Understanding Materials through Electron Microscopes: Realising the Potential. A workshop at Imperial College London, 22-24 April 2009.

Summary

Advances in our understanding of materials structure and properties are driven by the development of new characterisation techniques, both experimental and theoretical. On the experimental side, modern electron microscopes are capable of sub-Angstrom spatial resolution. In scanning transmission microscopes, the energy lost by the electrons traversing the sample due to excitation of core and valence electrons can yield chemical information at the atomic scale and with an energy resolution of 0.2 eV or better. Electron holography has been used to 'see' nanoscale particles in three dimensions and also to map the electrostatic potentials generated by the presence of dopants in semiconductor devices. The amount of information obtainable by all these techniques is impressive, and steadily increasing. Yet already in order to make the most of the information, state-of-the-art theoretical tools are essential. Such tools are embodied in large computer codes, many of which are still in a state of rapid development as new theoretical techniques are proposed and tested.

The workshop brought theorists into contact with the difficulties and capabilities of experimentalists in the fields of high-resolution imaging (HRTEM), Electron Energy Loss Spectroscopy (EELS) and electron holography. It included a session on the technical implementation of EELS/excitation theory into working computer code and approximations in different implementations. There were 60 participants, including 15 invited speakers.

In addition to experimental developments in imaging and electron spectroscopy, there have also been recent advances in the theory of these techniques. It is now possible to calculate Electron Energy Loss Spectra (EELS), which include many-body effects in an ab initio framework. The effects of lens aberrations, coherence and multiple scattering can be included in simulations of high-resolution images. Yet none of these theories is perfect; all are based on approximations, many of which are poorly understood outside a small circle of theorists, whose own understanding is far from complete. Although the positive developments have rightly attracted much attention, there has been less discussion of their inadequacies and how experiment and theory can best be combined to help us understand materials. In particular, what theoretical techniques now available could be more widely used in the experimental community in order to exploit the full power of their instruments? And what gaps in the theory are still holding back the full interpretation of data, both currently available or just around the corner? How can theorists advance their techniques in a way that will be useful to experimental microscopists and what theoretical tools do microscopists still most need in order to help them unravel the properties of materials?

Few conferences are specifically dedicated to problems associated with the theory-experiment interface, and given the increasingly interdisciplinary nature of materials research, we believe the workshop was especially timely. Furthermore, we found that the 'discussion meeting' format of the workshop had the desired effect of promoting discussion of the questions raised above, as the feedback confirmed.

Scientific Content

The following speakers were invited and took part:

Rik Brydson, Institute for Materials Research, University of Leeds, UK
Alan Craven, University of Glasgow, UK
Rafal Dunin-Borkowski, Technical University of Denmark, Copenhagen, Denmark
Christoph Koch, Max Planck Institute for Metals Research, Stuttgart, Germany
Hannes Lichte, Technische Universität Dresden, Germany
David McComb, Imperial College London, UK
Paul Midgley, University of Cambridge, UK
Guenter Moebus, University of Sheffield, UK
Peter Nellist, University of Oxford, UK
Tony Paxton, Queen's University Belfast, UK
Lucia Reining, Ecole Polytechnique, Palaiseau, France
Andrew Scott, Institute for Materials Research, University of Leeds, UK
Sangeeta Sharma, Freie Universität Berlin, Germany
Francesco Sottile, Ecole Polytechnique, Palaiseau, France
Andreas Thust, Forschungszentrum Jülich, Germany

An important theme was the availability of computational tools for experimentalists trying to understand their materials. Lucia Reining played an important role in this respect by introducing the European Theoretical Spectroscopy Facility (ETSF: http://etsf.eu/), which was a new concept to many participants. Experimentalists were encouraged to approach it as they might apply for beam time on a large scale facility for neutron or X-ray scattering. They could be put in touch with a theoretician competent with tools that should help solve the problem of interest. The important tools are public domain codes for density functional theory, GW, TDDFT and the Bethe-Salpeter equation, with many features for EELS and X-ray spectroscopy.

Some electron microscopists were apparently mostly concerned with the performance of their instruments and less about the properties of materials (see the first comment underlined in our feedback question 4 below). Alan Craven was the contributor who most clearly took the view that we sometimes need to work with the machines and materials we have to get imperfect answers with unsatisfactory specimens.

Holography was presented as an experimental technique that is within the capabilities of many if not most electron microscopy groups, but seldom exploited. It raised some interesting issues and comparisons. A particular need was expressed for theorists to concern themselves with the theory for magnetic materials. Theoretical tools are developed individually, and common documented codes are not generally available, as is the case for HRTEM and EELS codes.

For EELS calculations, practical advice was given by Andrew Scott to use codes that have a large user base already, so that experienced advice and help are at hand. The main codes to have penetrated the experimental community in a big way are WIEN2K and FEFF, with the newer codes being still mainly in the hands of developers and theorists.

Inadequacies in the paradigm for the interpretation of EELS in the core loss regime were demonstrated by Dave McComb. His examples showed clearly how the local approximation breaks down, since signals are recorded from elements that are not within the beam diameter, presumably due to some channelling effects. The material in question was strontium titanate.

Scientific Impact

It is impossible to measure the long-term impact of this meeting on the future direction of the field, such things are only seen when more time has passed. However, we are encouraged by the lively discussions before and after the meeting.

Summary of Feedback

A short questionnaire was distributed to gauge our success and learn what might be done better in the future. 14 responses were received, summarized below with the respondents' own words in italics, and including the most critical as well as a sample of the most positive. In general we seem to have fulfilled our aims. The full responses (unattributed) are available on request.

1. What do you think the aims of the workshop were?

To bring together the experimental and modelling communities to discuss research in a way that will be mutually beneficial. The focus was more on the discussion of how we can help each other rather than on particular research results.

The aims I felt were to provide an open forum for the interaction of theoretical and experimental electron microscopists.

It brings together the top researchers in the field of electron microscopy to show and discuss the current status of various TEM based techniques and the present difficulties and limitations. Through this young researchers could know better where they are and the possible directions to make effort towards, which is probably less possible anywhere else.

To find out about latest development in the field.

To get TEM-experimentalists who investigate atomistic structures and their EELS spectra to speak with people who look at the same thing from a theoretical perspective.

To promote better understanding between theorists and experimentalists for all aspects of characterisation of materials using analytical electron microscopy (tem) techniques. To provide a framework for future collaborations between the theoretical and experimental communities.

2. Do you think that the format was effective for fulfilling the aims?

The response was a unanimous 'Yes' with some qualifications. There were many more positive comments about the long discussion times, not reproduced here:

Due to the number of people at the meeting being quite small this gave more freedom to discuss issues more openly and for participation from a larger number of people than there is often time for at larger meetings.

In general yes. Having long discussion sessions can be risky, but in general they worked.

The format was ok. Not too long, nor dense. A bit tough the night session (especially because it was on a topic less obvious for me to catch: holography).

It was certainly effective in terms of highlighting challenges. Also I think that there was very good discussion on some topics, though not all sessions seemed to motivate discussion "between" the "two groups".

3. Would you attend a meeting on a similar theme in the future?

A unanimous `Yes' from all respondents.

4. What do you think worked and didn't work about the workshop?

Although not entirely consistent, the comments do make some useful suggestions (underlined) that could be addressed in future meetings of this kind.

The Thursday evening session was a struggle after the drinks. The imaging session contained mostly experimentalists, and the theory tends to be well developed here anyway.

The scope of putting people from different communities together, I believe it worked out well. I personally did learn a lot. Of course some topics were more interesting, for me, than others.

However I think we missed an electron microscopist of low losses. And, it goes with the same reasoning, a theoretician of core spectroscopies.

Time management is good and the team is well prepared.

There were many good things - plenty of social type things to facilitat[e intractions?]]

The programme was also wide ranging. All in all I hope you organise another one soon.
From my point of view, I think the HRTEM session was a bit too technique-y and did not focus on the challenges in obtaining "material" parameters for comparison. I would have liked the focus to have been "these are our problems - how can we get out useful materials information given these problems?", whereas it seemed to be "these are our problems - how can we solve them?" Of course the second question is important, but some of the microscopy-orientated problems (e.g. microscope stability and imaging theory) might take a very long time to solve, so we have to think about clever, robust methods to extract information from our HRTEM data even though it is not yet perfectly understood or problem-free. (or perhaps we can not get reliable data and that is an even bigger problem!)
The free afternoon was a good opportunity to meet up and discuss individual issues with other people, however, the evening session was a little bit of a struggle.
I realise the workshop was aimed at experienced researchers rather than students however I do feel that given the rather considerable student presence a small overview of the topic at the start of each session would have been nice. I personally found it a little hard to follow some of the presentations (e.g. holography) at first since I have never had any experience with these techniques. Other than that I thought the workshop was a success, very informative and enjoyable.
Some times discussions did not quite work: people were a bit shy at times to ask clear questions.
If we look generally most of the things that were discussed in workshop was about modeling more than imaging. We think that the sections could deal out more equally.
There was a lot of discussion on core-loss EELS, because most of the
EELS-Experimentalists present also try to do simulations with codes provided by theoreticians, and the corresponding theoreticians are very eager to make their theories match the experimental data or even have their codes being used by experimentalists. This sort of overlap seemed not as strong on the atomic structure and potential.
It would be nicer still to have a room that once the presentation is finished the discussions can be made more comfortable rather than people straining their necks to turn round etc.
I wonder if an afternoon of breakout sessions would be useful- especially in terms of specific problems that didn't have enough time to be discussed fully but ensuring this is in addition to the main discussion sessions.

5. Please send us any other comments you have.

Again, a cross-section here, with some practical constructive comments underlined.
Should this be made a regular event? I could try and interest the EMAG committee in getting involved, perhaps having it in the EMAG "off" years.
I would have personally liked a list of participants (not only invited) both on the website and a hard-written copy (you know, with contact details, emails), even on a plain a4 paper.
Overall I was very happy of my participation to this workshop, the organization was clean and flawless, the hotel good and the location superb.
The dialogue of ideas really got going on Friday with the EELS modelling. The holography session seemed quite focussed on experiment and perhaps there wasn't enough exchange between theory and experiment.
I thought some more structured discussion might have been useful. (perhaps if the session chairs or speakers were asked to prepare 2 specific and unresolved topics to lead in discussion.)
I have no problem with evening sessions, but talks scheduled after 9:30 seem to discourage a few people from attending, especially if they have to think about how to get home afterwards.

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Imperial College London, April 22nd – 24th, 2009

Wednesday, April 22nd
Session: EELS (G20, Royal School of Mines)
Chair: M. Finnis

13:45 – 14:00	Welcome	
14:00 – 14:30	Lucia Reining	*Electronic response – theoretical approaches and link to experiment*
14:30 – 15:00	Alan Craven	*The highs and lows of experimental EELS*
15:00 – 15:30	Discussion	
15:30 – 15:50	Coffee break	
16:00 – 16:45	Tony Paxton	*K-edge spectra in the local spin density approximation – application to strontium and barium titanates*
	Rik Brydson	*Current challenges in EELS modelling*
	David McComb	*TBA*
16:45 – 17:15	Discussion	
18:00	Dinner	

The workshop dinner will be held at Ognisko Restaurant, 55 Exhibition Road, London SW7 2PN (immediately opposite Imperial College).

Thursday, April 23rd (Day)
Session: Imaging (G01, Royal School of Mines)
Chair: N. Benedek

09:30 – 10:00	Andreas Thust	*Quantifying HRTEM images: New insights and challenges*
10:00 – 10:30	Peter Nellist	*Quantitative interpretation of STEM image data*
10:30 – 11:00	Discussion	
11:00 – 11:20	Coffee break	
11:30 – 12:15	David Cockayne	*Atoms at surfaces – TEM challenges the modellers*
	Günter Möbus	*Contrast mismatches at interfaces: Beyond the Stobbs Factor*
12:15 – 14:00	Lunch	

There are no sessions scheduled for the afternoon of Thursday, April 23rd. A drinks reception will be held shortly before the commencement of the evening session (∼19:00), on the roof terrace of the Blackett Laboratory (Level 8).

Thursday, April 23rd (Evening)
Session: Holography (Common Room, Level 8, Blackett Laboratory)
Chair: D. Cockayne

19:30 – 20:00	Hannes Lichte	*Structures and fields in solids – possibilities and limits of electron holography*
20:00 – 20:30	Paul Midgely	*Visualizing electrostatic potentials in two and three dimensions with electron holography*
21:00 – 21:20	Break	
21:30 – 22:00	Christoph Koch	*What can holography tell us about charges at grain boundaries in ceramics?*
	Rafal Dunin-Borkowski	*Challenges and opportunities for electron holography of magnetic materials*
22:00 – 22:30	Discussion	

Friday, April 24th
Session: EELS code development (G01, Royal School of Mines)
Chair: R. Nicholls

10:00 – 10:30	Francesco Sottile	*Plane-wave approach for the dielectric function*
10:30 – 11:00	Sangeeta Sharma	*Electron energy loss spectroscopy with the FPLAPW method*
11:00 – 11:30	Discussion	
11:30 – 11:50	Coffee break	
12:00 – 12:30	Andrew Scott	*EELS codes: An Electron Microscopist's Wish-List*
12:30 – 13:00	Discussion	
13:00	Closing remarks	