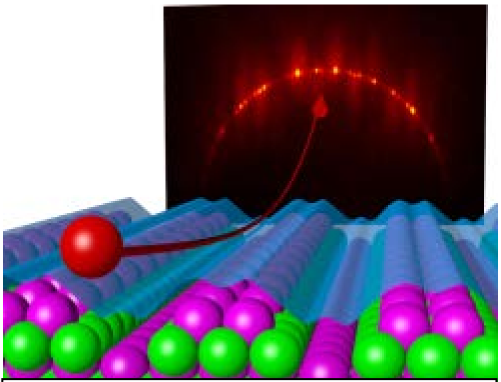
Proposition de thèse ECOLE DOCTORALE : ONDES ET MATIERE

Directeur de thèse : Philippe Roncin Directeur de Recherche au CNRS philippe.roncin@u-psud.fr

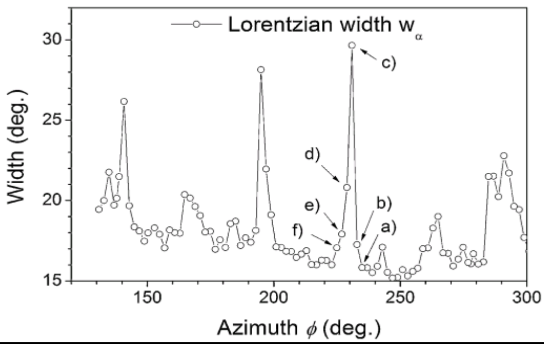
Laboratoire : Institut des Sciences Moléculaires d'Orsay,(ISMO) Université Paris-Sud http://www.ismo.u-psud.fr/

Title: Fast atom diffraction, from concepts to application to thin film growth.

Present status : Grazing angle fast atom diffraction (GIFAD) is a new diffraction technique discovered in our group at ISMO. By shooting a well collimated beam of neutral atoms at a crystal surface under grazing incidence, a diffraction pattern is observed which reflects the shape of the surface electronic density. This is analogous to light diffraction on a grating with the peculiar features of matter waves obeying Schrodinger equation, having large momentum and very short wavelength. Since the technique is fast and sensitive only to the topmost layer, it has been applied to track in situ the surface reconstructions and the growth of successive layers in a molecular beam epitaxy chamber at INSP[1,2,3]. More recently we have been able to propose a unified description of both the elastic intensity located on the Laue circle and of the inelastic diffraction intensity extending above and below [4,5]. In collaboration with A.G. Borisov we are now able to calculate efficiently the quantum dynamics of the projectile atom on the surface so that GIFAD should rapidly be able to provide elementary chemical identification of the atoms of the topmost layer (Work in progress).



In GIFAD, the crystal surface is aligned along a low index direction and the scattered beam forms a distinct diffraction pattern [1]



In triangulation, the crystal surface is rotated and simple properties of the scattered beam (here its full width at half maximum) indicate direction where molecules tend to align [4,5].

One of the limitations is that GIFAD needs well-ordered surfaces. With organic layers this order is more difficult to reach but before long range order starts to develop, short range order can be present in the form of local correlations between neighboring molecules. These correlations are revealed by the increased deflection of the projectile when entering a local valley formed along directions where these molecules tend to align [6] and [7,8] for interpretation.

Future developments during the thesis.

On the experimental side, both techniques; triangulation and diffraction rely on the same setup using a position sensitive detector[9,10]. The techniques can be applied to a wide range of thin films such as graphene[11,12], its insulator analog boron nitride and various new 2D materials as long as some crystallographic order starts to develop. These systems will be investigated in collaborations with the groups producing them around to world. We will also benefit from our new building where a UHV tunnel connects several experiments together, allowing for instance, spectroscopic diagnostic of molecular vibration at the surface. We will also chose simple test systems to investigate specific quantum effects associated with the wave nature of the projectile [13] or with energetic degrees of freedom of the surface. Since the technique is still comparatively new, a large part of the experimental activity can be devoted to developing new analysis and comparing predictions to experiments. The use of GIFAD inside MBE was extremely productive and, if possible, new experiment will be performed at INSP.

[1] Debiossac *et al* Phys. Rev. B. **90** 155308 (2014) [2] Debiossac *et al* App. Surf. Sci. (2017) [3] Atkinson *et al* App. Phys. Lett. **105**, 021602 (2014) [4] Roncin & Debiossac Phys. Rev. B. **96**, 035415 (2017) [5] Roncin et al submitted (2017) [6] Kalashnyk & Roncin App.Surf.Sci. **364** p235 (2016), [7] Debiossac &Roncin Phys. Rev. A. **88** 012904 (2013), [8] Zugarramurdi *et al* Rev. A. **90** 054701(2013), [9] Lupone *et al* Rev.Scient.Instr. **86** (2015), [10] Lupone *et al* submitted (2017), [11] Zugarramurdi *et al* App. Phys. Lett. **106**, 101902 (2015), [12] Debiossac *et al* Phys. Rev. B. (2016) [6] Debiossac *et al* Phys. Rev. Lett. **112**, 023203(2014).

keywords: Nanosciences, atomic diffraction, inelastic diffraction, thin films, molecular beam epitaxy, decoherence processes, electronic excitations, phonon excitations