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Experimental and Computational Electron Energy-Loss Spectroscopy : Enabling the Future

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Measuring the energy lost by the primary electron beam in an electron microscope, when travelling through the specimen, has been recognized as a powerful source of information since its early days. After having been instrumental to identify and investigate in the 60s and 70s plasmons (and surface plasmons) and core-loss signals, EELS spectroscopy has now reached a mature role and it constitutes a major component of any new electron microscope, in particular for materials science studies. It is commonly used for elemental mapping, in which case atomic resolution (1, 2) and single atom sensitivity (3) have been demonstrated, and it has found wide areas of applications in many scientific domains.

Recent achievements in instrumentation (spectrometers, monochromators, detectors) and in methodology (data processing) now provide access to increased performance, to upgraded accuracy and precision and also to unconventional domains lying out of the main stream. They are all associated to spatially-resolved EELS (as offered, for instance, in the spectrum-imaging mode (4), -see fig.1-), which intimately combines a very broad range spectroscopy (from 1 eV up to a few thousands of eV) with high spectral resolution (typically 0.1 to 0.5 eV), and an imaging microscopy with unique spatial resolution (down to 0.1 nm with C_s corrected instruments). However, the quality of the recorded data requires an equivalent development of the relevant theory and of associated numerical tools for an optimized information extraction through well suited modelling and computation.

Using the present or targeted ultimate performance, bond mapping deduced from the spatial variations of the fine EELS structures on characteristic core-edges (ELNES), constitutes a key to relate the transport properties to the interfacial electronic structure and atomic scale chemistry in artificially grown stacks of hetero-layers for microelectronics devices or in spin tunnel junctions (5). For this goal, refined ELNES measurements, close and at the apex of interfaces between different materials, have to be compared with simulated spectra, including as intermediate steps *ab initio* modelling of the local atomic structures and calculations of the electron density of states (DOS).

In the low energy-loss part of the spectrum, new routes are now being opened to disentangle the local electronic response of the material in terms of band structure (band gap, interband transitions, excitons) from the long-range response of the neighbouring architecture, encompassing the electromagnetic fields generated by surface and interface plasmons (6). In particular, when applied to individual metallic nanoparticles (7), see figure 2, it has recently been demonstrated that the measured EELS signal is closely related to the electromagnetic density of states (EMDOS) determined by the nanostructure shape and dimensions (8), thus opening new access to the comprehension of plasmon physics and to the mastering of plasmon engineering.

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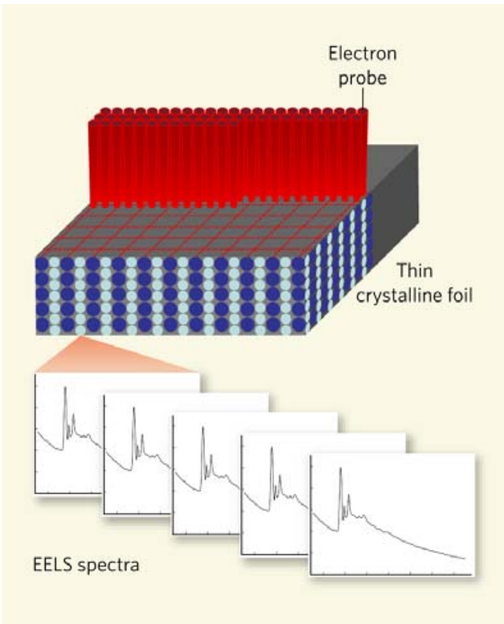
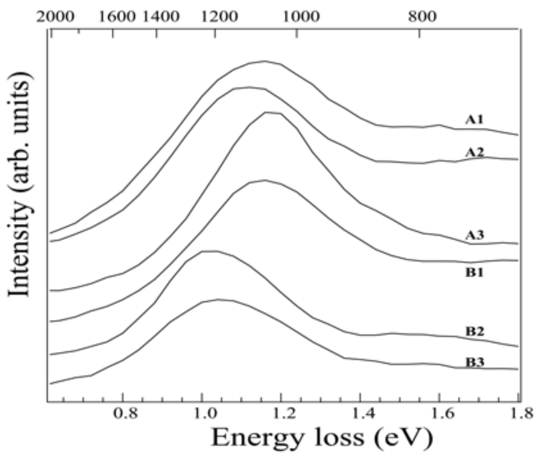


Fig.1: EELS spectrum-imaging acquisition in the STEM mode for achieving atomic resolution mapping of crystalline materials



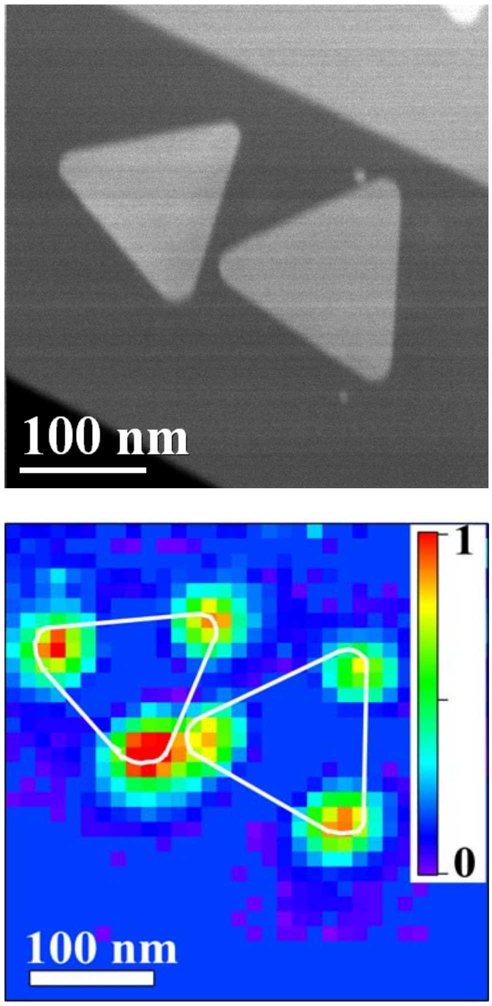


Fig.2: Mapping of the intensity of surface plasmon modes (see spectra recorded on different apex at left) on two neighbouring triangular silver platelets (from J. Nelayah)