BENEATH THE SURFACE

The LSNM combines unique facilities and experience to uncover the microscopic mechanisms of surface chemical modification and ultra-thin film growth, Professor Yves J Chabal explains

The ability to control the atomic structure and chemical composition of surfaces and interfaces remains the single most important challenge in the development of new devices, whether they involve charges, heat, electromagnetic radiation and even magnetic fields. Interfaces are becoming even more important as the size of devices is reduced. The demands for cheaper, sustainable and more efficient products has also motivated the development of new materials and compounds and introduced new types of interfaces. It is therefore critical to develop a fundamental understanding of surface processing and interface formation to cope with the wealth of systems currently being considered. Such efforts require a combination of techniques (to grow and characterise interfaces) and theoretical analysis (to understand atomic-scale mechanisms).

The Laboratory for Surface and Nanostructure Modification

The Laboratory for Surface and Nanostructure Modification (LSNM) is focused on understanding the atomic phenomena controlling the formation and behaviour of interfaces that are at the heart of selected devices. These include gas and biosensors, nano-electronic devices (e.g. transistors and storage elements), and structures for energy harvesting, storage and release. For all of these specific applications, the performance of devices is directly impacted by the nature and properties of their interfaces, such as electronic and energy conduction across or along interfaces. The goal of the LSNM is to understand the atomic mechanisms involved in the formation and therefore provide control in their fabrication.

To achieve this goal, the centre combines advanced deposition methods with *in situ* characterisation techniques, and establishes synergistic collaborations

The laboratory has developed capabilities to grow films by physical (e.g. electron beam evaporators) and vapour phase (e.g. atomic layer deposition and chemical vapour deposition) methods, as well as sputter and pulsed laser deposition. It also is equipped for advanced wet chemical surface modification of surfaces. Wet processing is critical to clean and passivate surfaces prior to processing, and constitutes a typical first step of all device fabrication. With the goal of performing *in situ* studies, homemade equipment to incorporate tools for *in situ* characterisation has been constructed in the LSNM, including spectroscopies such as infrared (IR) absorption, ellipsometry, Raman, X-ray photoelectron (XPS), and low energy ion scattering (LEIS). In fact, it boasts a unique cluster tool that combines IR, XPS and LEIS with various deposition and processing tools for accurate determination of the elemental composition, atomic position and bonding at the surface, illustrated in Fig. 1.

Collaborations have been established with leading theorists in Europe, industry (Schrödinger, Inc.), and universities who use advanced computing methods to calculate surface structures and reaction pathways involved in etching, deposition and more generally interface formation.

> ‘Fundamental progress is often based on our ability to prepare model surfaces with atomically well-defined surface structures, and to perform *in situ* measurements that can be directly linked to theoretical modelling.’

The LSNM has developed methods for perfecting surfaces with well characterised and defined atomic and chemical structures. For instance, despite the enormous importance of silicon (Si) surfaces, typical cleaning and fabrication methods do not lead to atomically smooth interfaces. By devising a wet chemical method to prepare atomically flat oxide-free surfaces and atomically straight, hydrogen-terminated steps of various geometries on the (111) face of silicon, much progress has been realised in understanding the etching process with hydrofluoric acid and its derivatives. This work has led to the control of the (100) faces of silicon as well, which are widely used in the microelectronic industry.

Subsequent organic functionalisation of these H-terminated oxide-free surfaces has made it possible to uncover new information on the chemical stability and electrical properties of such inorganic/organic hybrid interfaces. Most recently, a clear correlation has been established between atomic flatness of the surface and electrical quality of the interface, which is an important breakthrough for device fabrication, and is being applied to biosensors and single electron devices, for instance.

Importantly, model surfaces such as the one illustrated in Fig. 2 have been developed to attach a variety of molecules without oxidising the silicon surface, such as phosphonates, which are particularly useful for coatings, sensors, electronics and adhesive promoters, or arsenates that can be used for shallow doping in Si.

Novel materials

In addition to studying silicon-based structures, there have been recent investigations in the LSNM of the nature of interfaces between dielectrics or metal films with high mobility materials such as III-V

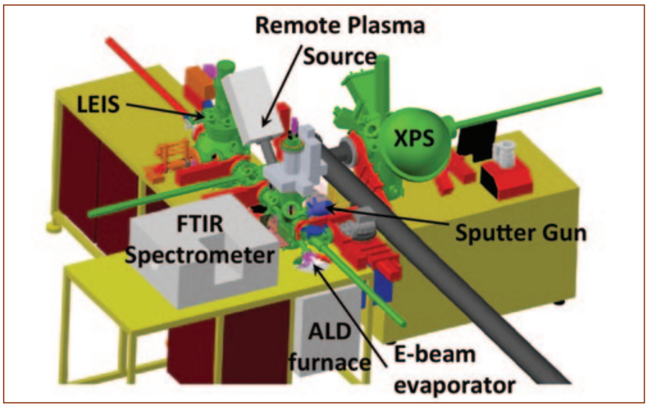

Fig. 1 Schematic diagram of the cluster tool for in situ infrared spectroscopy, X-ray photoelectron spectroscopy and Low Energy Ion Scattering

semiconductors, graphene, and two-dimensional transition metal dichalcogenides (TMDs). These materials are promising for future nanoelectronic applications for which reliable and controllable methods for gating the transistors and making contacts have not yet been developed. The LSNM is investigating the degree to which metal contacts perturb the electronic structure of (i.e. charge transport in) these two-dimensional materials. Collaborative work is also carried out on ultra-nanocrystalline diamond (UNCD) that is currently being developed as a coating for biomedical and mechanical devices.

ATLAB

The ATomically precise nano-engineering LABoratory (ATLAB) is a multidisciplinary French-US initiative launched by the Centre National de la Recherche Scientifique (CNRS) to bring fundamental understanding of interfaces between reactive materials and of DNA/inorganic surface interactions. It links the Laboratoire d'Analyse et d'Architecture de Systèmes (LAAS) in Toulouse (France) and the Laboratory for Surface and Nanostructure Modification (LSNM) in Dallas (USA). It combines the theoretical and technological expertise in the LAAS with the state-of-the-art deposition and characterisation facilities in the LSNM to develop novel micro-electromechanical systems (MEMS) and examine the interfacial chemistry of reactive nanolaminates and nanoparticles. The overall goal is to uncover new directions to develop tuneable materials through smart interfaces by:

- Providing a quantitative assessment of the interface parameters (structure, thickness and chemical nature) that control the kinetics and stability of reactive Al-CuO nanocomposites;
- Providing computational tools that enable understanding and prediction of interface formation under diverse experimental conditions;
- Exploring atomically precise technologies, such as atomic layer deposition, to tune the thermal properties on reactive nanolaminates coatings as a function of layer chemical composition; and
- Exploring alternative technological approaches such as DNA-directed assembly of nanoenergetic materials.

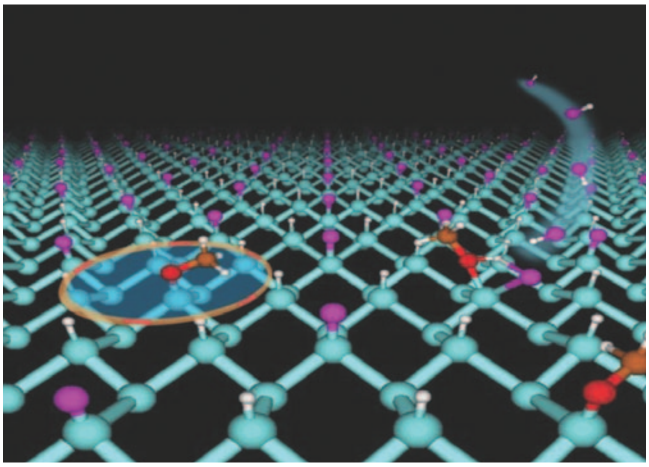

Fig. 2 Illustration of a nanopattern on the (111) face of silicon, obtained by immersion of an atomically flat H-terminated surface in methanol, then subsequent HF etching. By immersion of this F-terminated surface in water, a nanopattern of OH can then be obtained (Nat. Mat. 9, 266, 2010)

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