10 - 11 April 2014
North Campus Conference Centre, University of Sheffield

## Day One - 10.04.14

<table>
<thead>
<tr>
<th>Speakers/breaks</th>
<th>Start time</th>
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<th>Presentation title</th>
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<tr>
<td>Registration (tea and coffee available)</td>
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<td>09:00</td>
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<tr>
<td>Welcome from Prof David Lerner</td>
<td>09:00</td>
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<tr>
<td>Prof Nicholas Dobigeon</td>
<td>09:05</td>
<td>09:55</td>
<td>Bayesian linear unmixing for spectral mixture analysis - application to hyperspectral imagery</td>
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<td>Prof Bernhard Schölkopf</td>
<td>09:55</td>
<td>10:45</td>
<td>Machine learning and computational imaging</td>
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<tr>
<td>Refreshments and break</td>
<td>10:45</td>
<td>11:15</td>
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<tr>
<td>Dr Francisco De La Pena</td>
<td>11:15</td>
<td>12:05</td>
<td>HyperSpy, a software package for interactive data analysis of multi-dimensional datasets</td>
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<tr>
<td>Dr Paul R Edwards</td>
<td>12:05</td>
<td>12:55</td>
<td>Cathodoluminescence hyperspectral imaging in the scanning electron microscope</td>
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<td>Lunch</td>
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<tr>
<td>Alberto Eljarrat</td>
<td>13:55</td>
<td>14:25</td>
<td>Phase identification, hyperspectral segmentation and MVA for EELS of Si-NC embedded in dielectric matrices</td>
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<tr>
<td>Pierre Burdet</td>
<td>14:25</td>
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<td>3D EDS microanalysis by FIB-SEM: limitations, potential and perspectives</td>
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<td>Q&amp;A for speakers</td>
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<tr>
<td>Refreshments and break</td>
<td>15:10</td>
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<tr>
<td>Networking and poster presentation</td>
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<td>Free Time</td>
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<tr>
<td>Evening Dinner at Inox Dine - see next page for details</td>
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**Day Two - 11.04.14**

<table>
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<th>Practical/breaks</th>
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<th>12:05</th>
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<tbody>
<tr>
<td>Welcome</td>
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<tr>
<td>Practical applications: test software for hyperspectral image processing (Electronic and Electrical Engineering Lab) led by Dr Francisco De La Pena</td>
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<td>Lunch in the North Campus Conference Centre</td>
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<td>Opportunity to visit double aberration-corrected (scanning) transmission electron microscope (sign up for group slot on Thursday)</td>
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**Additional Information**

**Evening meal - 10th April 2014, 7.30pm**
If you are attending the evening meal this will be held at Inox Dine, Level 5, Students’ Union Building, Durham Road, Sheffield, S10 2TG. Please note that you need to use the west entrance to the building on Glossop Lane. Free parking is available in the University's Durham Road car park from 5pm or is easily accessible by public transport.

![Google Maps](https://via.placeholder.com/150)

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Bayesian linear unmixing for spectral mixture analysis - application to hyperspectral imagery

Nicolas Dobigeon
University of Toulouse, IRIT / INP-ENSEEIHT, 31071 Toulouse Cedex 7, France

Spectral unmixing is a crucial step while analyzing hyperspectral data in astronomy, remote sensing and spectroscopy. It consists of decomposing the measurements into a set of elementary spectra and quantifying their respective proportions in the observed mixtures. Unsupervised spectral unmixing can be formulated as a blind source separation problem. Bayesian estimation offers a convenient framework to tackle this problem. This talk presents a Bayesian estimation algorithm derived to recover the parameters of interest (spectral components and corresponding mixing coefficients). It is based on the wide assumption of a linear observation model. The physical constraints implied by this model are naturally ensured within the Bayesian framework by assigning appropriate priors to the unknown parameters. Inference is conducted using a Markov chain Monte Carlo algorithm. Examples on real hyperspectral data will be proposed.

Machine learning and Computational Imaging

Bernhard Schölkopf
Max Planck Institute for Intelligent Systems, Spemannstraße 41, 72076 Tübingen, Germany

Machine learning deals with the problem of extracting regularities from empirical data. This can beneficially be applied in situations where training data is available, but accurate physical models are missing. The talk will introduce basic ideas of machine learning, introduce examples of learning algorithms, and describe some applications in imaging.
Recent technological breakthroughs in the field of microscopy, such as fully computer-controlled microscopes and higher acquisition rates (sometimes of different signals simultaneously), have dramatically increased the level, rate and precision at which we can analyse matter in all branches of microscopy. Therefore, as in many other fields, the microscopy community is facing the challenge of how to better analyse large quantities of data extending over multiple dimensions. In some cases, analytical procedures developed for single-image and single-spectrum analysis can easily be extended to multi-dimensional datasets by performing the analysis individually on each signal in the set. However, this is not always possible as such procedures frequently require input parameters that are different for each element of the set. Moreover, multi-dimensional datasets usually contain highly redundant information, and methods that harness this property are becoming increasingly useful in the solution of problems that would be highly challenging, if not impossible, with more conventional methods.

In order to facilitate the interactive data analysis of multi-dimensional datasets and to foster interdisciplinary collaboration in the development of new data analysis methods we have developed a free, open-source and open-development software package, HyperSpy [1]. Specifically, it provides (amongst other things) easy access to curve fitting, machine learning algorithms, and multi-dimensional data visualisation as well as specialized routines for electron energy-loss (EELS) and energy dispersive X-rays (EDX) data analysis.
Cathodoluminescence (CL) is the phenomenon of ultraviolet/visible/infrared light emission from a material as a result of electron beam irradiation, and its measurement is well established as a characterization tool in the study of both semiconductors and minerals. CL has many of the same benefits as photo- and electro-luminescence measurements, allowing the investigation of various effects such as the presence of alloying, elastic strain, crystal defects, impurities and electric fields. However, CL has an advantage over these analogous techniques in that its spatial resolution is not limited by diffraction effects in the collection optics, making it possible to probe such properties on the nanoscale.

CL measurements in a scanning electron microscope (SEM) have conventionally been carried out in one of two modes: imaging, in which the intensity of either all the light or that of a discreet wavelength band is mapped under a scanning beam, or spectroscopy at a fixed spatial position. Extending the technique to the hyperspectral imaging (HSI) mode offers a number of advantages, while imposing additional constraints on the collection optics and challenges in the analysis of the multidimensional datasets [1,2]. In my talk I will discuss these aspects of the technique, and illustrate them with examples of CL-HSI taken from III-nitride semiconductor materials and nanostructures and from geological specimens.

One notable advantage of carrying out CL in the HSI mode is the ability to image variations in the wavelength of emission peaks. Such shifts commonly occur in semiconductor samples due to spatial variations in (for example) composition or strain. The ability to spatially map these is unique to the HSI mode, and I will show how nonlinear least-squares peak fitting has been used to extract high-resolution images of such shifts, e.g. in GaN nanorods.

Another advantage of CL hyperspectral imaging is the ability to spectrally deconvolve peaks. This allows imaging of the intensities of overlapping emission bands—not possible with simple monochromatic CL imaging—and I will show how we have used this to uncover previously unseen banding in calcite samples.

Unlike many HSI applications, CL data can often not be described adequately in terms of a combination of fixed “endmember” spectra, due to peaks shifting in wavelength. Nevertheless, for samples in which variations in CL emission are dominated by inhomogeneous impurity incorporation such methods can still be informative. Examples will be shown in which principal component analysis (PCA) has been used to identify dominant spectral features [1], to extract images from datasets with poor signal:noise, and to correlate CL with simultaneously-acquired X-ray microanalysis images.

Finally, this talk will describe aspects of the experimental setup, including the trade-offs in light collection and resolution imposed by optical étendue [2]. I will also outline recent developments, including the acquisition of CL in an environmental SEM; this has allowed measurements on less conductive samples such as undoped wide-gap semiconductors and uncoated mineralogical sections.

Phase identification, hyperspectral segmentation and MVA for EELS of Si-NC embedded in dielectric matrices

Alberto Eljarrat 1, Lluís López-Conesa 1, Julian López-Vidrier 1, Sergi Hernández 1, Sònia Estradé 1,2, César Magén 3,4, Blas Garrido 1 and Francesca Peiró 1
1. MIND-IN2UB, Departament d’Electrònica, Universitat de Barcelona, c/ Martí i Franqués 1, 08028 Barcelona, Spain.,
2. TEM-MAT, Centres Científics i Tecnològics (CCiT), Universitat de Barcelona, Solís Sabarís 1, Barcelona, Spain.,
3. Fundación ARAID, 50018 Zaragoza, Spain., 4LMA-INA, Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50018 Zaragoza, Spain.

In this work we have analyzed Si-nanocrystals (Si-NCs) embedded in three different dielectric matrices (SiO2, SiC and Si3N4). We present a characterization using hyperspectral imaging by electron energy loss spectroscopy (EELS) in the aberration corrected and monochromated scanning transmission electron microscope (STEM). The measured EELS is exploited by direct measure of relative thickness and plasmon peak energy in spectrum images, producing two-dimensional maps of these properties. The information within this maps is complemented by identification of the different phases, barrier dielectric, Si-rich layers and Si-NCs. Additionally, fast hyperspectral segmentation enhanced by mathematical morphology algorithms allows us to produce sub-datasets with irregular shapes defined by its pixels fulfilling a particular condition to the plasmon peak energy. This perspective proves more advantageous that the examination of the individual raw EELS or averaged spectra from square regions. However, by this method alone we are unable to obtain a measurement of the pure contribution of the Si-NC to the spectra, as all measured data present at least a mixture of Si-NC and dielectric substrate low-loss EELS.

After segmentation, selected sub-datasets were used for a detailed exploration of spectral factorization using multivariate analysis (MVA). These slices were suspected to contain a contribution to the EELS from a Si-NC that popular methods of MVA could not separate (principal component analysis and blind source separation by independent component analysis). However, the less common methods of non-negative matrix factorization (NMF) and bayesian linear unmixing (BLU) were successful on the separation of the contributions to the low-loss EELS from the Si-NC and the dielectric matrices. Finally, the possibility of extracting electro-optical properties by thickness-normalized Kramers-Kronig analysis of the average spectra and MVA factors was also be explored.
Two-dimensional (2D) energy dispersive X-ray spectrometry (EDS) mapping with a scanning electron microscope (SEM) can be extended to a three dimensional (3D) approach using focused ion beam (FIB) ‘slice-and-view’ methods. In a sequential acquisition, the surface, freshly milled by the FIB, is characterised by SEM imaging and 2D EDS mapping. A 3D elemental picture of the sample can be obtained this way.

This technique suffers from the same limitations as 2D EDS mapping, the most serious being linked to the volume of X-ray emission that is large due to the high accelerating voltage typically used. 3D EDS mapping also suffers from specific limitations due to the complex acquisition geometry and to time constraints. All these limitations will be discussed, as well as different ways to minimize them during acquisition and through post-processing.

3D SEM-EDS of metallurgic samples of practical interest are shown as examples. The complexity of the microstructure and composition in such samples is a challenge, but the rich elemental and spatial information obtained with the technique allows a deeper understanding of the formation of the phases and their morphologies during sample processing.

Acknowledgement: The research leading to these results has received funding from the European Research Council under the European Union’s Seventh Framework Programme (FP7/2007-2013) / ERC grant agreement 291522-3DIMAGE. SAC and PAM acknowledge financial support from Rolls-Royce plc. Thanks to F. de la Peña for the help with Hyperspy (hyperspy.org)
**Poster Presentations**

**Fluorescence spectral and lifetime imaging on nanopatterns of light harvesting complexes**

Lin Wang1,2, Cvetelin Vasilev2, Samson Patole3, C. Neil Hunter2 and Ashley J. Cadby1

1. Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK
2. Department of Molecular Biology and Biotechnology, University of Sheffield, Sheffield, S10 2TN, UK
3. Department of Chemistry, University of Sheffield, Brook Hill, Sheffield, S3 7HF, UK

One step toward understanding how light harvesting (LH) complexes in photosynthetic organisms capture and transfer energy in an efficient manner is to investigate the bottom-up fabrication of planar LH arrays on well-defined surfaces. In order to assess the localisation and the preserved functionality of the LH complexes attached along the nanopatterned lines, we developed a bench-top fluorescence spectral and lifetime imaging microscopy system capable of high-speed high-resolution spectral and time-resolved data acquisition. The fluorescence spectrum and lifetime measurement results show that biologically functional LH complexes can be site-specific immobilised onto chemically patterned substrates on dozens of nanometre scales. This paves the way of designing and constructing natural and bio-inspired systems for solar energy conversion.

**In situ Raman Spectroscopy for Solid Oxide Electrolysis Cells**

Jevgenija Manerova1, Dr Denis J. Cumming1, Prof Derek C. Sinclair2, Dr Rachael H. Elder1

1Department of Chemical and Biological Engineering, University of Sheffield, Mappin Street, Sheffield, S1 3JD.
2Department of Material Science and Engineering, University of Sheffield, Mappin Street, Sheffield, S1 3JD.

High temperature co-electrolysis of steam and carbon dioxide using solid oxide electrolysis cells (SOECs) is one of the most promising and economically feasible power-to-fuel technologies for CO2 utilisation. This process can be used to convert a surplus of renewable energy into syngas (H2 +CO), a common precursor for synthetic fuel production via Fischer-Tropsch synthesis, addressing the electricity supply-demand mismatch. Commercialisation of SOECs, however, requires extensive research to improve the performance of the cells and prolong their life-time. This project is part of 4CU, a wider programme investigation carbon dioxide utilisation, and applies in situ Raman Spectroscopy to understand the fundamental electrochemical processes occurring during operation of SOECs. Particular focus is placed on structural transformations and reaction intermediates formed at the triple phase boundary (TPB), where electron conducting, electron conducting and gaseous phases meet.

The preliminary Raman spectroscopy results of the yttria-stabilised zirconia substrates show a distinctive phase change upon increasing temperature. Ex situ measurements taken from post-analysis of cells used for CO2 electrolysis have shown carbon formation on the fuel side electrode.
Beef quality assessment based on NIR spectroscopy and hyperspectral imaging using classical feature extraction methods with support vector machines

Jaime Zabalza, Tong Qiao, Jinchang Ren, Stephen Marshall
Centre for excellence in Signal and Image Processing, Dept. of Electronic and Electrical Engineering, University of Strathclyde, Glasgow, G1 1XW, U.K.

Spectral data acquisition such as visible-Near InfraRed (NIR) and Hyperspectral Imaging (HSI) leads to extremely potential data analysis and mining in multiple applications, where emerging technologies related to medical, pharmaceutical and food quality are fast growing. Based on NIR spectroscopy and HSI, beef quality assessment is currently a topic under research, where different signal processing chains, mainly related to feature extraction and data reduction methods, are possible. In this paper, several well-known methods such as Principal Components Analysis (PCA), Robust-PCA and Independent Component Analysis (ICA) are evaluated, using Support Vector Machine (SVM) regression for prediction of slice shear force and ultimate pH as quality parameters in beef assessment. Results prove that alternative processing of the same data can lead to differences in the prediction ability. Also it is suggested that in general HSI outperforms NIR spectroscopy in accurate prediction of meat quality related metrics.