS (extended X-ray absorption fine structure). It spans up to 2000 eV above the edge and probes short-range atomic order.

XAS complements X-ray diffraction (XRD) and X-ray fluorescence (XRF). The method is particularly useful for liquids and amorphous materials. Moreover, the element-specificity of XAS allows one to distinguish similar atomic species in different environments.

Historically, XAS experiments were exclusively performed at synchrotron facilities. However, in the last decade the interest in laboratory-based XAS has grown [1,2], and several commercial instruments are now available. Conventional experimental configurations (Rowland circle and von Hamos geometries [3-18]) use focused X-rays for enhanced signal intensity. However, these setups increase mechanical complexity and are generally incompatible with standard laboratory powder diffractometers.

Recently we proposed a novel XAS setup with a flat analyzer crystal that can be readily implemented on a standard laboratory powder XRD instrument[19]. The present report gives the short setup description and demonstrates its feasibility using the example of the iron K absorption edge. For the detailed discussion and additional case studies, including in operando XANES of an NMC battery, please refer to the original publication [19].

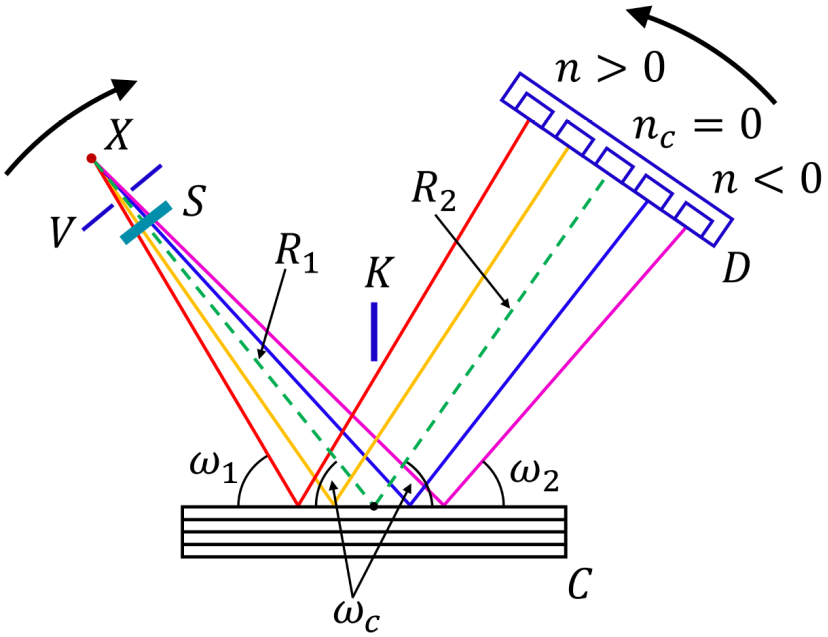

Figure 1. A schematic diagram of the experimental set-up. Polychromatic X-ray radiation is emitted by the X-ray source X, travels through specimen S and is diffracted by the flat crystal monochromator C. After diffraction, the X-ray photons are directed to the position sensitive detector D. Depending on the angle of incidence, photons with different energies will be diffracted at different points on the crystal surface. This is represented by lines of different colors. R1 and R2 are the distances between the source and the rotation axis (center) of the goniometer and between the goniometer center and the middle channel of the X-ray detector. The top surface of the crystal is aligned to be at the center of the goniometer. V is a divergence slit, and K is a beam shield.

XAS measurement configuration

A schematic overview of the proposed setup is shown in Figure 1. The configuration uses an X-ray tube with a line focus and a one-dimensional strip detector with high energy resolution (better than 500 eV). This helps to suppress background contributions such as higher harmonics, fluorescence, and characteristic radiation from the X-ray source. Other X-ray beam characteristics (size, axial divergence, and parasitic scattering) are controlled by standard diffractometer components.

The sample is mounted on a goniometer arm and is moved with the source. Depending on the experimental requirements, it may be beneficial to mount it on the detector arm. The setup operates in a wavelength-dispersive mode: X-rays transmitted through the sample impinge on the flat analyzer crystal at varying incidence angles. According to Bragg's law, only photons with specific energies are diffracted toward the detector. Because different parts of the incident beam satisfy the diffraction condition at different angles, a range of photon energies is spatially dispersed across the detector. This enables simultaneous acquisition of a range of different energies, significantly improving measurement efficiency compared to a point detector. By accounting for the geometry of the setup, the position on the detector (strip number) can be directly correlated with photon energy, allowing reconstruction of the transmitted spectrum and determination of the absorption at each energy.

The energy range accessible in a single measurement is defined by the detector solid angle. However, it can be extended using a scanning mode, in which the source and detector move synchronously over a defined angular range. Additional benefit of scanning is the lower sensitivity to local variations in thickness or composition of both, sample and analyzer crystal. Furthermore, the scanning mode allows for sub-strip angular sampling, improving the effective energy resolution.

Given the low intrinsic intensity of XAS signals, air absorption becomes a significant factor in XAS experiment design. For the configuration presented here, air absorption is negligible above ~8 keV (≈80% transmission over 480 mm); however, the transmission drops to about 10% near 5 keV. Performance at low energies can be improved by tuning the X-ray source settings for optimized emission in the required energy range. It should be noted that the performance of a tube (the number of photons with a specific energy) drops when the absorption edge of the investigated element is at a higher energy than the absorption edge of the anode element [19]. If it is not possible to select an optimal source for every element to be analysed, Cu or Ag tubes offer a good compromise. These tubes provide reasonable performance for a range of absorption edges [19].

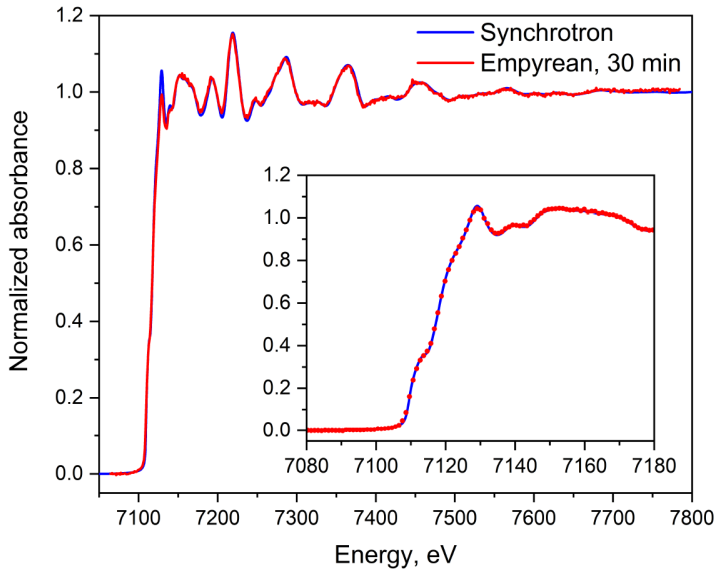

Figure 2. Experimental XAS spectrum of a 7.5 µm Fe foil collected in 30 min and covering a range of 700 eV (red) compared with a synchrotron reference (blue). The inset shows a 30 min scan in the XANES range optimized for better performance (red), compared to the synchrotron reference (blue).

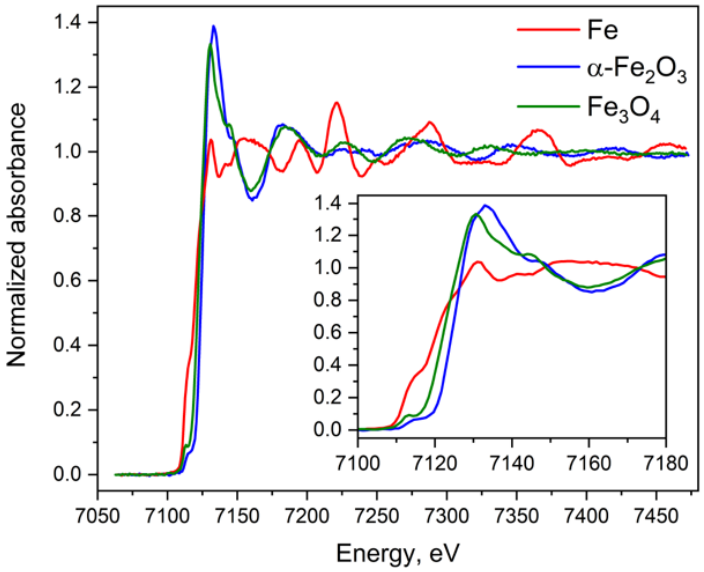

Figure 3: XAS spectra of α-Fe2O3 (blue) and Fe3O4 (green) powder samples, compared with the corresponding spectrum of a 7.5 μm Fe reference foil (red). The inset shows a magnified view of the XANES range.

Experimental details

The experimental configuration described above was realized on a Malvern Panalytical Empyrean multipurpose diffractometer, with a long-fine focus Cu or Ag tube, slit optics, solid-state 1Der Advanced Detector with the energy resolution of 320 eV. A flat Si (011) crystal was used as an analyzer crystal. R1 and R2 (Figure 1) were both equal to 240 mm. The energy resolution of the experimental setup was estimated to be ~2.2 eV at the energy of 8 keV when using Si[022] reflection. This results in a resolving power of E/δE = 3600, typical for many XANES experiments [13,14]. The energy resolution can be improved by using a different crystal reflection, for example Si [044] of the same crystal. In this case, the estimated resolution was ~1.3 eV.

The performance of the proposed setup was evaluated using 7.5 μm Fe foil reference material, supplied by EXAFS materials, Danville, CA, USA. The obtained spectra were compared with high quality synchrotron data obtained from the Materials Data Repository (https://mdr.nims.go.jp/). Metal oxides, used for the measurements, were prepared by mixing the corresponding powder materials with isopropyl alcohol and depositing them on a Kapton (polyimide) foil. The collected XAS spectra were processed using the program Athena [20].

Results and discussion

XAS spectra of the reference Fe foil, measured using the proposed setup, are shown in Figure 2. The EXAFS spectrum, collected in 30 minutes using the setup, optimised for intensity, covers an energy range of 700 eV. A small difference from the synchrotron spectrum is observed in the vicinity of the Fe absorption edge. However, despite this difference, the data quality is sufficient for the quantitative analysis of the EXAFS signal of Fe. The Fourier transform of the Fe foil EXAFS spectrum obtained with the present experimental setup is very similar to that calculated from the synchrotron data when the same k range is considered [19]. Better quality at the absorption edge can be achieved using XAS setup optimised for resolution (inset of Figure 2).

Figure 3 compares XANES spectra of α-Fe2O3 (hematite) and Fe3O4 (magnetite) samples prepared from powder with the reference Fe foil discussed above. All scans were measured using setup optimized for resolution with the data collection time of one hour. The differences in the absorption edge positions, near-edge structure and absorption behaviour in the higher-energy part of the spectra are clearly visible. These differences stem from the different oxidation states and coordination environments of the Fe atoms in the three materials. The presented data are consistent with previous reports based on synchrotron studies [21].

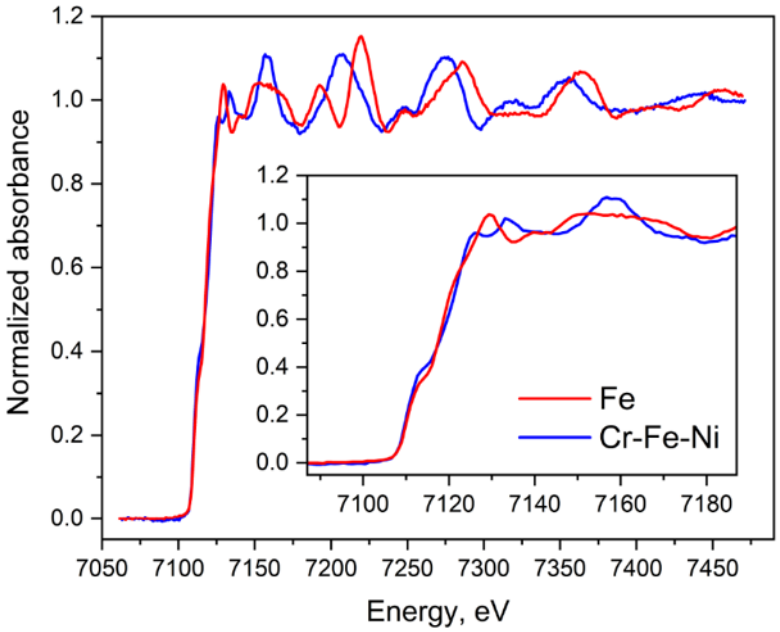

Figure 4. XAS spectrum of a Cr-Fe-Ni alloy measured around the absorption edge of Fe, compared with a reference Fe reference foil.

XAS spectrum of the same reference Fe foil was compared to that of a 5 µm thick austenitic steel foil with a nominal composition of 70% Fe, 16% Cr, and 14% Ni. Pure metallic Fe exhibits a body-centered cubic (*bcc*) structure at ambient conditions, with a transition to a denser face-centered cubic (*fcc*) structure at higher temperatures (~1200 K). However, additives, such as Cr and Ni, stabilize *fcc* structure at room temperature, which defines the high ductility and corrosion resistance of austenitic steel. As seen in Figure 4, both Fe and austenitic steel show nearly identical absorption edge positions. However, the post-edge structures are distinctly different, reflecting their differing crystal structures.

Conclusion

The proposed XAS experiment setup [19] has been implemented on a standard laboratory powder diffractometer with a few minor modifications to both hardware and control software. The approach has been validated across a variety of materials, demonstrating that high-quality data can be obtained within practical acquisition times ranging from several minutes to a few hours, depending mainly on the sample composition and the selected energy range.

Compared to conventional laboratory-based XAS instruments, the present setup exhibits several distinctive features commonly available in modern powder diffractometers: a position-sensitive detector with high energy resolution, a highly precise goniometer, enabling accurate alignment of the flat analyzer crystal, and the adoption of continuous scanning of both the X-ray source and detector during data collection. Apart from the straightforward reconfiguration from XRD to XAS mode, a key advantage of the proposed methodology is its ability to cover a broad energy range encompassing the absorption edges of multiple elements without requiring exchange of the analyzer crystal or other optical components. Furthermore, the system allows for rapid switching between high-intensity and high-resolution measurement modes by simply adjusting the goniometer angle to access a different crystal reflection.

The integration of XAS capabilities into a conventional powder diffractometer provides an accessible entry point for users familiar with diffraction techniques, facilitating the adoption of XAS in laboratory environments. This approach has the potential to significantly expand the accessibility and routine application of XAS in materials characterization.

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About

The Crystal36-AXAA2026 Conference is jointly organised by the Society of Crystallographers in Australia and New Zealand (SCANZ) and the Australia X-ray Analytical Association (AXAA). This is the first combined conference for the two organisations, which together represent a wide range of the structural science community in Australia and New Zealand.

This 3 day conference is bookended by satellite workshops, and will contain both concurrent and combined sessions.

Venue

The Adelaide Hills Convention Centre is located in Hahndorf, and is only a 20 min drive from the Adelaide city centre. Conference attendees can book to stay on site in cabin accommodation through the conference website. The township of Hahndorf also offers a range of accommodation options a short walk away from the conference venue.

Awards and Bursaries

Madsen-Gore Award for outstanding application of analytical technique/s using X-ray or Neutron scattering and/or major radiation facilities.

Early Career Scientist Award for outstanding development in, or application of, analytical methodologies to understand minerals or materials, with an emphasis on industrially relevant processes and technologies.

Applications for both awards close 30th September

Rising Star Awards for excellent abstracts from students and early career postdocs and will be giving oral presentation opportunities in a dedicated session.

This application will be open till 17th August 2026.

AXAA Student Travel Bursaries will be available for partial support of costs associated with travel to the conference. More details to come on the conference and AXAA websites.

Abstracts

The deadline for abstract submission is **Wed 15th of July**.
Apply on the conference website and select the theme which bests suits your submission.

Registration

Early bird registration closes on the **28th August**. Register here.

	Early bird *(Until 28th Aug)*	Regular
Full registrations		
SCANZ-AXAA Member	$580 AUD	$860 AUD
Non-member Registration	$620 AUD	$900 AUD
Student Registration		
Student SCANZ-AXAA Member	$290 AUD	$430 AUD
Student Non-member	$300 AUD	$440 AUD
Other Registrations		
Day SCANZ-AXAA Member	$275 AUD	
Retired SCANZ-AXAA Member	$430 AUD	

Membership

Discounted registration fees are available for members. If you are not a member yet, apply on our website now, and encourage any interested conference attendees to do the same.

42nd Ore and Mineral Analysis (OMA) Workshop Perth

Real applications across the critical minerals value chain

Malvern Panalytical
a spectris company

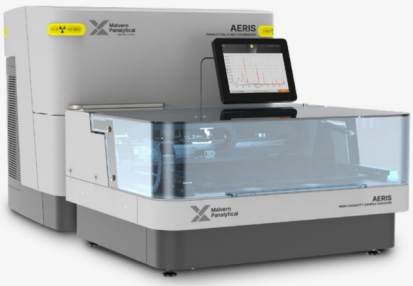
For
information & registration

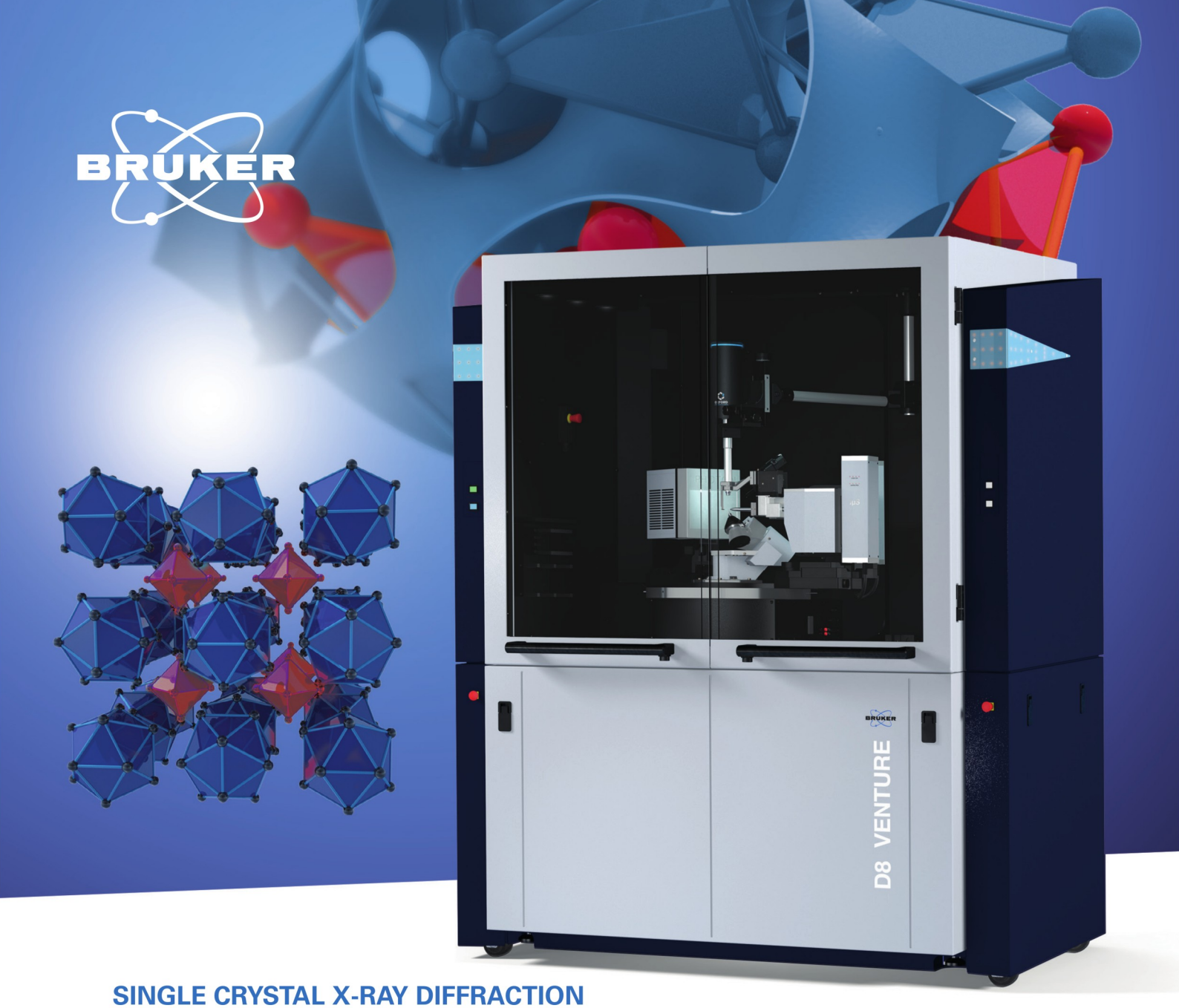
Date: 26th June 9:00 – 17:00
*Complimentary tea & Lunch will be served
Location: Karstens Perth
Level 1/111 St Georges Terrace, Perth WA

This one-day seminar will showcase analytical solutions supporting the mining and metals industry across the critical minerals value chain.

Topics include ore characterization, process optimization, quality control, and recycling.

The program features industry presentations and live demonstrations of XRF, XRD, NIR, and particle characterization technologies from Malvern Panalytical. Designed for professionals in mining, metallurgy, and mineral processing, the workshop offers practical insights and valuable networking opportunities.





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XRD MINERAL MAPPING

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Our advanced single-particle counting cameras, combined with energy dispersive X-ray diffraction (EDXRD) technology, allow for rapid scanning of the entire volume of a mineral sample within milliseconds. For example, a pint in a 5 mm thick piece of rack can be exampled in just 10 milliseconds.

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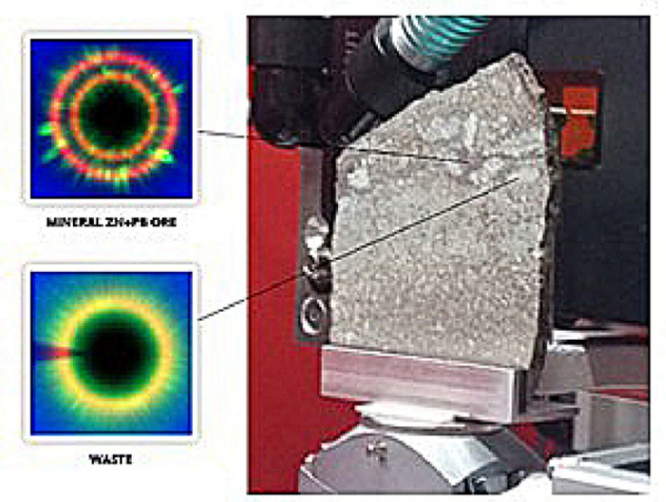

The diffractograms in this image visualize different materials inside the examined 5mm tick piece of mineral.

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Diffraction Technology
diffraction@bigpond.com

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NATIONAL COUNCIL PRESIDENT:

Tony Wang
Level 6, P Block
Gardens Point Campus
Queensland University of Technology
Brisbane, QLD, 4000
Telephone: (07) 3138 1904
e-mail: tony.wang@qut.edu.au

NATIONAL COUNCIL VICE PRESIDENT:

Jessica Hamilton
Australian Synchrotron (ANSTO),
800 Blackburn Road,
Clayton, VIC 3168
Telephone: (03) 8540 4297
e-mail: hamiltoj@ansto.gov.au

NATIONAL COUNCIL SECRETARY:

Daniel Fanna
Advanced Materials Characterisation Facility,
Division of Research and Innovation
Western Sydney University, NSW 2751
Telephone: 0414 288 919
e-mail: d.fanna@westernsydney.edu.au

NATIONAL COUNCIL TREASURER:

Ruoming Tian
University of New South Wales,
G65, XRD Lab
Mark Wainwright Analytical Centre
Chemical Sciences Building
Telephone: (02) 9385 4524
e-mail: r.tian@unsw.edu.au

NATIONAL COUNCIL COMMUNICATIONS EDITORS:

Rosemary Young
Australian Synchrotron (ANSTO),
800 Blackburn Road
Clayton, VIC 3168
Telephone: 0439 734 345
e-mail: youngr@ansto.gov.au

Valerie Mitchell
Australian Synchrotron (ANSTO),
800 Blackburn Road
Clayton, VIC 3168
Telephone: 0439 734 345
e-mail: mitchelv@ansto.gov.au

Rod Clapp
Diffraction Technology
194 Mt Eliza Way,
Mt. Eliza, VIC 3930
Telephone: 0418220672
Email: diffraction@bigpond.com

NATIONAL COUNCIL MEMBERS:

Matthew Rowles (Microanalysis Aus, WA)
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AXAA Membership

New memberships can be obtained free of charge, by making an application to the National Council.

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 Liam Tan.

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 late 2026. Please feel free to send contributions for the newsletter to the Communications Editors at *ausxray@gmail.com*. Any comments or feedback about the Newsletter are welcome.