



News from the Applications Lab.

Questions, highlights and collaborations

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Apprentice and former apprentice Alex and Phoebe

Making complicated simple

Improving ease of use of XPS instruments

Meet our Users

Dr Billy Murdoch, RIMT, Australia

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WELCOME TO THE WINTER KRATOS NEWSLETTER

Drive innovation together

Welcome to the Winter Newsletter. There's plenty of Kratos related content for you to read.

Have a look at News from the Apps lab for details of our new US office location. You can also see the dramatic delivery of an AXIS Supra⁺ to the Centre for Advanced 2D Materials at NUS. Our User interview is with Dr. Billy Murdoch who is a Senior Technical Officer in the RMIT Microscopy & Microanalysis Facility (RMMF) in Australia. Read about how the AXIS Supra⁺ supports research goals at the Royal Melbourne Institute of Technology.

To coincide with National Apprentice Week here in the UK, we interview two Kratos colleagues. Alex who is an Apprentice Fitter and Phoebe who has now finished her apprenticeship and is now working at Kratos as a Quality Engineer. In the article 'Making complicated simple' we consider how automation has made operation of complex analytical instruments easier but with the risk of inadvertently generating erroneous data. The article highlights the need for educating new instrument Users and the contribution of 'expert systems' guiding data acquisition.



Finally we present the headline results from the Users' survey conducted at the end of 2022. Thank you to everyone that took time to contribute. We're extremely pleased to report that >95% of Users rated our overall performance average or above.



UPDATES FROM THE APPLICATIONS LAB.

Our new US office !



At the end of 2022 we moved our North American office to new premises. The new postal address is:

Kratos Analytical Inc.

404 East Route 59, Nanuet New York 109540 USA

Our telephone, fax number and e-mail addresses remain unchanged:

+1 (845)-426-6700
+1 (845)-426-6192

Featured job opportunity in Manchester, UK

We have a vacancy for an **Applications Specialist**, based at our Manchester headquarters. This is an exciting role within Kratos Analytical's surface analysis business group, involved in sales and marketing of our XPS products. The ideal candidate will have a PhD or equivalent skills in surface or materials analysis and hands-on experience using scientific instrumentation. The successful applicant will have responsibility for sample analysis using our market-leading Apps. Lab. instruments. You will also be responsible for preparation of sample analysis reports that demonstrate the capabilities of the spectrometer. The job requires someone who is self-motived and can work to deadlines, with good attention to detail. As experience increases you will be able to initiate and develop collaborations, developing the technique and its application to materials analysis challenges. There will be ample opportunity for international travel to provide on-site instrument training and presentation of work at conferences and symposia. This is a job for someone who thrives on each day at work being different.

ANALYTICAL A SHIMADZU GROUP COMPANY	
Location	Manchester, UK
Salary	Competitive
Posted	18 th December
Closes	on successful appointment
Discipline	Applications Specialist
Position type	Permanent
Hours	Full time

If you would like to know more about the role or for an informal discussion contact our Applications Manager, Dr Sarah Coultas.

To see an up-to-date list of all vacancies based in Manchester, visit our recruitment portal.



Flying Supra's

Every installation of the AXIS Supra⁺ is different. Some instruments are delivered from the back of the air-ride suspension truck to an unloading bay and wheeled directly into the laboratory. Others, such as the AXIS Supra⁺ shown in the photograph above, have a more 'exciting' journey. After unpacking from the main instrument crate, the shock-absorbing base of which is still evident on the road, the Supra⁺ was lifted 5m onto a 1st floor walk way (inset). It then had a more conventional route down corridors into the lab. in the Centre for Advanced 2D Materials, National University of Singapore (NUS).

Our Test & Installation Engineer, David Richardson, commented 'although a difficult route to the lab, the freight handlers had the move under control at all times, which was reassuring. I guess we were lucky that we didn't get any tropical down-pours while the Supra was outside'.

i-work

Interview with our employees

Here we meet two Kratos colleagues, Alex Yates and Phoebe Barton. Alex is an Apprentice Fitter, working primarily on assembly of the Surface instruments and Phoebe is a Quality Engineer, having moved to a full-time job within Kratos after her apprenticeship. Apprenticeship schemes in the UK are vocational training programs that combine on-the-job experience with classroom instruction. They are intended to provide individuals with the skills and knowledge needed to succeed in a specific trade or occupation.



We sat down for a chat to learn more about what it's like to be an apprentice at Kratos and the route from school to employment.

How did you end up as an apprentice at Kratos?

Alex: In my last 2 years at school, I picked engineering subjects and Maths. I enjoyed Maths and the problem solving involved. After two years at college I knew I wanted to carry on with engineering so applied for an apprenticeship. After a couple of

interviews I was taken on by Kratos.

Phoebe: My dad works in a car body-shop and as a kid I was dragged to his work on Saturdays. We had an old Mini Cooper Classic that we were doing up, so I'd help with that. I knew from a young age that I didn't want a job sitting behind a desk. I started my apprenticeship at 16, straight out of school. Like Alex, I did a six-month block at college covering the basics of mechanical engineering. I completed my apprenticeship but by the end had moved from the shopfloor into the Quality Department.

What was it like starting as an apprentice at Kratos?

Phoebe: It was a bit strange on the shopfloor in such a male dominated environment, but they are great to work with. I think they took me on as a daughter and really looked after me!

Alex: It wasn't too daunting. I spent a week at Kratos, being shown around and working with someone on the shopfloor, getting to know the type of work involved. I was then on a three-month block release to college, learning skills like milling, lathe work, fitting, all the basics. It also involved mini-build projects, which really helped with the type of work I do at Kratos.

What's your current role at Kratos?

Alex: I build sub-assemblies, like sample magazines, the magnetic lens or gas cluster ion sources. Most of the work is described in SAMI's (scientific apparatus manufacturing instructions), but I still need to be able to read and understand technical drawings. I have also worked on main builds, assembling the complete instrument. I worked with a colleague on my first build and then was mainly on my own for the second build—I think that instrument is heading to a lab. in China!

Phoebe: As a Quality Engineer, I am involved in final inspection of our instruments before they ship to their new owners. I also inspect incoming parts, making sure they are manufactured correctly to drawing and within tolerance. I also am involved in problem solving, both those from our customers and also internal issues. It's a very varied and exciting job. I think having

a hands-on mechanical background is really helpful in my current role. Knowing how something is built allows me to discuss issues in detail with our suppliers and suggest solutions to identified problems.

What about your future employment?

Alex: Kratos has given me the opportunity to carry on with my apprenticeship and complete my Higher National Certificates for another 2 years. After that I'd like to look at moving into the Engineering Office, perhaps Mechanical Design or Production Engineering. Unfortunately, covid and now remote working has meant that I've not had the opportunity to shadow colleagues in the Engineering Office, but I'm sure the opportunity will come.

Phoebe: My journey was a little bit different. I did get to move around the different departments within Kratos quite early in my apprenticeship, spending a few days or up to a week in different roles. While I was part way through my apprenticeship there was a vacancy in the Quality Department. I applied and got the job, so that meant we had to change the direction of my apprenticeship, so as well as studying mechanical engineering, I was also focusing on Quality.

Would you recommend an apprenticeship as a route to employment?

Phoebe: Yes, definitely. I completed my apprenticeship after 3 years. It helps that I had an idea what I wanted to do but it was certainly a really good way to get to know a subject and get practical experience of working.

Alex: Definitely. The mix of college learning and practical engineering in a company is much more engaging. I think it's much more applied than going to university. It also has the advantage that you're earning while completing an apprenticeship. It means that I have developed and gained new skills but not got mounting debts like my mates that went to college and then University.

MAKING COMPLICATED SIMPLE

Improving ease of use of XPS instruments

Considering the complexity of a modern smart phone, they are staggeringly easy to use. I'm sure it's hard to remember a first encounter with a touch sensitive screen but it undoubtedly seemed intuitive. The tap of a finger to select, pick up and drag. The swipe left or swipe up to scroll. The pinch of thumb and forefinger to magnify or demagnify. All these actions to navigate and initiate processes, often with simple icons for guidance. Even though I struggle to remember *my* first encounter, I can distinctly remember my then 4-year-old daughter happily mimicking what she's seen me do so that she could watch Peppa Pig on my phone.



And I'm pretty sure that I've never opened, let alone read, a User manual for my smart phone, despite its functionality and complexity.

Which leads to the thought ' should analytical instruments have a similarly low barrier to entry?' It's a fact that the AXIS Supra⁺, with it's full automation, is significantly easier to operate than the manual, 'home-built' system I learnt on three decades ago. It's easy to forget the old potentiostat with jittery needle

display used to apply the acceleration voltage to the X-ray anode. It actually felt as though you were applying a highvoltage, rather than the abstract double digits of a software readback that we're used to today.

There is undoubtedly a growing trend. Analytical instruments are becoming easier to use, approaching 'smart phone' type

simplicity that any novice can walk up to an run. But where does that leave the analytical scientist?

As James Strachan highlights in his recent editorial of The Analytical Scientist [1], there are certain advantages to opening up analytical techniques to many more researchers. He continues 'there is a big gap between the cutting-edge and the truly accessible—and this middle ground must not become an open but confused playing field'.

As a manufacturer of XPS instruments we are acutely aware of our role in lowering the barrier to entry for use of the modern spectrometer. It is true to state that there has not necessarily been a step change in the ease of use. Over several generations of spectrometer, the level of automation and therefore ease of use has increased. Our current generation of spectrometer, the AXIS Supra⁺, is fully automated, from sample handling to gas admission for ion sputtering. Complete automation means that the spectrometer can be operated remotely from another room, site or even continent. It also means that the spectrometer is easier to operate for the novice User. Automation has great advantage in increasing sample throughput, lowering the cost of ownership when measured against the number of samples analysed. But, to quote Bill Gates 'automation applied to an inefficient operation will magnify the inefficiency' or to paraphrase 'garbage-in, garbageout'.

Having established that we can reduce complexity through hardware automation, what other support can be provided to the analyst? A growing area within analytical instrumentation is the incorporation of AI, artificial intelligence. Applying this to XPS surface analysis is still some way off, but the fundamentals exist and are available in the latest release of acquisition software. Robust peak identification with a high-degree of



ESCApe software User interface for 'Known Sample Workflow' method.

confidence in peak assignment is a non-trivial requirement, forming the starting point for any sample analysis. Improved computer derived peak identification from unknown samples minimises User error or bias. It also forms the starting point in an automated sample analysis workflow, known in Kratos' ESCApe as Data-dependent Analysis (DDA). This acquisition method identifies peaks in a survey spectrum and then acquires high resolution, narrow region spectra from the major components. We know from our recent User survey that 89% of our Users regularly employ the large area survey acquisition mode as the starting point for sample analysis. For an experienced analyst DDA can simply be considered a timesaving acquisition method. For the inexperienced analyst it provides confidence that elements will be correctly identified and appropriate high resolution spectra acquired.

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MAKING COMPLICATED SIMPLE (continued)

Thoughts on improving ease of use of XPS instruments

A further step in guiding analysis, simplifying spectral acquisition and interpretation in ESCApe is the use of the Known-Sample Workflow (KSW) method. As the name suggests, a standard acquisition is progressed to allow charge correction and fitting of pre-defined component models to narrow region spectra. This type of analysis is only appropriate for well-known, highly reproducible samples and currently finds primary use in QA and QC type application.

Data dependent acquisition and known sample workflow methods will not replace the knowledge of an experienced analytical scientist. Indeed, the concept of an 'expert system' is not a new one. Dr Jim Castle has championed this concept in the early 2000's [2]. Over two decades later, the analyst is still probably the single-most important component for materials characterisation. Dr Castle identifies the starting point in creating an expert system as the setting of goals, a series of steps leading to the reasonable outcome for the analytical investigation. This is analogous to the discussion between the subject specialist, usually the owner of the sample, and the analytical scientist responsible for using the spectrometer for the sample analysis. Knowledge and experience of the capabilities of the XPS instrument are fundamentally important for successful sample analysis.

It seems therefore that whilst the data acquisition has been simplified by instrument automation there is still no replacement for the detailed knowledge held by expert analytical scientists. There remains a responsibility of both manufacturer and User of the XPS instrument to educate. The education needs to be balanced between XPS application, understanding the information available from the technique and correct use of the instrument to acquire that data, and XPS fundamentals, understanding how to analyse the data KRATOS ANALYTICAL NEWS 09 generated from the instrument. As Strachan concludes in the Analytical Scientist [1], through education we ensure that the next generation of XPS Users have the skills and knowledge to apply and, perhaps more importantly, critically assess the latest generation of instruments provided by manufacturers.

In making the complicated simple, it's important to remember that the expert analyst must in fact struggle with the complexities and embrace the simplicities.

What would make your experience of using a Kratos XPS instrument better? Why not let us know by sending an e-mail to surface.applications@kratos.co.uk?

[1] J. Strachan. Will you play upon this HPLC? The Analytical Scientist Dec.2022 https:// theanalyticalscientist.com/issues/1222

[2] J.E. Castle. Developments in expert systems for automatic examination of samples by X-ray photoelectron spectroscopy Journal of Electron Spectroscopy and Related Phenomena 178:347-356 DOI:10.1016/j.elspec.2009.07.005



MEET OUR USERS

Dr. Billy Murdoch, RMIT, Australia

Name:

Dr Billy Murdoch

Affiliation:

Royal Melbourne Institute of Technology (RMIT)

Quick outline of your career to date?

I completed my PhD in Physics with RMMF Director Prof. Dougal McCulloch in early 2016. I then worked for Prof. Peter Cumpson at the National EPSRC XPS Users Service at Newcastle University (UK) before returning to RMIT for a 2nd postdoc, working on carbon-based neuromorphic electronics. I have been in my current role since the end of 2019

What is your role in the RMMF?

I am a Senior Technical Officer in the RMIT Microscopy & Microanalysis Facility (RMMF). We are a large, multi-user facility providing electron microscopy and related services to researchers and research students. My primary responsibilities are looking after the surface science equipment, including X-ray Photoelectron Spectroscopy (XPS) and scanning probe microscopy techniques.

Can you describe a typical day at work?

My days and weeks are dictated by the requirements of our users. Our XPS systems operate 24/7 and we have ~50 XPS users, so scheduling is very important. I usually try to reserve mornings for assisting users in setting up their XPS experiments or training new XPS users. In the afternoons I am often helping users with their XPS data interpretation, preparing and pumping down samples for the following morning or assisting users with the scanning probe instruments.



How do you use your AXIS Supra in your role?

In our labs, the AXIS Supra is used for surface analysis of a very wide variety of materials. We make use of every feature included on the instrument. We have researchers who use angle resolved XPS (ARXPS) in their work developing biomedical sensors using click chemistry. Concentration depth profiling using the gas cluster ion source (GCIS) and ultraviolet photoelectron spectroscopy (UPS) have been used in projects studying different aspects of photovoltaic cells. We've also recently had an exciting project using XPS and the high-pressure gas reaction cell to study CO_2 emission reduction using liquid metal catalysts. The projects are constantly changing, and our use of the AXIS Supra changes to reflect that, so it's nice to have an instrument with this many capabilities.

What's the most useful (or most used) feature of your instrument?

Recently, my favourite feature of the instrument has been the dual monochromated X-ray source. There's been an increase in supply of lab based XPS instruments with high energy X-ray sources. There's also been some nice work on methods allowing us to make quantitative measurements using these new tools. Performing XPS with both the Ag L α source and the Al K α source can be really useful when analysing samples that have a concentration that varies as a function of depth but can't easily be studied by ARXPS or sputter depth profiling (e.g., samples that are not flat or have laterally inhomogeneous chemistry). I think that we'll see this type of analysis, photoelectron spectroscopy combining data collected with multiple photon energies, becoming more common.

What do you see as the value of surface analysis?

Nobel laureate Herbert Kroemer famously said that "the interface is the device". I think that's true for more than just semiconductor technologies. Chemistry happens at short length scales so if we don't have the tools to study the surfaces and interfaces, as opposed to the bulk characteristics of a sample, then it's going to be hard to understand how a composite sample or product functions as a whole.

FEEDBACK FROM THE RECENT USERS' SURVEY

In autumn 2022 we circulated our biennial Users' Survey and received responses from just under 100 institutions. The data gathered from the survey forms an important overview of the performance of the Surface Analysis Business. We have been gathering the survey data through online, digital collection since 2016, allowing us to review trends in responses.

Here we share some of the highlights of the survey, demonstrating the 'health' of the business and that we're providing the best for our customers.



% Users interacting with Kratos communications

Keeping in contact with our Users is extremely important. Over 80% of our Users review new Kratos materials through the website. It's also pleasing to note that those seeing content distributed through the Newsletters has increased since the last survey in 2020.

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Large area spectroscopy measurements