nanocrystalline nature. The results cast light on the nature of pressure amorphization, and provide a potential route for the synthesis of new nano-materials.

Keywords: amorphization under pressure, X-ray diffuse scattering, diamond anvil high-pressure apparatus

MS.34.1

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HR-TEM imaging of the carbon networks

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Identification of individual C-C bonds is an ultimate goal of the carbon nanostructure characterization. We have been developping a high sensitivity transmission electron microscopy (TEM) which enables us to visualize a single C-C bond. A TEM equipped with an aberration corrector allows a higher spatial resolution without increasing its tension (the accelerating voltage). Then we have achieved the resolution of 0.14 nm, which corresponds to a typical C-C distance, at a moderate accelerating voltage (120kV). This merits a lot to realize the visualization of carbon atomic chain such as the alkyl chain without electron irradiation damage (1). Here we show some examples for atomic-level characterization of carbon nanostructures. The C_{60} fullerene molecule has been successfully identified its structure and orientation at a single-molecular basis (2). Also the active topological defects have been eventually caught red-handed (3). The technique can be widely applicable to visualize a biological activity, at an atomic level, for which any conformation change of the C-C bonds is responsible. The cis-/trans-isomerization of retinal molecules have been successfully visualized (4).

(1) M. Koshino et al., Science 316 (2007) p853
(2) Z. Liu et al., J. Am. Chem. Soc., 129 (2007) pp.6666-6667
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Keywords: electron microscopy, carbon nanotube, defects

MS.34.2

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Image contrast in atomic resolution high-angle annular dark-field images

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High-angle annular dark-field scanning transmission electron microscopy (HAADF or Z-contrast) is remarkably sensitive to the atomic number (Z). Quantitative HAADF imaging holds enormous potential for extracting chemical information in parallel with information on the atomic structure. To date, comparisons between experimental and theoretical HAADF images have been based on image contrast or scaling by an arbitrary amount. Such comparisons are only semi-quantitative and place severe limitations on identifying the origins of any contrast mismatch between experiments and simulations. In this presentation, we demonstrate that the HAADF detector can measure the incident beam intensity to normalize Z-contrast images onto an absolute intensity scale. We report on a practical approach that ensures that the detector is sufficiently linear over the intensity range of interest. Limitations of the current generation of HAADF detectors, such as scintillator heating and intensity saturation, will be discussed in the context of the probe intensity measurements. By normalizing the atomically resolved signal to the incident probe, we demonstrate quantified HAADF imaging of a $SrTiO_3$ single crystal as a function of sample thickness. Experimental images are compared with Bloch wave image simulations that incorporate thermal diffuse scattering. Provided that spatial incoherence in the probe is taken into account in the simulations, exellent agreement is found between simulation and experiment. The electron energy-loss spectroscopy (EELS) log-ratio method was used for determination of the local thickness. We will discuss how thickness determination by EELS can be combined with information from the HAADF background to provide improved estimates of the thickness.

Keywords: STEM, electron microscopy techniques, analytical electron microscopy

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In aberration corrected STEM, shrinking some dimensions expands others

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Crystallography is usually associated with coherent elastic scattering. Having atomically localised inelastic information, however, can allow the solving of crystal structures particularly when crystals are nanometres in size. A particular advantage of the STEM geometry is that inelastic signals, in particular electron energy loss spectroscopy (EELS), are localised and the high angle annular dark field image can be collected simultaneously with the spatially resolved spectroscopic information. Aberration correctors have improved the spatial resolution of EELS as well as significantly improving the signal-to-noise in both imaging and spectroscopy. Results on atomically resolved EELS data will be presented where light has been shed on a periodic structure. Necessarily the sample is only a few tens of nanometres thick in the beam direction but many structures are spatially of similar or smaller scale in one of the other dimensions as well. Systems that will be discussed include silicon/metal di-silicide interfaces and silicon nanowires. In addition to using these two dimensional projections of nanostructures, the three dimensional shape of nano-crystals is of crucial importance for heterogeneous catalysis. Conventional tomographic techniques are not expected to get down to the atomic scale. An alternative approach will be presented with data on the shape of gold nano-particles.

Keywords: aberration correction, HAADF, EELS

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Development of new electron diffraction microscope for diffractive imaging

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Using a relatively low-acceleration-voltage (a few tens of kilovolts) electron beam, we are researching diffractive imaging to achieve atomic-resolution observation with little damage to the specimen. Using the prototype microscope, we verified the reconstruction of the object image of a multiwall carbon nanotube (MWCNT) [1]. In this prototype, the resolution during specimen observation was not sufficiently high, and the camera length was fixed. To achieve high resolution imaging using the diffraction pattern with a variable camera length, we have developed a new diffraction microscope based on the conventional scanning electron microscope (Fig.1). The diffraction pattern is recorded on the imaging plate (IP) without projecting the back-focal plane. Development of the new microscope and examples of diffractive imaging will be presented.

[1] Kamimura O., et al., *Appl. Phys. Lett.*, 2008, **92**, 024106.

Keywords: electron microscopy and diffraction, electron diffraction techniques, scanning electron microscopy

MS.34.5

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Applications of aberration-corrected TEM-STEM and high-resolution EELS in materials research

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Aberration-corrected electron microscopy has the potential to significantly improve the quality of information retrieved from transmission electron microscopes and to help researchers understand the structure of materials and their defects. In our laboratory, two aberration corrected microscopes have been commissioned and have been used to study several materials ranging from oxides, multiferroic thin films, nanowires, nanoparticles and a variety of quantum structures. With a FEI Titan 80-300 Cubed equipped with an image corrector, located in an ultrastable environment, this instrumentation has demonstrated extremely low drift rates and better than 0.75Å information limit. The stability of the microscope is demonstrated in several examples of work where remarkable improved image contrast has been noted. With high-angle annular dark field imaging, we have been studying polarity of nanowires and nanoparticles as well as defects in layered multiferroic materials. Early results on a double-corrected and monochromated FEI Titan 80-300HB equipped with a SuperTwin lens have demonstrated better than 1.4Å STEM resolution with a monochromated beam of 0.14eV energy resolution. A second instrument equipped with a CryoTwin lens, an image corrector and a monochromator has demonstrated better than 1Å information limit. Results of these instruments installed in our laboratory will be presented. Particular emphasis will be given to the enhanced contrast and benefits of aberration-correction for solving materials science problems. The combined benefits of high-resolution electron energy loss spectroscopy and high spatial resolution will be shown with examples related to materials exhibiting interesting magnetic properties.

Keywords: high-resolution electron microscopy, electron energy loss spectroscopy, perovskites

MS.35.1

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Comprehensive structural characterisation of local and bulk structure in disordered systems

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The detailed structure around physico-chemically active atomic sites and their incorporation within a structurally disordered bulk supporting medium is an important aspect of modern materials physics and chemistry. The interplay between these two issues often defines a system's technological properties. Though many experimental techniques have been applied to the challenging task of elucidating this structure over the past few decades, the results have mostly been interpreted in isolation. This has led to a range of conflicting findings in the literature due to the distinctly different and often poorly defined structural sensitivities of the various probes. With the advent of modern inverse modeling techniques, whereby computer simulations are driven to reproduce structural models that are consistent with experimental data, it has now become possible to resolve this problem. Here I will illustrate how to combine the strength of neutron or X-ray scattering for bulk structural studies, with the chemically specific short ranged structural sensitivity of EXAFS spectroscopy. This analytical approach is particularly advantageous as it allows us to compensate for the poor sensitivity of the scattering experiments to dilute components whilst simultaneously removing the need for large numbers of free parameters in modelling spectroscopy data. The technique will be illustrated with results on a range of liquid and glassy systems.

Keywords: scattering neutron, EXAFS spectroscopy, liquids structure

MS.35.2

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Developments of advanced XAFS analysis techniques with Ifeffit

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Advances in XAFS modeling and error analysis procedures that allow easier and more robust modeling of experimental XAFS data will be discussed. For example,the ability to simultaneously co-refine different XAFS data sets parameters can greatly reduce issues of uniqueness and correlations between model parameters. Using mathematical constraints and restraints to describe prior knowledge of the system and the impact this has on data refinement will be emphasized. Examples of using such a priori chemical information from bond valence sums and a priori physical information about partial pair distribution functions will be given. In addition, the impact of theoretically-derived XAFS scattering factors as from FEFF will be discussed in terms of the current limits on resolution and precision for the refinement of XAFS data.

Keywords: XAFS data analysis, XAFS, computer modelling