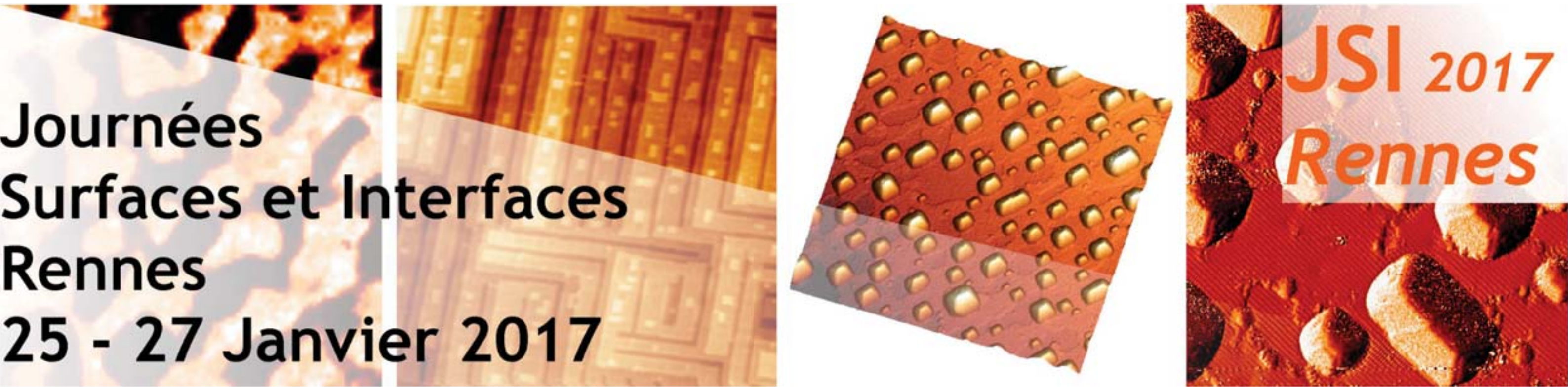

Résumés des conférences et affiches

Pôle Numérique Rennes Beaulieu, Campus de Beaulieu,
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Heure	Mercredi 25	Heure	Jeudi 26	Heure	Vendredi 27
			Session 2 **9h-12h30**		**Session 4** **9h-12h30**
		09:00	**Tao ZHOU** ESRF	09:00	**Anne-Laure BIANCE** ILM
		09:45	**Anny MICHEL** Institut P’	09:45	**Matthieu BUGNET** MATEIS
		10:30	**Pause-café** **10h30-11h**	10:30	**Pause-café** **10h30-11h**
		11:00	**Thomas JAOUEN** IPR et Univ. Fribourg	11:00	**Fabrice COUSIN** LLB
		11:45	**Jacek GONIAKOWSKI** INSP	11:45	**Véronique VIE** IPR
12:00	**Accueil** **12h-14h** *Hall PNRB* **Buffet de bienvenue** 2ème étage Espace co-working	12:30	**Buffet** **12h30-14h** 2ème étage PNRB Espace co-working	12:30	**Buffet** **12h30-14h** 2ème étage Espace co-working
	Session 1 **14h-18h15**		**Session 3** **14h-16h15**		
14:00	**Xavier MARIE** LPCNO	14:00	**Elena SAVINOVA** ICPEES		
14:45	**Jérôme LAGOUTE** MPQ	14:45	**Samy BOUKARI** IPCMS		
15:30	**Pause-café** **15h30-16h**	15:30	**Mikaël KEPENEKIAN** ISCR		
16:00	**Christophe BRUN** INSP	16:15	**Session Posters** **16h15-19h30**		
16:45	**Franck PALMINO** FEMSTO-ST				
17:30	**Laurence MASSON** CINaM				
		20:30	**Dîner de Gala**		

Journées Surfaces Interfaces, Rennes 25-27 Janvier 2017

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Session 1

Mercredi 25 janvier
14h-18h15

MoS_2 et ses Cousins : Nouveaux Matériaux Bidimensionnels aux Propriétés Prometteuses

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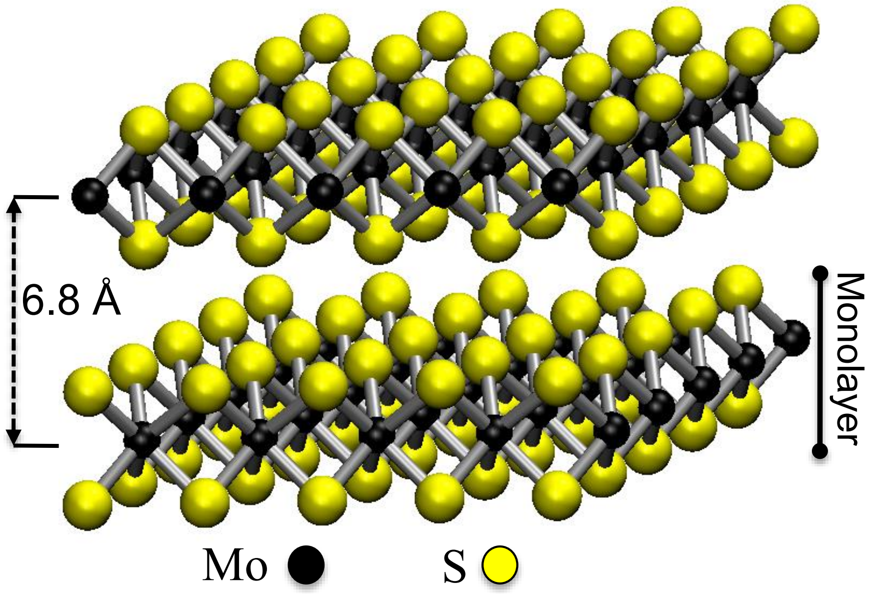
Les progrès spectaculaires sur le contrôle des propriétés électroniques du graphène ont stimulé la recherche de nouveaux matériaux bidimensionnels (2D). Les monocouches de Dichalcogénures de Métaux de Transition tels que MoS_2 (et ses cousins $MoSe_2$, $MoTe_2$, WS_2, WSe_2…) sont apparues très récemment comme des nanostructures très prometteuses pour des applications variées à la fois dans le domaine de l'optique et de l'électronique.

Dans cet exposé, je donnerai un aperçu des propriétés physiques de ces semiconducteurs 2D (structure de bande, excitons, polarisation de spin/vallée…) et des composants prototypes (transistor, photodiode, LED ...) basés sur cette nouvelle classe de matériaux.



Mercredi 25 janvier 14h

Dopage du graphène par l'azote mesuré à l'échelle atomique

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La modulation des propriétés du graphène est un enjeu important pour envisager l'utilisation de ce matériau bidimensionnel dans différents domaines comme l'électronique moléculaire ou l'énergie. Dans ce contexte, l'insertion d'azote dans le réseau carboné est très étudiée car cela permet de réaliser un dopage de type n avec peu d'effet de relaxation. Pour comprendre comment ce dopage modifie la structure électronique du graphène et les implications qui en résultent, la microscopie à effet tunnel (STM) est un outil de choix pour mesurer à l'échelle atomique la structure électronique du graphène dopé. L'imagerie STM permet d'identifier des atomes d'azote isolés insérés dans le graphène ainsi que des paires d'azote [1]. La spectroscopie locale permet de voir comment la densité d'états est modifiée à l'échelle atomique. En particulier, nous verrons que le dopage induit non seulement un décalage du point de Driac, mais également la formation d'états résonants localisés autour des atomes d'azote ce qui implique qu'il faut aller au-delà d'un modèle de bande rigide pour décrire l'effet du dopage.

Le dopage du graphène modifie également sa réactivité chimique. Afin de comprendre comment l'interaction du graphène avec avec des molécules organiques est modulée par le dopage, les propriétés électroniques de molécules de porphyrine sur le graphène dopé ont été étudiées (voir figure 1). Un décalage en énergie du spectre électronique des porphyrines met en évidence une interaction électronique locale entre les sites dopants du graphène et les molécules adsorbées. [2,3].

Ces effets seront discutés dans le but de appréhender la manière dont le dopage du graphène modifie ses propriétés électroniques.

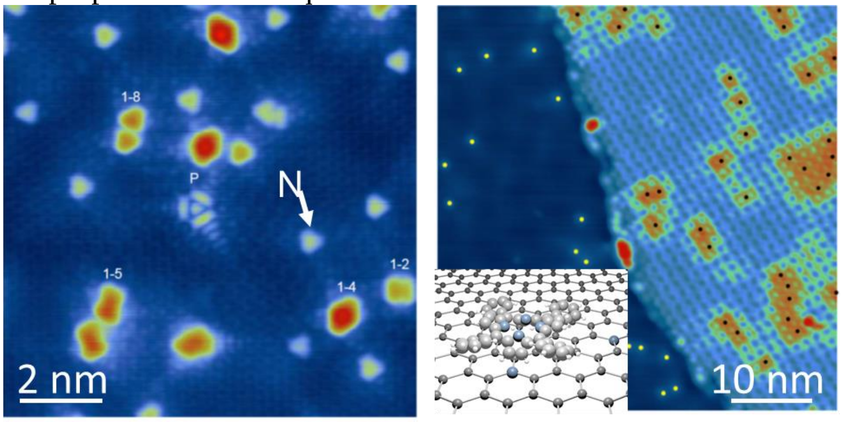

Fig. 1*: Gauche: Image STM d'une surface de graphène dopé par de l'azote montrant des atomes et paires d'atomes d'azote [1]. Droite : Image STM d'un îlot de molécules de tétraphénylporphyrines sur graphène dopé par de l'azote. Les points jaunes et noirs indiquent la position des atomes d'azote sur le graphène et sous l'îlot de molécules respectivement. [3]*

Bibliography

[1] Y. Tison et al., *ACS Nano* **9**, 670 (2015).
[2] V. D. Pham et al., *ACS Nano* **8**, 9403 (2014).
[3] V. D. Pham et al., *Scientific Reports* **6**, 24796 (2016).

Mardi 25 janvier 14h45

Remarkable superconducting properties of single atomic layers of lead on silicon

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Institut des Nanosciences de Paris, CNRS and Université Pierre et Marie Curie, Paris, France

It is well known that conventional superconductivity is very robust against non-magnetic disorder [1]. Nevertheless for thin and ultrathin films the structural properties play a major role in determining the superconducting properties, through a subtle interplay between disorder and Coulomb interactions [2]. Unexpectedly, in 2010 superconductivity was discovered in single atomic layers of lead and indium grown on silicon substrate using scanning tunneling spectroscopy [3] and confirmed later on by macroscopic transport measurements [4]. Such well-controlled and tunable crystalline monolayers are ideal systems for studying the influence of various kinds of structural defects on the superconducting properties at the atomic and mesoscopic scale. In particular, Pb monolayers offer the opportunity of probing new effects of disorder because not only superconductivity is 2D but also the electronic wave functions are 2D. Our study of two Pb monolayers of different crystal structures by very-low temperature STM (300 mK) under magnetic field reveals unexpected results involving new spatial spectroscopic variations [5]. Our results show that although the sheet resistance of the Pb monolayers is much below the resistance quantum, strong non-BCS corrections appear leading to peak heights fluctuations in the dI/dV tunneling spectra at a spatial scale much smaller than the superconducting coherence length. Furthermore, local evidence of the signature of strong spin-orbit coupling of Rashba type on the superconductivity of the Pb/Si(111) monolayer is revealed through filling of in gap states and local spatial variations of this filling. Additionally, the nature of superconducting vortices in a monolayer is found to be very sensitive to the properties of step edges areas. Finally, we will show that by combining the strong spin-orbit coupling at play in Pb monolayers grown on Si(111) with magnetic clusters, we should be able to realize and study 2D topological superconductivity [6,7].

[1] P.W. Anderson, J. Phys. Chem. Solids 11, 26 (1959)
[2] M.V. Feigel'man et al., Ann. Phys. 325, 1390 (2010)
[3] T. Zhang et al., Nature Phys. 6, 104 (2010)
[4] Y. Yamada et al., Phys. Rev. Lett. 110, 237001 (2013)
[5] C. Brun et al., Nature Phys. 444, 10 (2014)
[6] G. Ménard et al. arXiv:1607.06353v1 (2016)
[7] C. Brun, T. Cren and D. Roditchev, Supercond. Sci. Technol. 30, 013003 (2017)

Mercredi 25 janvier 16h

Molecular self-assembled networks on silicon surface

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Nowadays more than 90% of published results show molecules adsorbed onto metallic or HOPG surfaces. This is explained by the low reactivity between molecules and these surfaces which induce a molecular diffusion and the possibility to observe large and perfect self-assemblies. Nevertheless, there are a real economic and technological interests to develop molecular self-assembled layers onto semiconductors and in particular onto silicon surfaces. Actually, due to the existence of Si dangling bonds which induce a strong interaction between molecules and substrates, the formation of such molecular layers is still a real challenge. To circumvent this problem, we need atomically passivated Si surface. Here, an original unreactive silicon surface is presented: the high boron doped silicon √3x√3-SiB (111) reconstruction. Since 10 years, very amazing results have been obtained showing large and perfect molecular self-assemblies by deposition of home-made and specifically designed aromatic molecules on this silicon surface [See Fig. 1]. The morphology of each supramolecular network is explained by the competition between molecule-moleucle and molecuel-surface interactions [1-4].

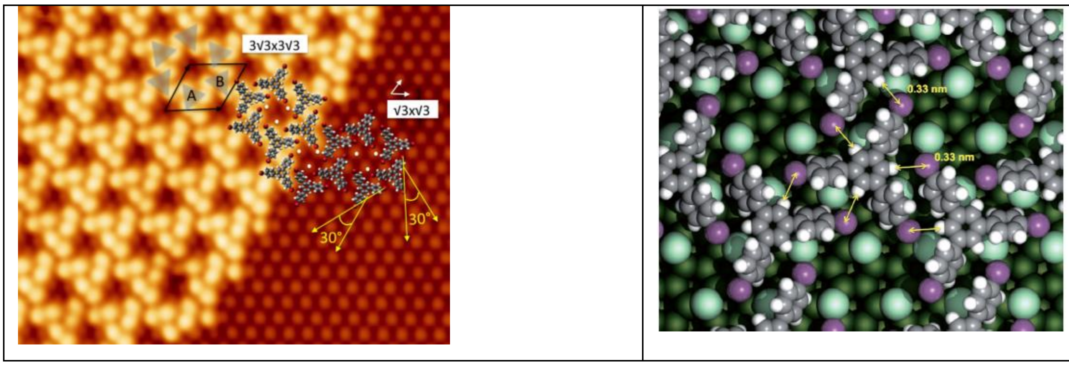

Fig. 1*: Left: STM image of the molecular network (Vs=2.3 V, It=0.037 nA, 15x15 nm2).*
Right: molecular model adsorbed onto Si(111)-B showing pi-stacking and halogen bonds interactions

Acknowledgements
Financial support from the French National Research Agency through contracts ORGANI'SO (ANR-15-CE09-0017) and ACTION (ANR-15-CE29)

Bibliography

[1] *B. Baris, V. Luzet, E. Duverger, P. Sonnet, F. Palmino, F. Cherioux, Angew. Chem. Int. Ed.* ***50****, 4094 (2011)*
[2] *Y. Makoudi, M. Beyer, S. Lamare, J. Jeannoutot, F. Palmino, F. Chérioux, Nanoscale* ***8****, 12347-12351 (2016)*
[3] *G. Copie, F. Cléri, Y. Makoudi, C. Krzeminski, M. Berthe, F. Chérioux, F. Palmino, B. Grandidier, Phys. Rev. Lett.* ***114****, 066101 (2015)*
[4] *Y. Makoudi, M. Beyer, J. Jeannoutot, F. Picaud, F. Palmino, F. Chérioux, Chem. Commun.* ***50****, 5714-5716 (2014)*

Mercredi 25 janvier 16h45

Two-dimensional Si layers on silver substrates

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The large interest in graphene layers and their applications has motivated scientists to investigate other group-IV two-dimensional (2D) layers that could be graphene's analogous, i.e. with a honeycomb structure and sp^2 bonding. Among these, silicene, a single sheet of silicon, has aroused considerable interest in the last past five years due to its fundamental interest [1] and compatibility with Si based-electronics [2]. As solid phase of silicon similar to graphite does not exist, silicene sheets cannot be synthetized through exfoliation methods as it was initially done for graphene. One possible route is to grow Si epitaxial sheets on substrates with expected immiscibility and high commensurability. Pioneering works concern the Si/Ag system and it has been shown that 2D epitaxial layers can be grown on Ag(110) and Ag(111). A graphene-like signature in photoemission spectra has been reported on such films, attributed to the formation of silicene with sp^2-sp^3 hybridized Si atoms arranged in a 2D honeycomb lattice [3-5]. However, recent experimental [6-7] and theoretical [8-9] studies have shown that these conclusions have to be reconsidered. In this talk, it will be shown that the strong Si-Ag interaction has to be taken into account to interpret the structural, electronic and optical properties of the Si/Ag interface. Apart from these investigations, 2D Si layers on Ag(110) can be advantageously used as a template for the self-organized growth of nanostructures. Recent results concerning the magnetic properties of Co nanolines grown on Si/Ag(110) studied with X-ray magnetic circular dichroism will be presented [10].

Bibliography

[1] S. Cahangirov, M. Topsakal, E. Aktürk, H. Şahin, S. Ciraci, *Phys. Rev. Lett*. **102**, 236804 (2009).

[2] L. Tao, E. Cinquanta, D. Chiappe, C. Grazianetti, M. Fanciulli, M. Dubey, A. Molle, D. Akinwande, *Nature Nanotech*. **10**, 227 (2015).

[3] P. De Padova, C. Quaresima, C. Ottaviani, P.M. Sheverdyaeva, P. Moras, C. Carbone, D. Topwal, B. Olivieri, A. Kara, H. Oughaddou, B. Aufray, G. Le Lay, *Appl. Phys. Lett.* **96** 261905 (2010).

[4] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M.C. Asensio, A. Resta, B. Ealet and G. Le Lay, *Phys. Rev. Lett.* **108**,155501 (2012)

[5] H. Jamgotchian, Y. Colignon, N. Hamzaoui, B. Ealet, J.Y. Hoarau, B. Aufray, and J.P. Bibérian, *J. Phys. Condens. Matter* **24** 172001 (2012)

[6] R. Bernard, Y. Borensztein, H. Cruguel, M. Lazzeri, G. Prévot, *Phys. Rev. B* **92**, 045415 (2015).

[7] G.Prévot, C. Hogan, T. Leoni, R. Bernard, E. Moyen, L. Masson, *Phys. Rev. Lett.* accepted (2016)

[8] S. Cahangirov, M. Audiffred, P. Tang, A. Iacomino, W. Duan, G. Merino and A. Rubio, *Phys. Rev. B* **88**, 35432 (2013).

[9] P. Gori, O. Pulci, F. Ronci, S. Colonna and F. Bechstedt, *J. of Appl. Phys.* **114**, 113710 (2013).

[10] L. Michez, K. Chen, F. Cheynis, F. Leroy, A. Ranguis, H. Jamgotchian, M. Hanbücken, L. Masson, *Beilstein J. Nanotechnol.* **6**, 777 (2015).

Mercredi 25 janvier 17h30

Session 2

Jeudi 26 janvier
9h-12h30

In situ synchrotron X-ray scattering of SiGe nanowires: growth, strain and bending

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The INS (In situ - Nanostructure - Surface/interface) end station of the BM32 beamline at the European Synchrotron Radiation Facility (ESRF) has been used for years to analyze the structural properties of nanoparticles in situ, during their growth, combining Grazing Incidence X-ray Diffraction (GIXD) and Grazing Incidence Small Angle X-ray Scattering (GISAXS) [1]. An auxiliary UHV-CVD injection system has been recently added to allow investigations of the VLS and VSS growth of Si/Ge NWs [2].

Results on the growth of Si NWs on Si(111) will first be presented, to demonstrate the in situ capability of the instrument. The real time NWs length and their size distribution can be measured with X-ray techniques without removing the sample from the UHV chamber. The deposition of the metal catalysts and the injection of the precursor gases were carried out side by side, making it possible to probe the very early stage of growth. The well-known sidewall dodecagon sawtooth faceting is clearly recognizable from reciprocal space mapping of both GIXD and GISAXS.

The strain relaxation in Si-Ge core-shell NWs will be presented next. The samples were kept under UHV during the entire process to avoid oxidation and contamination. The level of strain was measured in situ as a function of the overgrowth amount. The composition distribution in the heterostructure was determined using anomalous X-ray scattering, from which the evolution of the composition during growth was then deduced [3].

Results on the in situ bending of as-grown NWs will also be presented. The bending was induced, in our case, by depositing a second material on one side of the NWs and was measured solely by X-ray diffraction techniques. For the quantitative interpretation of the data, we employ the so-called Displaced Bragg Method (DBM) [4]. The strain profile along the longitudinal direction of the NWs was obtained by analyzing the position shift of the displaced Bragg peaks whereas the total stress applied on the NWs was deduced by fitting the NW curvature, retrieved from integrated intensities of the displaced Bragg peaks, with a formula based on classic beam theory. Two cases will be presented to illustrate the use and capability of DBM. We found that the bending induced by Ge deposition on Si NWs sidewall at 220°C is mainly driven by the misfit stress, which scales almost linearly with Ge film thickness. On the other hand, the bending induced by the same deposition on Si NWs sidewall at RT is driven by the surface stress, which evolves from tensile eventually to compressive in the later stage of Ge growth. Finally, the so-called Stationary Method will be presented, which allows us to follow in real time, though mostly qualitatively, the entire bending process in a time efficient manner. The NWs were seen dancing back and forth with increasing amount of deposition as revealed by live stationary measurements with a 2D detector.

[1] G. Renaud, R. Lazzari, F. Leroy Surf. Sci. Rep. (2009) 64, 255.
[2] V. Cantelli, O. Geaymond, O. Ulrich, T. Zhou, N. Blanc and G. Renaud, submitted.
[3] T. Zhou, O. Geaymond, G. Renaud et al., in preparation.
[4] T. Zhou, O. Robach, G. Renaud et al., in preparation.

Jeudi 26 janvier 9h

Premiers stades de croissance de films minces métalliques

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Comprendre le développement de la microstructure et la morphologie de surface durant la croissance de films minces est d'une importance capitale pour contrôler la texture et la rugosité des films, mais également la nucléation et la croissance de nanoparticules, la formation d'îlots, ou les transformations de phase. Ainsi les premiers stades de la croissance revêtent une grande importance, pour des applications allant des nanoparticules (catalyseurs, plasmonique) aux composants semiconducteurs de dimensions nanométriques,

La pulvérisation magnétron offre des conditions de dépôt fortement hors-équilibre, ainsi les aspects cinétiques peuvent prévaloir sur les prédictions thermodynamiques lors de la croissance. On observe que, sans négliger l'importance des réactions interfaciales, pour des métaux à forte mobilité, une croissance en îlots est privilégiée alors qu'une croissance bidimensionnelle sera favorisée à basse mobilité.

En nous situant dans cette problématique, nous avons étudié la croissance de films minces de différents métaux, sur substrats de silicium oxydé ou sur silicium amorphe, en privilégiant l'utilisation de techniques de suivi *in-situ*. Durant la croissance des films, la mesure optique multi-faisceau de courbure du substrat *in-situ* et en temps réel est conjuguée à la spectroscopie de réflectivité différentielle de surface (SDRS), ainsi qu'au suivi en résistivité électrique, toutes techniques ayant une sensibilité de l'ordre de la monocouche, afin de relier l'évolution en contrainte des films au mode de croissance adopté. La mesure de courbure traduit l'évolution de la contrainte dans le film, la SDRS est notamment sensible au mode de croissance (2D, 3D) par l'identification de résonances de plasmons de surface, tandis que la résistivité électrique présente une chute brutale lorsque la couche métallique déposée présente des chemins continus. Nous montrons ici la convergence de ces techniques pour identifier la croissance en îlots, la percolation puis la continuité du film lors de la croissance de métaux de forte mobilité (Ag, Cu…).

La croissance de films de basse mobilité est aussi abordée à travers l'étude de la croissance d'alliages $Mo_{1-x}Si_x$. Dans ce cas, une transition de phase amorphe-cristal est mise en évidence à une épaisseur critique de film déposé, rendant très fructueuse la combinaison de trois méthodes d'analyse *in-situ* : la réflectivité X, la diffraction X et le suivi optique des contraintes. Ces mesures ont été réalisées sur la ligne MPI de la source ANKA (Karlsruhe). Les résultats démontrent que l'évolution de la contrainte est une traduction directe du changement de phase. Cette méthodologie unique permet de relier l'épaisseur critique de cristallisation à la teneur en Si de l'alliage, et par-delà ces résultats l'étude en fonction du temps de l'épaisseur du film, de sa rugosité et du développement de contraintes donne de précieuses informations sur la nucléation et la cinétique de formation de la phase cristalline.

Bibliographie

[1] G. Abadias, L. Simonot, J.J. Colin, A. Michel, S. Camelio, D. Babonneau, *Appl. Phys. Lett* **107**, 183105 (2015).

[2] B. Krause, G. Abadias, A. Michel, P. Wochner, S. Ibrahimkutty, T. Baumbach, *ACS Appl. Mater. Interface***,** DOI: 10.1021/acsami.6b12413 available on line (2016).

Jeudi 26 janvier 9h45

Nature and control of MgO/metal interfaces at the ultrathin limit

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Metal-supported ultrathin oxide films constitute a class of materials whose interesting and novel properties have raised several questions on the nature of interactions at the interfaces. In this talk, we address the intimate nature of the model MgO/Ag(001) system. First, we present a strong manifestation of the image potential screening acting at the interface through the layer-resolved Mg KLL Auger transition. This layer-sensitive spectroscopic probe is used for the full determination of the atomic structure of MgO ultrathin films as well as the study of a controlled Mg intercalation at the interface [1]. Next, we demonstrate how obtaining spectroscopic insights on empty states by using resonant Auger spectroscopy. We show that the evolution of the Auger spectra through the absorption edge allows a layer-by-layer mapping of the local density of unoccupied states therefore giving access to interface and surface electronic states that are hardly probed in conventional photoemission-based techniques [2].

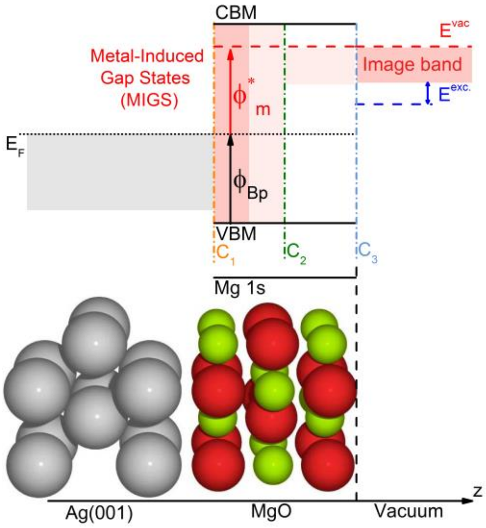

Fig. 1*: Schematic band diagram of the MgO(3ML)/Ag(001) interface*

Acknowledgements

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Bibliography

[1] T. Jaouen *et al.*, Phys. Rev. Lett. **111**, 027601 (2013).
[2] T. Jaouen *et al.*, Phys. Rev. B **91**, 161410(R) (2015).

Jeudi 26 janvier 11h

Nano-polarity: electrostatic effects in free and supported oxide nano-objects

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The advances in the fabrication and control of ultra-thin oxide films have fostered the development of theoretical concepts related to confinement and low dimensionality effects in these objects. This concerns in particular the electrostatically-driven polarity effects, which appear to have a sound influence on the stability and properties of ultra-thin films, 2D ribbons, or nano-islands. Indeed, below a critical size, nano-objects may sustain finite dipole moments which drive strongly size- and dimensionality- dependent properties. At small sizes, polarity effects may also extend beyond the surface region and drive structural transformations of the entire object, resulting in novel structures, with no bulk counterparts. Finally, since oxide nano-objects are often synthesized on metal substrates, their characteristics are additionally modified by the electrostatic coupling between their structure and the interface charge transfer.

Relying on selected examples which were the subject of recent experimental and/or theoretical works, we will exemplify such novel manifestations of polarity in free and supported nano-scale oxide films and discuss the consequences for their physico-chemical properties.

Bibliography

C. Noguera, J. Goniakowski, *Chem. Rev.* **113**, 4073 (2013).
C. Noguera, J. Goniakowski, in *Oxide Materials at the Two Dimensional Limit*, ed. F.P. Netzer and A. Fortunelli, Springer Series in Material Science **234**, 201, Springer (2016).

Jeudi 26 janvier 11h45

Session 3

Jeudi 26 janvier
14h-16h15

Investigation of electrocatalytic materials *in operando* with Near-Ambient Pressure XPS (NAP-XPS)

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Global pursuit of clean and sustainable energy is guiding the development of electrochemical energy conversion and storage technologies, including fuel cells, batteries, and electrolyzers, where the interface between an electronic and an ionic conductor (solid, liquid or polymer) plays a central role. The development of efficient energy conversion systems not only requires potent, durable and cost-effective materials, but also asks for precise engineering of electrochemical interfaces where molecular, ionic and electronic flows merge. Future progress in the field thus relies heavily on the availability of in situ and in operando techniques to probe structure and composition of the dynamic electrode/electrolyte interfacial region.

X-ray Photoelectron spectroscopy (XPS) is one of the most powerful techniques for studies of the chemical composition and the oxidation state of components located within the near-surface region. Recent advances in vacuum and analyzer technologies have resulted in the development of specialized instruments which allow performing the so-called Near Ambient Pressure Photoelectron Spectroscopy (NAP-XPS) measurements in the pressure range of millibars [1,2].

In this presentation we will discuss recent insights into the structure and dynamics of electrode/electrolyte interfaces from NAP-XPS measurements of electrocatalytic materials *in operando* conditions [3-5]. We will see XPS not only provides information on red-ox transitions and segregation/dissolution phenomena of the electrode constituents, but also offers insights into reversible and irreversible electrolyte transformations under polarization [5].

Acknowledgements

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Bibliography

[1] M. Salmeron, R. Schlögl, *Surf. Sci. Rep* **63**, 169 (2008).
[2] A. Knop-Gericke, E. Kleimenov, M. Hävecker, R. Blume, D. Teschner, S. Zafeiratos, R. Schlögl, V. I. Bukhtiyarov, V. V. Kaichev, I. P. Prosvirin, A. I. Nizovskii, H. Bluhm, A. Barinov, P. Dudin, M. Kiskinova, Adv. Catal. **52**, 213 (2009).
[3] V. Papaefthimiou, M. Diebold, C. Ulhaq-Bouillet, W. H. Doh, R. Blume, S. Zafeiratos, E. R. Savinova, *ChemElectroChem* **2**, 1519 (2015).
[4] V. A. Saveleva, L. Wang, W. Luo, S. Zafeiratos, C. Ulhaq-Bouillet, A. S. Gago, K. A. Friedrich, E. R. Savinova, *J.Phys.Chem.Lett*. **7**, 3240 (2016).
[5] Y. T. Law, S. Zafeiratos, S. G. Neophytides, A. Orfanidi, D. Costa, T. Dintzer, R. Arrigo, A. Knop-Gericke, R. Schlögl, E. R. Savinova, *Chem. Sci*. **6**, 5635 (2015).

Jeudi 26 janvier 14h

Interactions between molecules and metals

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To ensure the long-term progress of information technology, radically new concepts, materials and processing methods are required to circumvent the limitations of traditional electronics. Spin electronics, or spintronics, adds a new spin degree of freedom to conventional charge-based electronics. By injecting, transporting, controlling and detecting spin-polarized currents, new spin-based devices can be obtained, including spin valves (magnetoresistive devices), spin-FETs (field-effect transistors with spin-polarized source and drain), spin-LEDs (spin-polarized light-emitting diodes), and quantum bits for quantum computation and communication.

Separately, organic electronics offers the advantages of low-cost materials and processing, the tuning of electronic properties by simple chemical routes to build multifunctional devices, and self-organization. In a more long-term perspective, organic electronics at the nano- or molecular scale will exploit intriguing electric properties of nanoscopic objects down to single molecules in electric circuits.

The combination of these two approaches, spin and molecular electronics, gave rise in the last decade to a new emerging field – termed organic spintronics – that has received considerable interest since it's expected to produce devices that could enter in the growing organic electronics market. Within this field, it appeared that interface properties are important to understand how devices are working. Indeed, to build a device, molecules will be chosen a priori on their intrinsic properties. However, once integrated into a device, their intrinsic properties may change radically. For instance we have shown that phthalocyanine (Pc) semiconductor molecules turn metallic when adsorbed on cobalt [1], or that the spin transition of Fe-phenanthroline molecules is precluded when adsorbed on bare Cu(100) but restored by inserting a CuN layer [2]. The interactions between molecules and metals are not necessarily deleterious but can be the source of new properties that are hardly predictable. As an example, Mn-phthalocyanine that present in the bulk no magnetic order above ~9K, can bias a ferromagnetic Co layer [3]. Therefore, the interactions between molecules and metals is a fundamental issue for the future of organic spintronics and multifunctional devices.

Bibliography

[1] S. Javaid et al. Phys. Review Lett. **105** 077201 (2010).
[2] T. Miyamachi et al. Nat. Commun. **3** 938 (2012).
[3] M. Gruber et al. Nature Mater. **14** 981 (2015).

Jeudi 26 janvier 14h45

Towards highly cooperative spin-crossover metal-organic frameworks on metallic surfaces

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The design of molecular-based devices to manipulate spin has driven many investigations opening the field of molecular spintronics [1]. In this context, molecular bistability has drawn much attention and the most promising objects arise from molecular magnetism. Although recent realizations have been achieved with single molecules, such setups disrupt the required inter-site cooperativity that turns a slowly commuting system into a rapidly switching set of molecules. An auspicious path comes from the use of metal-organic frameworks (MOF) self-assembled on surfaces, which offer the opportunity to tailor interactions between magnetic sites.

Based on density functional theory, we first elucidate the structure, electronic structure and magnetic properties of a recently proposed Fe-based MOF self-assembled on the Au(111) surface [2]. We then propose a chemical strategy to turn a weakly interacting magnetic system into a strongly cooperative spin-crossover monolayer. Finally using a thermodynamic model, we demonstrate how the dimensionality reduction combined to deposition on a metal surface enhance the electrostatic contributions to spin-crossover cooperativity, going from $\Gamma_{3D} = 16$ K for a bulk materials to $\Gamma_{2D}^{supp} = 386$ K for its 2D supported derivative [3]. With the ability to enhance cooperativity in a rational way, a promising route is opened towards the design of molecular spintronic devices.

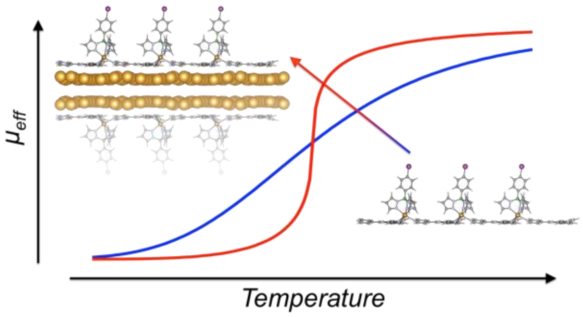

Fig. 1*: The presence of a metal surface turns a slowly transiting spin-crossover network into a highly cooperative system displaying a sharp transition.*

Bibliography

[1] L. Bogani, W. Wernsdorfer, *Nature Mater.* **7**, 179 (2008). S. Sanvito, *Chem. Soc. Rev.* **40**, 3336 (2011). S. V. Aradhya, L. Venkataraman, *Nature Nanotech.* **8**, 399 (2013).
[2] T. R. Umbach, M. Bernien, C. F. Hermanns, A. Krüger, V. Sessi, I. Fernandez-Torrente, P. Stoll, J. I. Pascual, K. J. Franke, W. Kuch, *Phys. Rev. Lett.* **109**, 267207 (2012).
[3] T. Groizard, N. Papior, B. Le Guennic, V. Robert, M. Kepenekian, *manuscript submitted.*

Jeudi 26 janvier 15h30

Session 4

Vendredi 27 janvier
9h-12h30

Grosseur et décadence de films de savon

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Les films de savon sont un des constituants élémentaires des mousses liquides, matériaux rencontrés dans l'industrie ou dans la vie de tous les jours. Nous nous intéressons ici expérimentalement à la dynamique de ces films dans des architectures savonneuses modèles et dans diverses situations.

Nous étudierons tout d'abord le cas de films au bord desquels est appliquée une différence de potentiel, ce qui permet dans certains cas d'induire des écoulements et d'augmenter considérablement le temps de vie de ces films [1,2]. Grâce à une méthode d'optique non linéaire, nous avons déterminé la répartition des tensio-actifs aux interfaces lors de ces écoulements [3]. Nous nous intéresserons ensuite aux conséquences de ces phénomènes dans les mousses macroscopiques. Enfin, nous revisiterons le problème très classique de la dynamique de films qui éclatent [4].

Dans toutes ces situations, nous montrerons que la physicochimie des tensioactifs peut modifier considérablement les mécanismes observés.

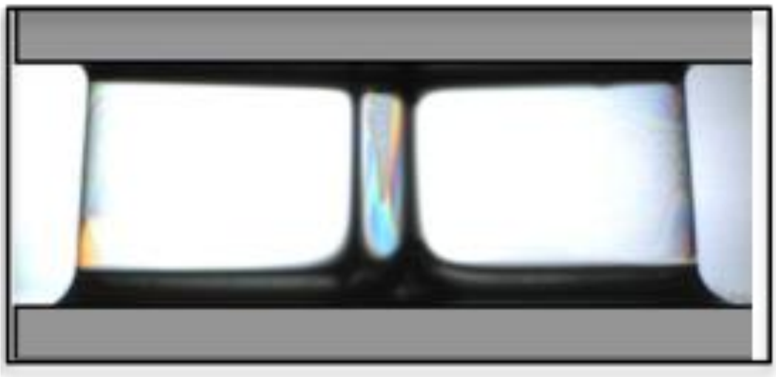

Fig. 1*: Deux bulles de savons confinées entre deux électrodes horizontales. Hauteur de 3 mm.*

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The authors would like to acknowledge ANR for funding through the EFOAM project.

Bibliography

[1] Bonhomme, Liot, Biance*, Bocquet, *PRL* **110**, 054502 (2013).
[2] Joly, Detcheverry, Biance, *PRL* **113**(8), 088301 (2014)
[3] Petit, Le Merrer, Biance, *Journal of Fluid Mechanics* **774** R3 (2015)
[4] Blanc, Bonhomme, Ybert, Biance, *submitted* (2016)

Vendredi 27 janvier 9h

Contributions of environmental TEM to operando surface analysis

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Transmission electron microscopy (TEM) is a well-established characterization technique to combine bulk as well as surface analysis in a wide range of materials at the nanoscale. Since the large majority of materials are not utilized in moderate or high vacuum, investigating them *in situ* in the TEM in more realistic environmental conditions appears necessary to understand fundamental structural and chemical aspects at surfaces in several fields of research such as catalysis, corrosion, or crystal growth. In this respect, control of the nature and the pressure of the atmosphere surrounding the specimen while allowing nanoscale down to atomic resolution in a transmission electron microscope is of great importance [1, 2].

Surface phenomena induced by the partial pressure and temperature within a dedicated Cs-corrected environmental TEM (ETEM) will be presented, with a particular focus on heterogeneous catalysis applications. For example, tuning the reduction state at surfaces of ceria (CeO_2) nanocubes under reducing and oxidizing conditions brings light on the surface structure and chemistry of their organization [Fig. 1], and opens a field of study for direct visualization of atomic scale phenomena such as carbonate adsorption. The current capabilities and limits of such approaches in the ETEM will be discussed.

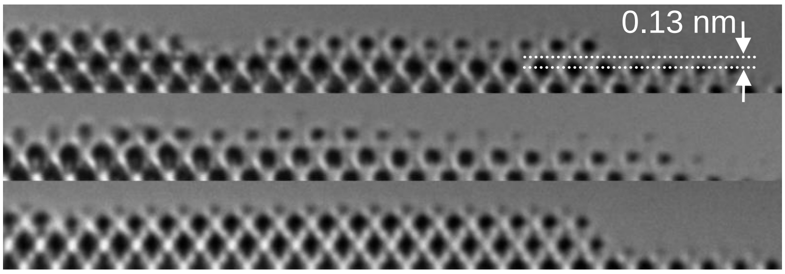

Fig. 1*: (001) surface of a ceria nanocube observed along [110] in (from top to bottom): O_2 (5 10^{-2} mbar), HV (5 10^{-6} mbar) and CO_2 (2.5 10^{-2} mbar). Each 'dark atoms' image is averaged over 2 seconds according to original micrographs recorded at 25 fps. This procedure shows that the terminating layer is mainly constituted by oxygen atoms with some mobility under O_2, cerium atoms with a great mobility under HV and oxygen (most probably CO_x complexes) without any mobility under CO_2 (FEI Titan ETEM 300 kV at 20°C).*

Acknowledgements

The authors thank A. K. P. Mann, Z. Wu, and S. H. Overbury from Oak Ridge National Laboratory for providing the ceria nanocubes. The electron microscopy presented here has been performed at the CLYM: Lyon-St-Etienne centre for electron microscopy, a node of the French CNRS METSA network providing access to advanced EM and ATP instruments.

Bibliography

[1] H. Yoshida et al., *Science* **335**, 317 (2012).
[2] M. Aouine et al., *ACS Catalysis* **6**, 4775-4781 (2016).

Vendredi 27 janvier 9h45

Neutron scattering : a unique tool for probing sot matter systems at surfaces and interfaces

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"Soft Matter" deals with systems made of individual building blocks (e g colloidal nanoparticles, polymers, surfactants,) whose characteristic sizes lay in the 0.1–10 nm range. In such systems, the delicate balance of interactions (of the order of kBT) can lead to the formation of large self-assembled complex architectures showing specific dynamics, kinetics. Understanding the underlying mechanisms of their self-assembly and dynamics is then the key to control and tune their very specific properties at the nanometer scale (1-100 nm). In this framework, the neutron scattering techniques combined with H/D isotopic labeling are a unique tool to characterize the systems at the relevant spatial scales of the systems owinf to the possibilities provided by contrast variation methods.

In this lecture, I will show how such contrast variation methods can be applied to probe polymer systems at interfaces with neutron reflectivity on three examples. First, it will be shown how specific deuteration can demonstrate the inner superstrcuture of polyelectrolyte multilayers [1]. Second, it will shown how the kinetics of interdiffusion between a polymer brush and a melt of the same polymer can be followed [2.a] and, on the same system, how neutron reflectivity can highlight a partial disentanglement of the brush from the melt if this latter is strechted [2.b] ([Fig. 1]). Third, it will be shown how contrast variation can probe selectively the behavior of each block of a copolymer block adsorbed at the air/water interface as function of physico-chemical conditions [3]. I will show how specular neutron reflectivity combined by GISAXS enabled to get the full picture of the system, both perpendicular to the interface and within the interface. Finally, if time permits, I will show that Small Angle Neutron Scattering, the counterpart technique of reflectivity for bulk samples, can also be successfully used to probe interfaces if contrast conditions are smartly chosen. This will be illustrated by a recent example on Pickering emulsion [4].

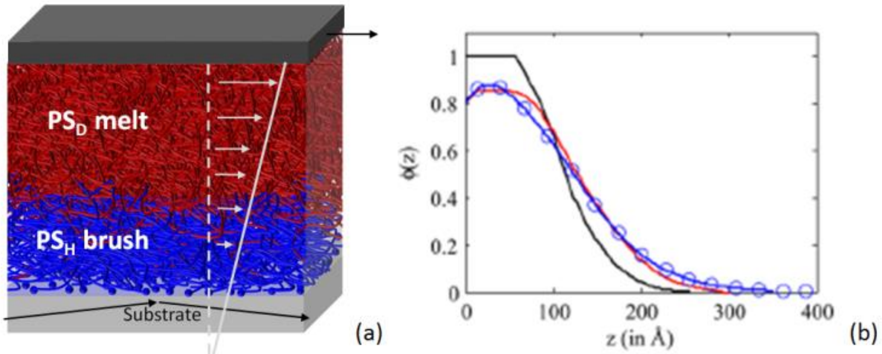

Fig. 1*: (a) Stretching of a hydrogenated polystyrene melt (in blue) interdigitated with a polystyrene brush (in red). (b) Profiles obtained from reflectivity curves: at rest (red) and after shear (black).*

Bibliography

[1] O. Félix, Z. Zheng, F. Cousin, G. Decher, *C. R. Chimie*, **12**, 225-234 (2009).

[2.a] A. Chennevière, E. Drockenmuller, D. Damiron, F. Cousin, F. Boué, F. Restagno, L. Léger, *Macromolecules*, **46(17)**, 6955–6962 (2013). [2.b] A. Chennevière, F. Cousin, F. Boué, E. Drockenmuller, K. Shull, L. Léger, F. Restagno, *Macromolecules*, **49(6)**, 2348-2353 (2016).

[3] Z. Guennouni, F.Cousin, M.-C. Fauré, P. Perrin, D. Limagne, O. Konovalov, M. Goldmann, *Langmuir*, 2016, **32 (8)**, 971–1980 (2016).

[4] F. Cherhal, F. Cousin, I. Capron, *Biomacromolecules*, **17(2)**, 496–502 (2016).

Vendredi 27 janvier 11h

Air/liquid interface: relevance of Langmuir film as biological membrane model

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Biological membranes are composed of a lipid bilayer in which proteins are more or less embedded. Now, these lipids are amphiphilic molecules which form spontaneously a monolayer at the air/liquid interface. Choosing specific lipids, this monolayer is used as simple model mimicking either the inner or the outer leaflet of the membrane. Combination of different biophysical tools such as ellipsometry, atomic force microscopy or interfacial rheology allows the characterization of the lipid film's behavior (Fig.1). For example, the lateral organization and its dynamic can be related to segregation phenomena observed in cell membrane [1]. Moreover, it is also possible to evaluate the ability amphiphilic compounds (peptides, proteins or nanoparticles) to interact or insert in these monolayers [2, 3].

After the biophysics tool description, I will present our work focused on interaction of dystrophin fragments with lipid monolayers mimicking the inner leaflet of the muscle membrane [4]. Indeed, the dystrophin is a long protein located close to the muscle membrane and confers resistance to muscular cells during elongation/contraction cycles. Dystrophin is involved in Duchenne and Becker muscular dystrophies and a better understanding of the molecular function (interaction with the membrane) can provide new insights in gene therapy.

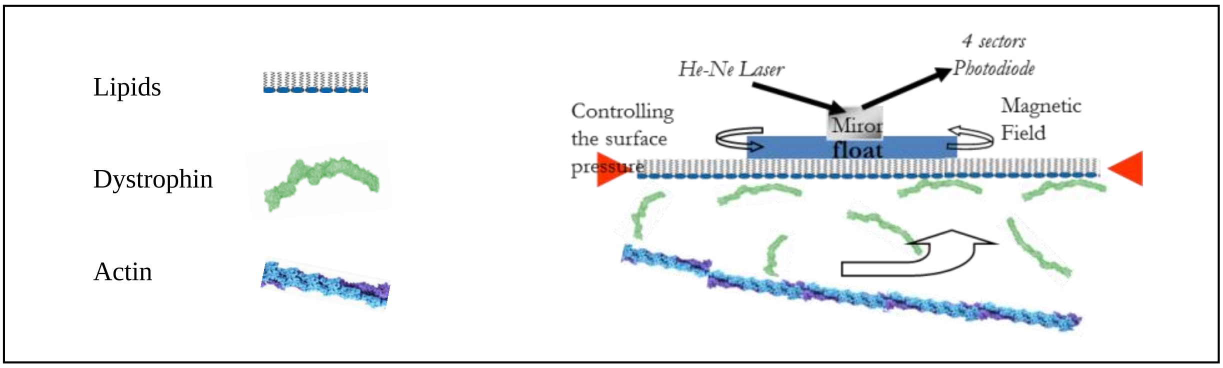

Fig. 1*: Setup to measure the shear elastic constant of interfacial layer.*

Acknowledgements:
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Bibliography

[1] K. Simons and E. Ikonen, *Nature*, **397**, 569-572 (1997).
[2] R. Maget-Dana et al., *Biochim.Biophys. Acta*, **1462**, 109-140 (1999).
[3] V. Vié et al., *Biochim.Biophys. Acta*, **1798**, 1503-1511 (2010).
[4] J. Sarkis et al., *FASEB journal*, **27(1)**, 359-367 (2013).

Vendredi 27 janvier 11h45

Session Posters

Jeudi 26 janvier
16h15-19h30

Comparative adsorption study of copper phthalocyanine on Si(111)(√3 ×√3)R30°Ag and Si(111)(√3 ×√3)R30°B surfaces

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The adsorption of copper phthalocyanine (CuPc) molecules on both Si(111)(√3 ×√3)R30°Ag and Si(111)(√3 ×√3)R30°B surfaces is studied at room temperature under ultra high vacuum. Crystallographic, chemical and electronic properties of the interfaces are investigated by low energy electron diffraction (LEED), ultraviolet and X-ray photoemission spectroscopies (UPS, XPS) and X-ray photoemission diffraction (XPD). On both surfaces, LEED and XPD results indicate that after one monolayer deposition the molecular layer is highly ordered. While on the first surface (Si-√3Ag) the adsorption is according to a flat lying configuration, on the second surface (Si-√3B) the CuPc molecules are aligned in a standing manner (Fig. 1). On the second surface, the molecular packing appears very close to the one of the bulk CuPc α phase. XPS core level spectra of the two substrates reveal that there is no discernible chemical interaction between molecules and substrates; however there is evidence of Fermi level movement. During the growth, the work function was found to decrease in the two cases. Within a thickness of two mono-layer deposition an interface dipole and a substrate band bending have been found. UPS spectra indicate the existence of a band bending of the highest occupied molecular orbital (HOMO). The changes in the work function, in the Fermi level position and in the HOMO state have been used to determine in each case the energy level alignment at these interfaces. The deduced differences in results for both surfaces are related to the surface morphology.

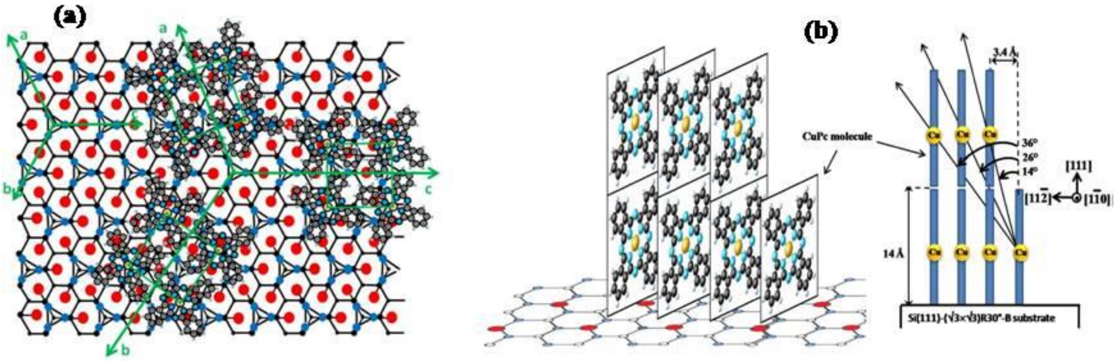

Fig. 1: *Schematics of the molecular arrangement for the one monolayer coverage on (a) the Si(111)-(√3 × √3)R30°-Ag surface and (b) the Si(111)-(√3 × √3)R30°-B surface.*

Structure and plasmonic properties of Al nanoparticles self-aligned in Si_3N_4 thin films

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Aluminum is one of the most promising materials for the future of plasmonics and is thereby attracting an ever growing attention [1-3]. Indeed, in comparison with the more traditional plasmonic metals (Ag and Au), the localized surface plasmon resonance (LSPR) of Al nanoparticles can be tuned from the deep ultraviolet to the near infrared range. Furthermore, Al nanoparticles show good field enhancement performances. However, Al nanoparticles are difficult to synthesize and quickly oxidize upon exposure to atmosphere. In this presentation, we will report on the plasmonic response of Al nanoparticles prepared at room temperature by glancing-angle ion-beam sputtering deposition onto nanorippled Si_3N_4 surfaces, and then covered with a transparent Si_3N_4 capping layer to protect them from oxidation. Combining energy-filtered transmission electron microscopy (EFTEM) and selected area electron diffraction, we will demonstrate that such a fabrication method enables the formation periodic chains of elongated Al nanoparticles surrounded by an AlN shell [**Erreur ! Source du renvoi introuvable.**]. Far-field optical properties were investigated by transmittance measurements showing that the as-deposited core-shell nanoparticles exhibit a polarization-dependent LSPR (in the 1.5–3 eV range), while thermal annealing causes a shift of the LSPR towards higher energies (~3.8 eV) as well as a progressive disappearance of the plasmonic dichroism. Moreover, calculations of the near-field optical properties based on the finite-difference time-domain method were performed. Due to the presence of the AlN shell, two LSPR are observed (*i.e.*, one at the Al/AlN interface and the other at the AlN/Si_3N_4 interface), thus generating a high density of hot spots at various energies with estimated field-enhancement ratios up to almost 10.

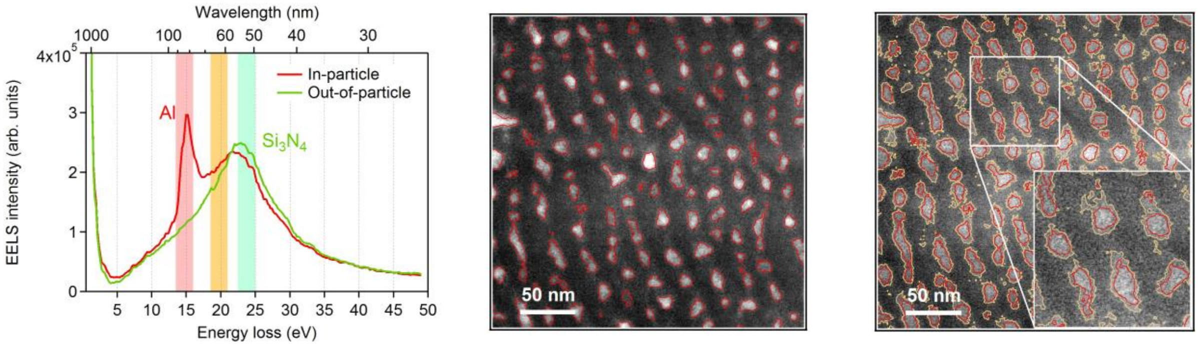

Fig. 1*: (left) Characteristic electron energy-loss spectra. (center) EFTEM image collected in the [13.5-16] eV range showing the presence of Al nanoparticles. (right) EFTEM image collected in the [18.5-21] eV range suggesting the presence of AlN shells surrounding the Al nanoparticles.*

Bibliography

[1] J. Martin and J. Plain, *J. Phys. D: Appl. Phys.* **48**, 184002 (2015).
[2] D. Gérard and S. K. Gray, *J. Phys. D: Appl. Phys.* **48**, 184001 (2015).
[3] F. Bisio *et al.*, *ACS Nano* **8**, 9239-9247 (2014).

Vectorial method: new method to analyze evolving thin films

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Understanding the chemical information at the surface of thin films is a key to predict the behavior of the material, especially in case the surface evolves under different stimuli. A hybrid sol-gel[1–3] based on titanium oxide has been developed and shows evolution under UV illumination with the reduction of Ti(IV) to Ti(III) and the apparition of an intermediate band in its band gap. However, Ti cation is not the only specie impacted by the reduction. To understand the chemical evolution of those thin films, XPS and Infra-Red measurements were performed under continuous UV illumination and controlled atmospheres. Information can be qualitatively extracted from the evolution of spectra but it can be difficult to quantify the evolution.

The vectorial method[4,5] is a method that can, once applied to the set of spectra generated, provide at least two vectors which will be used to describe the original set of spectra. Based on CasaXPS software[6], this mathematical method generates a weighted difference from an initial spectrum (before any evolution) to the final one according to the equation: $X_i = (1-c_i)S_o - c_iS_f$, i=1 to 200, with X_i, the vector generated, S_o and S_f the initial and final spectra and c_i, a coefficient varying from 0 to 1 with an interval of 0.005.

Applied to XPS spectra, this method allows the discovery of a new contribution for Ti(IV) in Ti 2p spectra, correlated to the appearance of Ti(III) specie under UV illumination. Applied to Infra-Red spectra, two states of the films, with different organic species, can be described, corresponding to neutral and photo-reduced states, respectively. The vectors can be used to describe the whole set of spectra and a percentage of reduction can be extracted. This percentage is then compared to the one obtained by XPS measurements and shows good correlation.

Bibliography

[1] Cottineau, T. *et al. Chem. Mater.* **20,** 1421–1430 (2008).
[2] Cottineau, T., Rouet, A., Fernandez, V., Brohan, L. & Richard-Plouet, M. *J. Mater. Chem. A* **2,** 11499 (2014).
[3] Cottineau, T., Richard-Plouet, M., Mevellec, J.-Y. & Brohan, L. *J. Phys. Chem. C* **115,** 12269–12274 (2011).
[4] Baltrusaitis, J. *et al. Appl. Surf. Sci.* **326,** 151–161 (2015).
[5] d'Halluin, M. *et al. Carbon N. Y.* **93,** 974–983 (2015).
[6] Fairley, N. Casa Software Ltd.

S-segregation anisotropy in Ni grain boundaries: consequences on embrittlement

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Sulphur is one among many non-metallic elements that favor the embrittlement of a polycristalline nickel sample that is undergoing a tensile test. In the case of the well documented bicrystal containing the Σ5(012) grain boundary (GB), atomic-scale computations revealed a strong segregation of sulphur at the GB [1], that leads to a strong decrease of both tensile and shear strengths of the bicrystal [2].

However, NanoSIMS experiments showed some years ago that this segregation can be very different with regards to the GB under investigation. For instance, clean coherent-twin GBs can coexist with fully segregated other GBs [3]. As such interfaces will not participate in failure, the description of their interfacial properties (structure, configuration) as a function of S composition is out of experimental reach via classical techniques such as AES.

We computed the segregation enthalpy and embrittling potencies of one S impurity on 3 different GBs (Σ5(012), Σ5(013) and the coherent-twin GB Σ3(111)) using the ReaxFF potential initally developed by Van Duin et al [2]. For each interface under investigation, the sign of these quantities respectively indicate if S would segregate at the interface and if it would participate in embrittling or strengthening the interface. We show that this behaviour is strongly dependent on the atomic-scale structure of the GB plane. Nevertheless, the limitations of the ReaxFF potential in describing the segregated interface are also emphasized and lead to new requirements mostly on the nickel description.

Acknowledgements
This work has been supported by ANR 15 – CE30 – 0016 (GiBBS).

Bibliography

[1] M. Yamaguchi, M. Shiga and H. Kaburaki, *Science* **307**, 393-397 (2005).
[2] H. P. Chen, R.K. Kalia, E. Kaxiras, G. Lu, A. Nakano, K.I. Nomura, A.C.T. Van Duin, P. Vashishta and Z. Yuan, *Physical Review Letters* **104**, 155502 (2010).
[3] F. Christien, C. Downing, K.L. Moore and C.R.M Grovenor, *Surface and Interface Analysis* **3**, *377-387.*

Physical properties of epitaxial Fe films on $SrTiO_3$ (001)

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$SrTiO_3$ is one of the most studied oxides for its own properties and as a substrate for epitaxial growth of oxides and metals. It has many potential applications in the field of thin films electronics, in particular memory devices based on a non-volatile resistive switching [1]. In that case, it is important to understand the electronic properties of metal thin films deposited on $SrTiO_3$. In the field of multiferroic heterostructures, it is also interesting to compare the well-known Fe/$BaTiO_3$ system to the Fe/$SrTiO_3$ one, in which ferroelectricity does not exist.

Here we present a detailed study of the electronic and magnetic properties of iron films deposited on $SrTiO_3$(001) substrates as well as the growth of Fe on this substrate using x-ray Photoemission Spectroscopy (XPS), Reflection High Energy Electron Diffraction (RHEED), Atomic Force Microscopy (AFM) and Magneto-Optical Kerr Effect (MOKE). Fe films from 0.1 nm to 8 nm in thickness were deposited by Molecular Beam Epitaxy (MBE) at room temperature on Nb-doped and un-doped $SrTiO_3$ (001) substrates. We found that the Fe films grow with a 45°-rotated cube-on-cube epitaxy on $SrTiO_3$ (001) with a mode close to the two dimensional mode. The roughness is about 1 nm for an iron thickness of 8 nm. We also observed that the Fe deposition induces a reduction of the substrate and that only few planes of TiO_2 near the Fe/$SrTiO_3$ interface are implied in this process.

Magnetic properties of Fe films depend on the thickness. The in-plane biaxial anisotropy constant (>0) decreases linearly with the inverse of thickness. We propose that this change is linked to the surface in-plane magnetic anisotropy that becomes dominant for the lowest coverages with a related constant negative.

Finally the Schottky barrier height (SBH) for the Fe/$SrTiO_3$ (001) n-doped junction was determined from XPS data. We found a value of ~0.2 eV indicating that the contact is ohmic. Our results disagree with theoretical works which have shown that the SBH for the Fe/$SrTiO_3$ junctions should be higher than 1.0 eV [2]. The difference between those theoretical works and our data comes from the fact that the theoretical model does not take into account the presence of reduced titanium cations at the Fe/$SrTiO_3$ interface.

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Bibliography

[1] K. Szot *et al.* Solid State Physics **65** 353 (2014)
[2] M. Mrovec *et al.* Physical Review B **79** 245121 (2009)

Structural and mechanical properties of TiCu metallic glass thin films deposited by DC and RF magnetron co-sputtering

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Abstract:

Since the first discovery of metallic glasses in 1960 [Klement-1960], researchers have been interested in their unique atomic structures and their mechanical [Xu-2005, Du-2007], electronic [Banerjee-2008], and magnetic [Zhang-2000] properties. Simple systems such as binary alloys either Bulk Metallic Glasses (BMGs) or Thin Films Metallic Glasses (TFMGs) [Chu-2012] are easily elaborated since a few ten years and their mechanical properties systematically studied using nanoindentation and µ-compression techniques.

This study focuses on the structural mechanical properties of binary Ti_xCu_{1-x} (TiCu) thin films metallic glass deposited by magnetron co-sputtering on silicon substrate from Ti and Cu targets in pure Ar DC and RF plasma discharge, respectively. Process parameters such as DC and RF power, working pressure, substrate temperature were varied and experimental conditions leading to glass forming ability were identified. Their influence on the film thickness, microstructure, chemical composition and mechanical properties were investigated. In particular, the structural properties of the metallic glass were characterized by X-ray Diffraction (XRD) and X-ray Reflectivity (XRR). Chemical composition was characterized both by Energy Dispersive X-ray Spectroscopy and X-Ray Photoelectron Spectroscopy (XPS) leading to bulk and surface insights, respectively. Besides, the picosecond ultrasonics, the Brillouin light scattering and the nanoindentation techniques were involved to characterize their acoustic, elastic and hardness properties. A synthesis of main results will be presented.

References

[Chu-2012]	*J. P. Chu, J.S.C. Jang, et al, Thin Solid Films 520, 5097 (2012)*
[Du-2007]	*X.H. Du, J.C. Huang, et al, Appl. Phys. Lett. 91, 131901(2007)*
[Klement-1960]	*W. Klement, R.H. Willens, P. Duwez, Nature 187, 869 (1960)*
[Xu-2005]	*Y.K. Xu, H. Ma, et al, Acta Mater. 53 1857, (2005)*
[Zhang-2000]	*Z.S. Zhang, M. Ding, et al, Phys. D: Appl. Phys. 33, 185(2000)*

Scanning tunneling microscopy investigation of GaP MBE growth on nominal and vicinal Si(001) substrates for optoelectronic applications

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The monolithic integration of III-V based optical functions on Si(001) substrates requires suppression of antiphase disorder in the III-V active region.[1] We present a detailed scanning tunneling microscopy (STM) study of epitaxial GaP layers grown by molecular beam epitaxy on nominal and vicinal Si(001) substrates. The surface morphology of GaP films with thickness varying between 3 and 220 nm is investigated from large scale down to the atomic level. We show that the use of vicinal substrates presenting bi-atomic steps only promotes anisotropic growth of the dominant polarity at the early deposition stages, allowing further annihilation of the antiphase boundaries (APB) on 6°-off Si(001) substrates.[2] From atomically resolved STM images, we also report on the presence of clearly different terminal GaP facets on nominal and vicinal substrates. These preliminary results give new ideas on the effect of a controlled substrate miscut on APB formation and annihilation mechanisms. Finally, the dependence of thick GaP layer's roughness with various growth parameters (substrate miscut angle, V/III flux ratio during growth[3]) is also presented and analyzed.

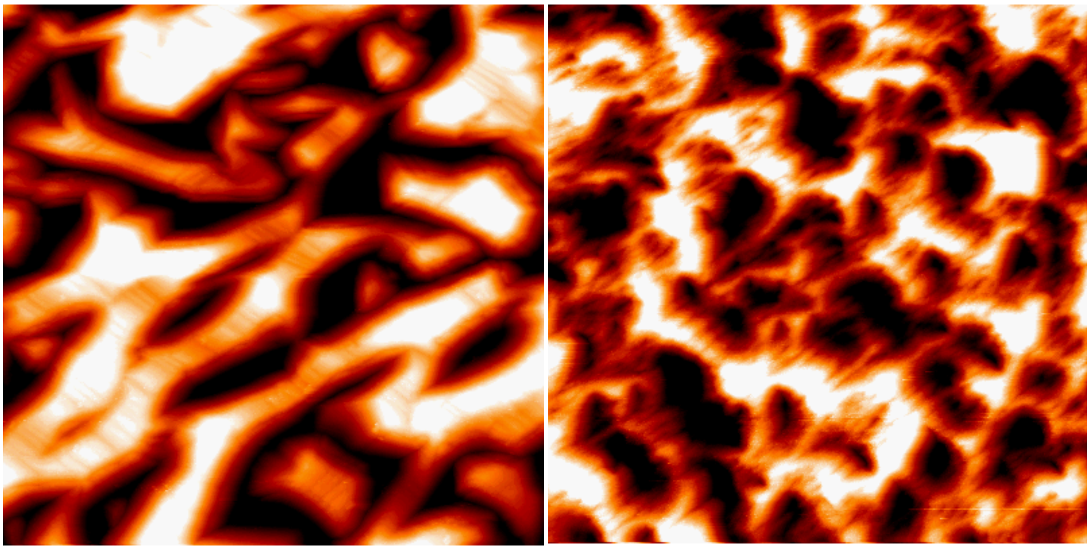

*Fig. 1 (1.4*1.4)µm^2 STM images of 200nm thick GaP epilayers grown on Si(001) nominal surface (left) and on a 6°-off Si(001) vicinal surface (right). Antiphase domains are still observed on the nominal Si substrate while antiphase boundary annihilation was achieved on the vicinal substrate.*

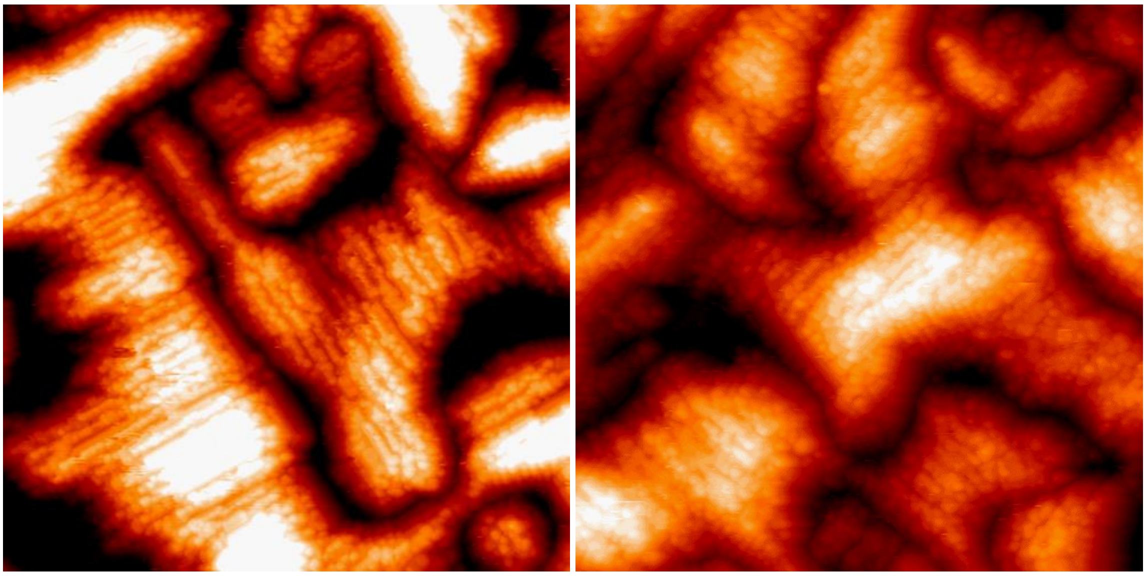

*Fig. 2 (60*60)nm*^{2} *STM images of 10nm thick GaP epilayers grown on Si(001) nominal surface (left) and on a 6°-off Si(001) vicinal surface (right). At this growth stage, antiphase domains are present for both substrates. Atomically resolved images evidence various terminal facets for the emerging antiphase domains on nominal and vicinal Si(001) substrates.*

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Bibliography

[1] K. Volz et al., *J. Cryst. Growth*, **315**, 37-47 (2011).
[2] Herbert Kroemer, *J. Cryst. Growth*, **81**(14), 193-204 (1987).
[3] A.C. Lin, M.M. Feyer, J.S. Harris, J. Cryst. Growth, 363 : 258-263, 2013.

Effect of a normal stress on the shear-coupled grain boundary migration

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Grain boundary (GB) migration occurs in stressed nanocrystalline materials(grains sizes <100 nm) as an alternative vector of plasticity compared to the usual dislocation activity. The shear-coupled GB migration, the expected most efficient GB based mechanism, couples the GB motion to an applied shear stress [1,2]. Stresses on GB in polycrystalline material have however seldom a unique pure shear component.

The influence of a normal stress on the shear coupled GB migration is investigated in a copper bicrystal studying the Σ13 (320) GB. Using molecular dynamic simulation, we theoretically show that the yield shear stress inducing the GB migration strongly depends on the applied normal stress. Moreover, we show that the application of a normal stress may induce a modification of the observed GB migration mechanism (mode). We evidence the existence of the $[010]$ GB migration mode, theoretically predicted but never observed. We characterize this mode both structurally and energetically using the Nudeg Elastic band Method.

Bibliography

[1] Rajabzadeh, A.; Mompiou, F.; Legros, M. and Combe, N. Phys. Rev. Lett., 110, 265507 (2013)
[2] Combe N.; Mompiou, F.; Legros, M. Phys. Rev. B, 93, 024109 (2016)

Poster 9

Structure And Growth Mechanism Of Single Layer And Multi-Layer Silicene

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The last years have seen a growing interest in the research and characterization of 2D materials, due to their interesting and exotic properties. In particular, for free-standing silicene, the 2D allotrope of silicium, DFT simulations predicts the existence of Dirac cones in the electronic structure. This makes silicene an appealing candidate for microelectronic devices. Experimentally, 2D Si arrangements have been reported on several substrates, among which Ag(111) is by far the most thoroughly studied.

Silver was thought to weakly interact with the Si sheet; however joint experimental studies and density functional theory (DFT) simulations have shown a non-negligible interaction [1]. The various structures observed are predicted to be buckled honeycomb lattices. The electronic band structures computed are however far from the one of free-standing silicene and depend on the precise atomic positions. In order to decouple the Si layer from the Ag substrate, researchers have tried to synthetize multi-layer silicene. The structure of the films obtained is however highly controversial. Whereas some claim that it corresponds to silicite, a graphite analogue for Si, others affirm that it corresponds to diamond-like Si covered with Ag.

Combining grazing incidence X-ray diffraction (GIXD) and DFT simulations we managed to give an accurate structure model of the (4x4) reconstruction of silicene on Ag(111), putting in evidence the role of the substrate relaxation[3]. The silicene layer shows a buckling of 0.76 Å and the relaxation of the substrate results in a vertical displacement of the Ag atoms at the interface layer of about 0.25 Å. The relaxation decreases exponentially in the layers deeper beneath the surface.

Regarding the synthesis of multi-layer silicene, we have performed real-time GIXD and scanning tunneling microscopy (STM) during Si evaporation. Diffraction results demonstrate that the film has a diamond-like structure, Fig. 1, with a large density of stacking faults. Comparing the experimental structure factors with the theoretical ones obtained from models known in the literature, we conclude that the surface is terminated with the $(\sqrt{3}\text{x}\sqrt{3})$ Ag/Si(111) reconstruction, showing the surfactant behavior of Ag atoms in the growth of Si/Ag(111). This behavior is also confirmed by real-time STM. Moreover, as for the single layer growth [1], the thick film growth is characterized by Si/Ag atomic exchanges. Indeed, the formation of thick islands terminated with the $(\sqrt{3}\text{x}\sqrt{3})$ reconstruction Fig 2a-c is accompanied by the release of Ag atoms that intercalate beneath the remaining silicene layer, Fig. 2b. This shows that Si islands grow in the Ag bulk.

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Bibliography

1. R. Bernard et al., *Phys. Rev. B* **92** (2015) 045415
2. Y. Borensztein et al., *Phys. Rev. B* **92** (2015) 155407
3. A. Curcella et al., *Phys. Rev. B* ***94*** *(2016)* 165438

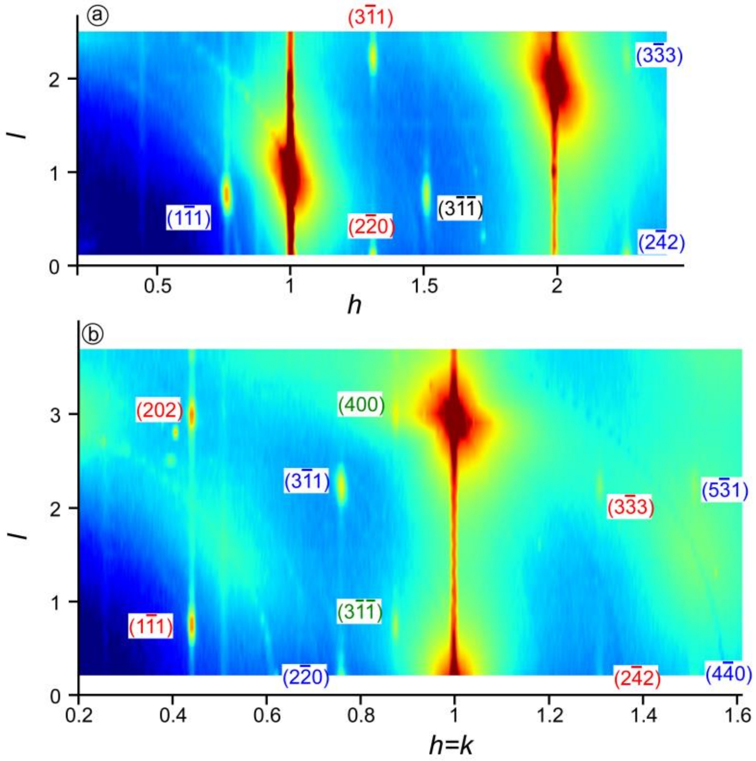

Fig 1.: *Maps of the intensity diffracted by 8 ML Si evaporated on Ag(111) at* $T_{growth} = 520\mathrm{K}$ *Measurements are performed at the same temperature. a) for* $k = 0$, *b) for* $h = k$. *The color scale is logarithmic and ranges from blue to red on 6 decades. The indexed spots belong to diamond-like silicon with four orientations (corresponding to blue, red, green and black labels).*

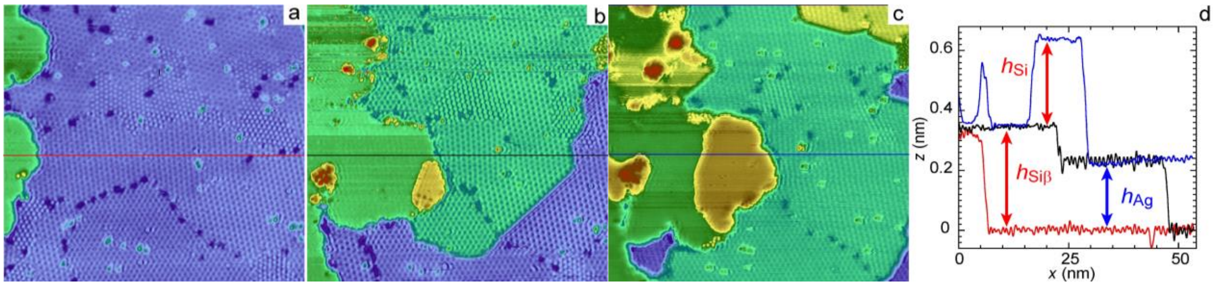

Fig. 2*: a) silicene layer (blue) and* 2^{nd} *Si layer (green). b)* 2^{nd} *Si layer (green) and silicene layer lifted of one Ag step (structured green). c)* 3^{rd} *layer appearing (yellow) with the height of one Si plane. d) Height profiles along the lines in a), b) and c)*

Ga on SiO_2 as catalyst for nanowire growth: Investigation by x-ray photoelectron spectroscopy

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GaAs nanowires (NWs) are studied in view of applications in optoelectronic and photonic devices. In our case, GaAs NWs are grown by Molecular Beam Epitaxy using the Vapor-Liquid-Solid method, using Ga as catalyst (auto-catalyzed growth) in order to avoid Au, which endangers optoelectronic performances. Typically, this auto-catalyzed growth is performed directly on Si substrates without any removal of the native oxide [1-2] or on a SiO_2 layer previously deposited on GaAs wafers [3]. This oxide layer is thought to favor droplet formation with enhanced chemical potential compared to the Si layer. However, despite this strong interest for the Ga/SiO_2/Si system, the mechanism of the droplet formation and the nature of the chemical interaction between the metal and the substrate is not yet fully understood.

The Ga-Si system is rather different from the Au-Si one. First, unlike gold, gallium is liquid at low temperature (about 30 °C). Second, the eutectic $Ga_{1-x}Si_x$ contains a very small amount of silicon: only 5.10^{-8} % vs 18.5 % in $Au_{1-x}Si_x$ eutectic, for bulk materials. Third, Ga can be easily oxidized and most Ga oxides are stable: for example, thermal and ozone Ga oxides cannot be removed below 582 ± 1 °C and 638 ± 1°C, respectively. However, it has been shown that the removal of native oxides from GaAs wafers can be obtained at lower temperature by converting stable Ga_2O_3 to volatile Ga_2O by exposure to Ga metallic flux.

Using atomic force microscopy and X-ray Photoelectron Spectroscopy (XPS) we have studied the effect of the growth temperature (from 50 °C to 700 °C) on the formation of the Ga droplets, and the annealing temperature. Our results show that the size and density of Ga droplet can be controlled by the growth temperature. This initial configuration of the Ga droplets is of special interest as it determines NWs dimensions and repartition. The evolution of the Si2p, O1s, Ga3d and As3d core levels as a function of the growth temperature allows for displaying interfacial Ga oxides in association with a dewetting phenomenon. Finally, the mechanism of formation of pinholes catalyzed by droplets in the SiO_2 film is discussed.

References

[1] Colombo, C., Spirkoska, D., Frimmer, M., Abstreiter, G. & Fontcuberta I Morral, A. Ga-assisted catalyst-free growth mechanism of GaAs nanowires by molecular beam epitaxy. *Phys. Rev. B - Condens. Matter Mater. Phys.* **77,** 2–6 (2008).

[2] Jabeen, F., Grillo, V., Rubini, S. & Martelli, F. Self-catalyzed growth of GaAs nanowires on cleaved Si by molecular beam epitaxy. *Nanotechnology* **19,** 275711 (2008).

[3] Fontcuberta I Morral, A., Colombo, C., Abstreiter, G., Arbiol, J. & Morante, J. R. Nucleation mechanism of gallium-assisted molecular beam epitaxy growth of gallium arsenide nanowires. *Appl. Phys. Lett.* **92,** (2008).

C_{60} Thin Films On Co(0001) : A Structural Study To Understand Magnetic Properties

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Due to their long spin relaxation time and the possibility to functionalize them at will, the use of organic materials is a promising way for the development of new spintronic applications, especially for the realization of vertical spin valves in which the non-magnetic spacer is made of an organic film. Promising results have already been obtained on C_{60} based spin-valve presenting a magneto-resistance at room temperature [Gobbi2011]. But, Surprisingly, the magnetic properties of thin Cobalt films can be drastically modified by the deposition of C_{60} molecules [Bairagi2015]. Thus, it is crucial to understand how the interface structure affects magnetic properties in order to improve spintronic devices.

To determine the structure of the interface and its link with magnetism, we are studying the structure of a model sample of C_{60} thin films on a Co(0001) single crystal by surface x-ray scattering and scanning tunneling microscopy, two complementary techniques giving reciprocal and real space information respectively. Ab-initio calculations complete the panel of tools used for the investigations. Our studies on C_{60}/Co(0001) monolayer structure, before and after annealing (Fig. 1), evidence a 4x4 reconstruction of the C_{60} on Cobalt, as well as an irreversible structural transition in temperature while annealing. We were also capable of growing a highly crystalline C_{60} fcc crystal on Co(0001).

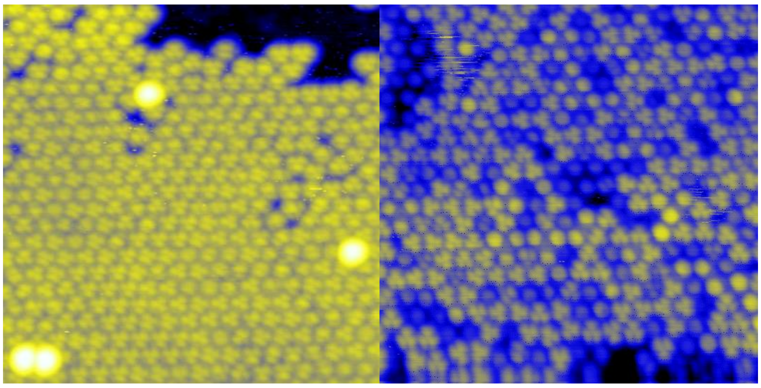

Fig. 1: *(20x20) nm² STM images at 2V of a C_{60} monolayer on Co(0001) before (left image) and after annealing up to 300°C (right image). One can see that after annealing C_{60} can have two different apparent heights within a domain. Thanks to GIXD measurements, we can conclude that it is due to the creation of Cobalt vacancies under some C60 molecules.*

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Bibliography

[Bairagi2015] K. Bairagi et al., *Phys. Rev. Lett.*, **114**, 247203 (2015)
[Gobbi2011] M. Gobbi et al., *Adv. Mater.*, **23**, 1609-1613 (2011)

Photoelectron Energy Loss Spectroscopy : Retrieval of the Energy Loss Function by a Fourier Transform method

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Photoelectron Energy Loss Spectroscopy (XPS-PEELS) is a non-destructive tool which extends analytical capabilities of XPS (chemical composition obtained from core level peak intensities) to detailed insight in electronic properties (near-surface dielectric function derived from kinetic energy losses resulting essentially from plasmon excitation).[1,2]

Using standard spectrometers without monochromatized X-ray source, the intensity measured over a broad kinetic energy range results from convolution of four spectral distributions: (i) X-ray source, (ii) Gaussian broadening of photoelectron analyzer, (iii) theoretical photoemission line shape and (iv) multiple plasmon loss probability. The latter being a self-convolution of the differential inverse inelastic mean free path, a Fourier transform method is proposed to retrieve the effective energy loss function and the dielectric function of the solid.

This method is applied to Aluminum single crystal Al(001) where the photoemission line shape can be computed accurately beyond the Doniach-Sunjic approximation to take into account the density of states distribution near the Fermi level. Adjustable parameters consist in broadening energy Γ which results from the core hole lifetime and creation rates for intrinsic and extrinsic plasmon excitation. After correction for surface plasmon excitations, the effective dielectric function $\varepsilon(\omega, \boldsymbol{q})$ of Al(001) differs from the optical limit $\varepsilon(\omega, \boldsymbol{q} = 0)$ and is well described by the Lindhard and Mermin dispersion relations.

Acknowledgements

Funding and grants: CNPq, Rennes Métropole.

Bibliography

[1] Derivation of the near-surface dielectric function of amorphous silicon from photoelectron loss spectra D. David *et al.*, *J. Non-Cryst. Solids* **358**, 2019-2022 (2012).

[2] Derivation of dielectric function and inelastic mean free path from photoelectron energy-loss spectra of amorphous carbon surfaces. D. David *et al.*, *Appl. Surf. Sci.* **387**, 1125-1139 (2016).

Ballistic Electron Emission Microscopy (BEEM): a local and quantitative probe to study the quality of Au/hexadecanethiols/GaAs(001) heterostructures by imaging buried interfaces and drawing local energy band alignments

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In molecular electronics, metallic top-contact deposition on organic molecular monolayer(OML)/semiconductor hybrid heterostructures is still a critical issue, leading to metal penetration through the molecules and monolayer's damage. Here, we report on the potentialities of BEEM (technique derived from the Scanning Tunneling Microscopy one) to quantitatively characterize the local transport properties at the nanometer scale and the degree of this penetration through the organic monolayer on Au-hexadecanethiols-GaAs(001) heterostructures. At room temperature, BEEM imaging mode provides mapping of the local hot-electron transmission and demonstrates pronounced inhomogeneities at buried interfaces. Using local transport measurements in spectroscopy mode, local barrier heights and the BEEM current attenuation are measured in each area and compared with the well-known Au/GaAs(001) Schottky contact [1-2]. In order to minimize the degree of gold penetration and obtain homogeneous heterojunctions, an alternative top-contact deposition method is used, based on Buffer-Layer Assisted Growth (BLAG) [3]. BEEM results obtained on such heterostructures are discussed and compared with macroscopic measurements [4]. In this framework, BEEM further appears as a highly powerful and complementary tool to commonly used spatially averaged diffusive transport experiments, essential for understanding such hybrid heterostructures of major interest for molecular electronics.

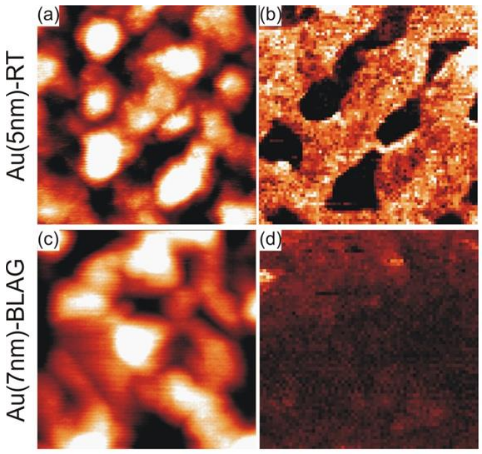

Figure 1: *50x50nm² STM images of Au surfaces deposited on hexadecanethiols/GaAs(001) (a) at room temperature and (c) by BLAG method. (b) and (d) Corresponding BEEM images of buried interfaces.*

Bibliography

Investigation of the Schottky barrier with ab-initio calculation and the real space multiple scattering BEEM.

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The Ballistic Electron Emission Microscopy (BEEM) [1,2] is a powerful technique to investigate interfaces of bulk systems. The experimental setup of BEEM is basically based on the Scanning Tunneling Microscope (STM), so that the spatial resolution is very high. When we cover the surface of a semiconductor with a metal thin layer, Schottky barrier is generated at the interface and behaves as an additional barrier to the tunneling barrier from the tip to the sample. Due to these two barriers, a hot electron, whose kinetic energy is about 1 eV, is created and travels in the bulk "ballistically", namely the scattering should be elastic without loss by excitons or plasmons. (See Fig. 1)

Theoretical studies for BEEM have been implemented by means of k-space band calculation [3] and tight-binding method [4,5]. k-space band study is very convenient to interpret the phenomena in qualitative way, however the diffusion process of the hot electron in real space is not be able to considered. While the tight binding method can treat the transport problem in the real space, the approximation is not suitable for the long traveling delocalized state due to the use of localized basis. Multiple scattering theory gives a good representation for a large-scale system within real space formalism. [6,7] We applied the full potential Multiple Scattering theory [8,9] to BEEM (MSBEEM) to describe the transport phenomena accurately.

For the first step of practical calculations, we performed ab-initio calculations of Schottky barrier of Au/GaAs by VASP code [10]. For a study of band gap of a semiconductor system, we used the HSE exchange functional [11]. We have obtained very good agreement with experimental values for the Schottky barrier. The calculated charge density will be used for MSBEEM calculation via an interface ES2MS [12].

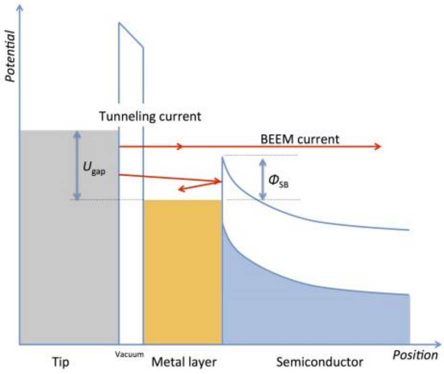

Fig. 1*: A scheme of BEEM current within an STM setup. Electrons on the tip is transported by tunneling effect to the metallic surface, then they meet Schottky barrier at the interface. Since the electrons have just about 1 eV of kinetic energy, they can be ballisticaly transported in the semiconductor.*

Acknowledgements

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Bibliography

[1] W. J. Kaiser and L. D. Bell, *Phys. Rev. Lett*. **60**, 1406 (1988).
[2] L. D. Bell and W. J. Kaiser, *Phys. Rev. Lett*. **61**, 2368 (1988).
[3] M. Hervé, S. Tricot, Y. Claveau, G. Delhaye, S. Di Matteo, P. Schieffer, and P. Turban, *Appl. Phys. Lett.* 103, 202408 (2013).
[4] P.L. de Andres, F.J. Garcia-Vidal, K. Reuter, and F. Flores, *Prog. in Surf. Sci.* 66, 3 (2001).
[5] Y. Claveau, arXiv:1501.06458[cond-mat.mes-hall] , PhD thesis (2014).
[6] J. Xu, K. Hatada, D. Sébilleau and L. Song, arXiv:1604.04846[quat-ph].
[7] J. Xu, P. Krüger, C. R. Natoli, K. Hayakawa, Z. Wu, and K. Hatada, *Phys. Rev. B* 92, 125408 (2015).
[8] K. Hatada, K. Hayakawa, M. Benfatto and C. R. Natoli, *Phys. Rev. B* 76, 060102(R) (2007).
[9] K. Hatada, K. Hayakawa, M. Benfatto and C. R. Natoli, *J. Phys. Cond. Matt.* 22, 185501 (2010)
[10] G. Kresse, D. Joubert, Phys. Rev. B **59** (3), 1758 (1999).
[11] J. Heyd, G. E. Scuseria, and M. Ernzerhof, *J. Chem. Phys.* **118**, 8207 (2003).
[12] J. Xu, C. R. Natoli, P. Krüger, K. Hayakawa, D. Sébilleau and L. Song and K. Hatada, *Comp. Phys. Comm.* **203**, 331 (2016)

Towards ferromagnetic resonance in skyrmionic spin structure using a spin polarized scanning tunneling microscopy

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In this communication we report on the experimental development of a new technique to measure locally ferromagnetic resonance signal with a SP-STM. The concept of this experiment, inspired by the spin torque diode effect [2], is based on the homodyne detection of the resonance signal in the sample. A continuous radio-frequency (rf) voltage (up to 3 GHz) is mixed to the bias voltage of the STM. If there is a magnetisation precession under the STM tip, the tunneling conductance will be modulated at the resonance frequency. When the high frequency signal mixed to the tunneling junction reach the resonance frequency of the precession, the tunneling current is rectified. This rectified current, measurable by conventional STM transimpedance amplifier correspond to a ferromagnetic resonance signal in the sample.

The experiment is carried out in a home-built STM operated at 4.2 K under ultra-high vacuum. The continuous electromagnetic wave is provided by a rf generator and sent to the STM sample stage through a 50 Ω transmission line [3]. The system we choose to study with this method is the skyrmionic spin structure Fe(0.4ML)/Ir(111) [4]. Figure 1(a) display a SP-STM topography revealing the magnetic structure. On several position of the spin structure, the additional DC component of the tunnelling current generated by the introduced microwave is recorded versus the rf-frequency (figure 1(b). This experiments allowed to reveal a signal at 615 MHz. Figure 1(c) and (d) present the lateral dependency of amplitude (figure 1(c)) and frequency position (figure 1(d)) of the peak. The spatial dependency on the signal is directly correlated to spin structure. The origin of this feature can be a ferromagnetic resonance.

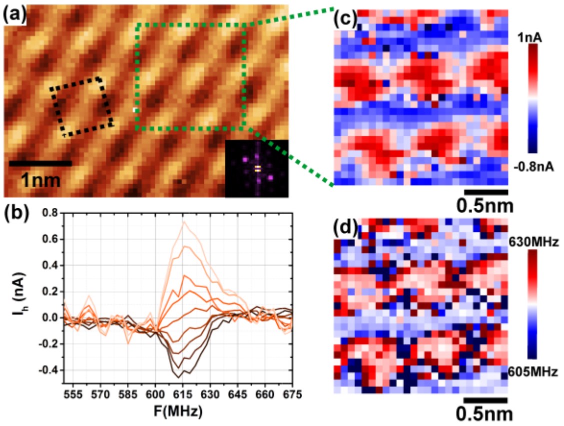

Fig. 1: *(a) SP-STM topography revealing the skyrmionic spin structure on Fe(1 ML)/Ir(111) – (b) Additional DC component of the tunneling current versus the rf frequency recorded on several location of the spin structure – Spatial variation of the amplitude (c) and frequency position (d) of the peak within an area of 2x2nm^2 of the skyrmionic lattice.*

Bibliography

[1] R. Wiesendanger, Rev. Mod. Phys. **81**, 1495 (2009)
[2] A. A. Tulapurkar, Y. Suzuki, A. Fukushima, H. Kubota, H. Maehara, K. Tsunekawa, D. D. Djayaprawira, N. Watanabe and S. Yuasa, Nature **438**, 339 (2005)
[3] M. Hervé, M. Peter, and W. Wulfhekel, Appl. Phys. Lett. **107**, 093101 (2015)

Poster 15

[4] S. Heinze, K. von Bergmann, M. Menzel, J. Brede, A. Kubetzka, R. Wiesendanger, G. Bihlmayer and S. Blügel, Nature Physic **7**, 713 (2011)

Non collinear magnetism in a Co monolayer probed by spin resolved scanning tunnelling microscopy

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In magnetic thin films, different magnetic orders can be observed. The most common ones are the ferromagnetic and antiferromagnetic order. These orders are stabilized by the Heinsenberg exchange interaction leading to a parallel or antiparallel alignment of neighboring spins in the crystal. When the structure of the crystal is noncentrosymmetric (or when the inversion symmetry is broken by a surface or an interface), a noncollinear spin interaction, called the Dzyaloshinskii-Moriya interaction (DM), competes with the Heinsenberg exchange interaction. This competition can lead, in some case, to the stabilization of complex spin textures such as spin spiral or skyrmion.

We report here on the characterization of a non collinear magnetic structure in Co(1 ML)/Ru(0001) with spin polarized scanning tunneling microscopy (SP-STM). 1.2 ML of cobalt was epitaxially grown on a clean Ru(0001) surface at 180°C. At this deposition temperature, the 1st cobalt monolayer forms a wetting layer in hcp stacking on the Ru(0001) substrate [1]. The experiment was carry out in a home built STM operated at 4.2 K under ultra-high vacuum. SP-STM measurement reveal the presence of a chiral spin spiral of 50 nm periodicity in the 1st monolayer as a ground state (fig. 1.a). Under magnetic field skyrmion can be stabilized (fig. 1.b).

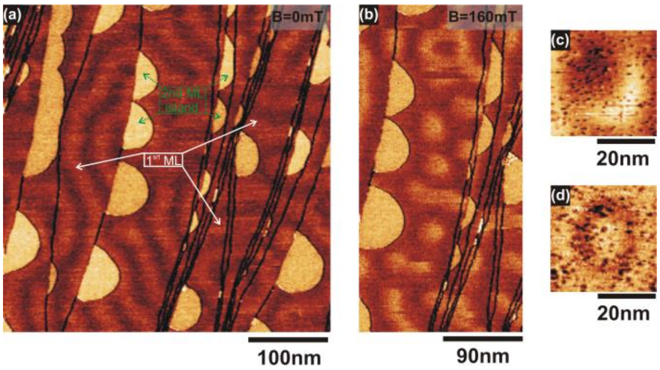

Fig. 1: *conductance map recorded on the Co monolayer using an out of plane spin polarized tip, revealing (a) a spin spiral at zero magnetic field and (b) the stabilization of magnetic skyrmion under magnetic field – Magnified conductance map of a skyrmion using an in-plane spin polarized tip (c) and a non-spin polarized tip. The image realized with a non-spin polarized reveal a tunnelling anisotropic magnetoresistance of 2 %.*

Bibliography

[1] F. El Gabaly, J. M. Puerta, C. Klein, A. Saa, A. K. Schmid, K. F. McCarty, J. I. Cerda and J. de la Figuera, New Journal of Physics **9**, 80 (2007).

Photoelectron Diffraction Modeling: Plasmon Effect in Pt and Bi

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We report on the multiple scattering modeling of photoelectron diffraction to investigate two different effects. Photoelectron diffraction is a technique derived from photoemission which is very much used to characterize the crystallographic structure of materials. It is generally modeled using a multiple scattering approach [1] . Here, we use the MsSpec code [2] in order to compute the photoelectron diffraction angular modulations. As is well-known, these angular variations are strongly dependent of the angular momentum of the initial state in the low kinetic energy regime while they are initial state-independent for high kinetic energies [3]. Therefore, we propose first here, to use this effect as a way to reveal the nature of the experimental feature nearby the 4f core-level peak for Pt and Bi metals which is supposed to be either 5s or plasmon peak. The probabilities of shake-effects (simultaneous excitation of 4f-electron and additional electron – 5d, 6s, 6p) were also calculated in the approximation of sudden perturbations [4].

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No. PIRSES-GA-2012-317554

Bibliography

[1] D. Sébilleau, R. Gunnella, Z.-Y. Wu, S. Di Matteo and C. R. Natoli. *“Multiple-scattering approach with complex potential in the interpretation of electron and photon spectroscopies”*, J. Phys.: Condens. Matter **18**, R175-R230 (2006)
[2] D. Sébilleau, C. R. Natoli, G. M. Gavaza, H. Zhao, F. Da Pieve and K. Hatada, *“MsSpec-1.0: A multiple scattering package for electron spectroscopies in material science”*, Comp. Phys. Comm. **183**, 1567-2579 (2011)
[3] D. Naumović, A. Stuck, T. Greber, J. Osterwalder, and L. Schlapbach. *“Full-hemispherical photoelectron-diffraction data from Cu(001): Energy dependence and comparison with single-scattering-cluster simulations”*, Phys. Rev. B **47**, 7462 (1993)
[4] V. P. Sachenko, and V. F. Demekhin, Satellites of X-Ray Spectra Zh. Eksperim. i Teor. Fiz., **49**, 765-769 (1965)

Poster 18

Band Alignments in Fe/Graphene/Si(001) Junctions Studied by X-ray Photoemission Spectroscopy

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The control of tunnel contact resistance is of primary importance for semiconductor-based spintronic devices [1]. This control is hardly achieved with conventional oxide-based tunnel barriers due to deposition-induced interface states. Manipulation of single 2D atomic crystals (such as graphene sheets) weakly interacting with their substrate might represent an alternative and efficient way to design new heterostructures for a variety of different purposes including spin injection into semiconductors [2].

We studied by x-ray photoemission spectroscopy the band alignments and interface chemistry of iron–graphene-hydrogenated passivated silicon (001) surfaces for a low and a high n-doping concentration. We found that the hydrogen passivation of the Si(001) surface remains efficient even with a graphene sheet on Si(001) surface. For both doping concentrations the semiconductor is close to flat-band conditions which indicates that the Fermi level is unpinned on the semiconductor side of the Graphene/Si(001):H interface [Fig. 1]. When iron is deposited on the graphene/Si(001):H structures the Schottky barrier height remains mainly unaffected by the metallic overlayer with a very low barrier height for electrons, a sought-after property in semiconductor based spintronic devices.

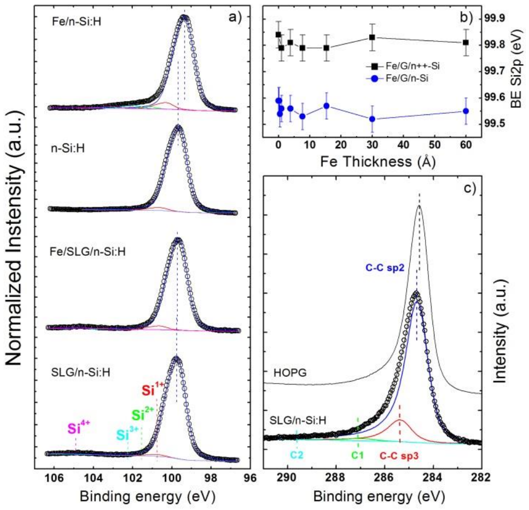

Fig. 1*: **(a) XPS spectra of Si2p core level for n-Si:H and SLG/n-Si:H before and after deposition of 15Å Fe. (b) Binding energy of the Si bulk component of the Si2p$_{3/2}$ core level for SLG/n-Si and n++-Si as a function of iron thickness. (c) XPS spectra of C1s core level of HOPG and SLG/n-Si:H.***

Bibliography

[1] A. Fert and H. Jaffrès, Phys. Rev. B **64**, 1 (2001).
[2] O. M. J. van 't Erve, a L. Friedman, E. Cobas, C. H. Li, J. T. Robinson, and B. T. Jonker, Nat. Nanotechnol. **7**, 737 (2012).

Effet de la transition de phase structurelle sur la structure de bande résolue en k de la pérovskite hybride organique-inorganique $CH_3NH_3PbI_3$

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Les pérovskites hybrides organiques-inorganiques d'halogénure de plomb sont devenues des matériaux prometteurs pour le photovoltaïque en raison de leur rendement élevé de conversion d'énergie solaire, ainsi que de leur fabrication à basse température et à bas coût en solution.[1,2,3] Une des performances la plus remarquables (22%[4]) est celle des pérovskites d'halogénure de plomb méthylammonium ($CH_3NH_3PbI_3$, MAPI). L'optimisation des performances au-delà nécessiterait d'une meilleure compréhension de la structure de bande électronique, qui est demeurée jusqu'à présent difficile à déterminer expérimentale. De plus, l'effet de la transition de phase structurelle sur la structure de bande dans la plage de température de fonctionnement des cellules solaires doit être éclairci. Ici, nous présentons la première détermination expérimentale de la structure de bande de MAPI avec résolution en k. Nos résultats montrent que la périodicité électronique dans la phase tétragonale de MAPI (inférieure à 50 ° C) correspond à celle de la phase cubique au haute température. Cela explique l'insensibilité des cellules solaires dans la gamme habituelle des températures de fonctionnement malgré la transition structurelle de tétragonale-cubique.

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Bibliography

[1] Burschka, J., Pellet, N., Moon, S.-J., Humphry-Baker, R., Gao, P., Nazeeruddin, M.K., & Grätzel, M., Nature **499**, 316 (2013).
[2] Jeon, N.J., Noh, J.H., Kim, Y.C., Yang, W.S., Ryu, S., & Seok, S.I., Nature Materials **13**, 897 (2014).
[3] Lee, M. M., Teuscher, J., Miyasaka, T., Murakami, T. N. & Snaith, H. J., Science **338**, 643-647 (2012).
[4] Yang WS, Noh JH, Jeon NJ, Kim YC, Ryu S, Seo J, Seok SI., Science **348** (6240), 1234–1237 (2015).

Molecular Magnets: From the single molecule to the 3D self-assembly

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Real materials are not pure. Impurities can bring to light beautiful physics: they are crucial, for instance, in achieving the functionality of doped semiconductors. In general, the response of a physical system to disorder can lead to elucidating details of its electronic properties.

In particular, magnetic impurities in superconductors are able to reduce the superconducting BCS gap and may ultimately destroy the superconducting state. A single classical spin of a magnetic atom is able to create a localized bound state within the BCS gap (Shiba state). Consequently, a finite concentration of magnetic impurities can form an impurity band within the superconducting gap. The spatial decay of these bound states critically depends on the dimensionality of the system, i.e. it increases by reducing the dimensionality [1].

The Pb/Si(111) system is one of the most remarkable examples of 2D superconductors in which superconductivity arises in a single atomic plane of Pb [2,3]. The use of magnetic phthalocyanines as magnetic impurities, by evaporating them on the Pb monolayer (UHV conditions), might lead to some advantages. For instance, their self-assembly properties together with substrate anisotropy allow tailoring both 1D and 2D arrays of magnetic centres [4]. For this reason, it is very intriguing to investigate the superconducting substrate-mediated interaction [5] between two Shiba states, which could be used as building block in order to coherently couple distant magnetic molecules. Such long-range coupling of magnetic impurities through a 2D superconductor could be an efficient way to create new topological phases.

Acknowledgements

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Bibliography

*[1] G. Ménard et al. Nature Physics **11**, 1013 (2015)*
*[2] T. Zhang et al. Nature Physics **6**, 104 (2010)*
*[3] C. Brun et al. Nature Physics **10**, 444 (2014)*
*[4] Gargiani et al. Phys. Rev. B **87**, 165407 (2013)*
*[5] Braunecker, et al. Phys. Rev. Lett. **111**, 147202 (2013)*

3D GaP nucleation as the origin of the antiphase boundaries

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The monolithic integration of GaP grown by MBE on Si(001) is very promising for photonics but crystal defects at GaP/Si interface can affect the GaP-based photonic device performances. We have shown by TEM the influence of the first layer of the Si surface on the quality of the heteroepitaxial GaP[1]. In this work, the GaP/Si 3D growth mode is described in terms of surface/interface energies computed by ab-initio calculations. We explain the origin of antiphase boundaries (APBs) by the initial GaP 3Dislands coalescence at the very beginning of the growth [Fig. 1]. We then highlight the impact of the APDs on the surface morphology thanks to the atomic force microscopy, scanning tunneling microscopy and TEM[2].

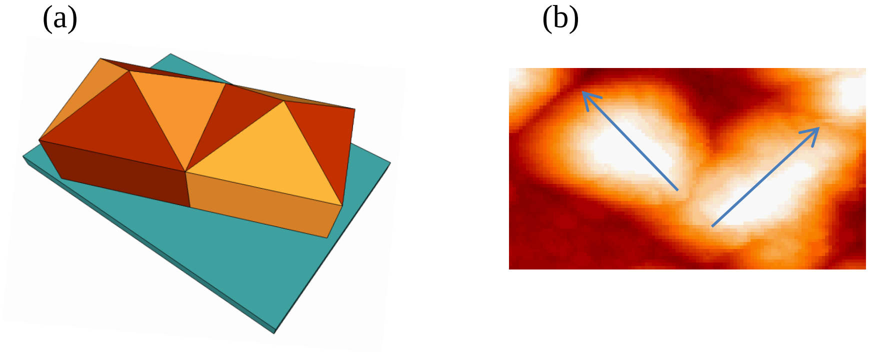

Fig. 1*: 3D coalescence of two GaP antiphase domains island (a) graphic representation and (b) STM image*

Acknowledgements
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Bibliography

[1] Y. Wang *et al.*, ‘Abrupt GaP/Si hetero-interface using bistepped Si buffer’, *Appl. Phys. Lett.*, vol. 107, no. 19, p. 191603, Nov. 2015.

[2] A. C. Lin, M. M. Fejer, and J. S. Harris, ‘Antiphase domain annihilation during growth of GaP on Si by molecular beam epitaxy’, *J. Cryst. Growth*, vol. 363, pp. 258–263, Jan. 2013.

Electrochemical, electrical and physical studies of the electrical double layer at the solid (304L) / liquid (NaCl solution) interface

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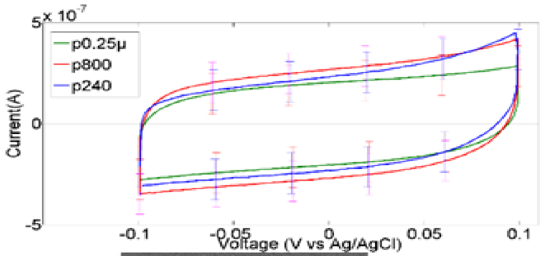
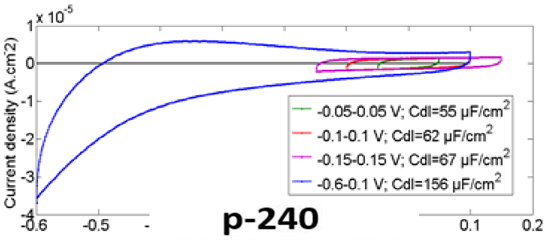
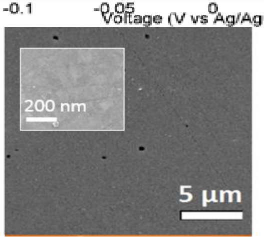
When a solid is immersed into a liquid solution, whatever their nature (dielectric or conductive), physicochemical phenomena lead to polarize a solid—liquid interface. Two zones with opposite sign of charge appear, one in the solid and the other in the liquid, forming thus the electric double layer (EDL). Various electrical and electrochemical methods have been combined in this work to determine the characteristics of the EDL at the interface between polycrystalline austenitic stainless steel 304L immersed in NaCl aqueous solution (0.01M, 0.1M and 1M). Its effective capacity $\mathbf{C_{dl}}$ was determined by both cyclic voltammetry (CV), for various electric fields and with different voltage scan speeds **[1],** and by electrochemical impedance spectroscopy (EIS) using an electrical equivalent circuit (EEC) **[2].** Another electrical method by flow electrification allows to measure the space charge density $\boldsymbol{\rho_w}$ at the wall **[3]**. The results demonstrate that the double layer capacitance depends mainly on the concentration of the electrolyte and the applied potential [

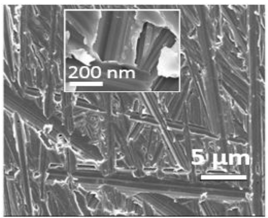
Fig. 1] and that the space charge density is also proportional to the concentration. The influence of the surface roughness (various preparations with SiC papers 240 or 800, or with diamond paste 0.25 µ) on the EDL was then studied by EIS and CV. It appeared that on a macroscopic scale, the roughness has a little influence on the capacity of the EDL at the 304L / NaCl (0.01M) interface [

Fig. 1]. These results were discussed in regards with physical and chemical characterisations operated by XPS, MEB, AFM and WLI.









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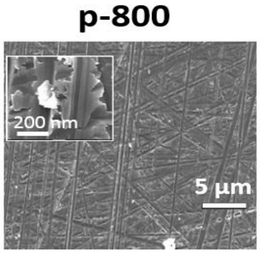

Fig. 1*: Electrochemical measurement and physical characterization of the roughness influence on the 304L / NaCl(0.01M) interface*

Bibliography

[1] Allen J. Bard, Electrochemical Methods. Fundamentals and Applications (1983)
[2] G.J. Brug, A.L.G. van den Eeden, J. Electroanal. Chem 176, p275 (1984)
[3] Thierry Paillat, Eric Moreau, Gérard Touchard, Journal of electrostatics 53, p171 (2001)

Interaction of native and dry-heated ovotransferrin with *E.coli* lipopolysaccharide monolayer

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The constant development of bacterial multiresistance to antibiotics and nosocomial infections is a permanent concern towards the public health authorities. In addition, the development of new antibiotics is constantly faced with bacterial adaptive strategies to establish a resistance process. Otherwise, some peptides/proteins possess an antibacterial activity leading to limit resistance development. They thus appear to be an alternative to face the bacterial resistance process and provide an opportunity for the current research.

Ovotransferrin is an egg white protein with an antimicrobial broad-spectrum activity. Especially, *Escherichia coli* is sensitive to the ovotransferrin which disrupts the bacterial outer membrane [1, 2]. The dry-heating ovotransferrin treatment modifies its properties with consequences on its antibacterial activity. In order to understand the mechanisms underlying the antibacterial activity of native ovotransferrin, and the effect of dry-heating on its activity, it is necessary to investigate the interactions of the protein with the *E. coli* outer membrane.

In this study, these interactions were characterized by using an *in vitro* membrane model which is a lipopolysaccharide monolayer at the air-water interface. Protein-membrane interactions were examined by ellipsometry, tensiometry and imaging techniques (Brewster Angle Microscopy and Atomic Force Microscopy).

The results showed that ovotransferrin had an affinity to lipopolysaccharides and inserted into the monolayer, the delta signal and the surface pressure increased. Therefore, the AFM images showed an increase of the monolayer roughness and changes on the lipopolysaccharide organization. Dry-heating enhanced the ovotransferrin affinity to lipopolysaccharides and increased its membrane activity. Moreover, this affinity was impacted by the molecular state of lipopolysaccharides which can be modulated changing the surface pressure.

The insertion into *E. coli* outer membrane and the disorganization of lipopolysaccharides due to ovotransferrin could explain its antibacterial activity. Otherwise, dry-heating appeared as a simple way to enhance the ovotransferrin antibacterial activity.

[1] P. Valenti, G. Antonini, C. Von Hunolstein, P. Visca, N. Orsi, and E. Antonini, "Studies of the antimicrobial activity of ovotransferrin," *International journal of tissue reactions*, vol. 5, pp. 97-105, 1982.

[2] O. Aguilera, L. M. Quiros, and J. F. Fierro, "Transferrins selectively cause ion efflux through bacterial and artificial membranes," *FEBS Letters*, vol. 548, pp. 5-10, 2003.

Effets de ségrégation de surface et d'alliage dans les nanoparticules Pt-Ag

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L'intérêt porté aux nano-objets, notamment aux nanoalliages, est dû aux nombreuses propriétés physico-chimiques qui en découlent, elles-mêmes dues aux effets de réduction de taille des objets qui seraient trop simpliste de résumer au seul effet de surface. En effet, un autre effet apparait, c'est celui de la quantité finie d'atomes qui en font des objets très différents du massif et de la surface infinie. Ces caractéristiques modifient en premier lieu la structure atomique et chimique des nanoalliages : l'arrangement des atomes, mais également les déformations internes induites par cette échelle nanométrique.

L'étude à l'échelle macroscopique de l'alliage Pt-Ag montre un diagramme de phase [1] intéressant mais complexe notamment à basse température : présence d'un alliage ordonné uniquement à l'équiconcentration AgPt, une immiscibilité presque totale pour les fortes concentrations en Pt mais partielle à forte concentration en Ag. La réduction de taille peut conduire à une modification de la stabilité des alliages ordonnés ou induire une ségrégation entre les deux éléments pour former une particule de type cœur-coquille, janus-like…

Trois forces principales permettent de prédire la tendance du système (alliage / ségrégation) : le désaccord de maille, la différence d'énergie de surface entre les deux éléments ainsi que l'énergie de mélange du système. Dans le cas de Pt-Ag, des études numériques basées sur la méthode Monte Carlo [2], prenant en compte ces forces motrices, ont tendances à prédire une ségrégation de type cœur(Pt)-coquille(Ag), en compétition avec un effet de mélange selon la composition. Notre objectif est de déterminer expérimentalement, en fonction de la composition de la nanoparticule, quelle sera la conséquence des effets de surface : l'effet de ségrégation de surface de l'argent va-t-il être prédominant sur les effets d'alliage qui ont été montrés sur le massif ?

Les particules Pt-Ag sont préparées en co-dépôt sous ultravide par évaporation des deux éléments. La structure et la configuration chimique du système ont pu être observées d'une part *ex situ* par microscopie électronique à transmission à très haute résolution notamment en mode HAADF, et d'autre part *in situ* et en temps réel sur la ligne SIXS du synchrotron SOLEIL par diffusion des rayons X en incidence rasante montrant une phase alliée avec une tendance à l'ordre après recuit thermique. Ainsi une phase d'alliage $L1_1$ (alternance de plans Ag puis Pt dans la direction [111]) avec une déformation rhomboédrique très marquée a été observée, mais aussi une ségrégation cœur-coquille, comportement dépendant de la composition.

Bibliographie

[1] M H. F. Sluiter, C. Colinet, A. Pasturel, *Ab initio calculation of the phase stability in Au-Pd and Ag-Pt alloys,* Phys. Rev. B, 2006.
[2] K. Yun et al, *Monte Carlo simulations of the structure of Pt-based bimetallic nanoparticles,* Acta materiala 60,12, 4908-4916, 2012.

Surface composition of Ir anode as revealed from in-situ NAP-XPS

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Iridium-based anodes are state-of-the-art catalysts for proton exchange membrane water electrolyzers [1]. The surface state of the Ir anode under the oxygen evolution reaction (OER) conditions remains a crucial issue for the understanding of the OER mechanism and strive for the enhancement of the PEM electrolyzer performance [2, 3].

In this work we applied synchrotron radiation-based (Soleil, Paris) near-ambient pressure x-ray photoelectron spectroscopy (NAP-XPS) to nanoparticulated Ir anodes to follow their surface composition under controlled potential. The analysis of the XP spectra at key potentials and different photon energies revealed the presence of a layered structure of various electrochemically formed Ir oxides [Fig. 1]. While below the onset of the OER the metal Ir core is coated with Ir(IV) and Ir(III) oxides, the latter is oxidized into Ir(IV) which is dominating the catalyst surface during the OER. The simulations of XP spectra (SESSA) suggest that the thickness of the Ir(IV) oxide shell is similar to a monolayer.

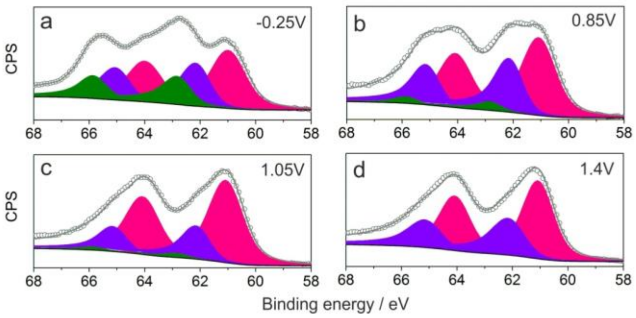

Fig. 1*: Ir4f XP spectra of Ir electrode obtained under 3 mbar water vapor and different polarization conditions (U_{WE-CE}): -0.25V; 0.85V; 1.05V (OER region); 1.4V (OER region). Color codes: Ir met (pink); Ir III (olive); Ir IV (violet), fitted line (grey). The raw data are presented as open circles. Photon energy 595 eV*

Acknowledgements

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Bibliography

[1] M. Carmo, D. L. Fritz, J. Mergel, D. Stolten, *Int. J. Hydrogen Energy* **38**, 4901 (2013)
[2] V. Pfeifer, T.E. Jones, S. Wrabetz et al. *Chemical Science* **7**, 6791 (2016)
[3] S. Cherevko, S. Geiger, O. Kasian, A. Mingers, K. J. J. Mayrhofer, *JEAC* **773**, 69 (2016)

Poster 26

MsSpec-1.1 : a multiple-scattering package for spectroscopies using electrons

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We present a package to compute the cross-section of photoelectron diffraction (PED), Auger electron diffraction (AED), X-ray absorption (XAS), low energy electron diffraction (LEED) and Auger photoelectron coincidence spectroscopy (APECS). It is based on multiple scattering theory [1]. This package allows to cover kinetic energies ranging from 0 to 1.5 keV, due to the use of three different algorithms for the evaluation of the multiple scattering. A light Graphical User Interface (GUI) called µ-GUI is also provided [**Fig. 1**]. The package makes use of free software to plot and visualise the results [2]. A Python binding of the package based on the Atomic Simulation Environment (ASE) allows intensive scripting support for the user and provides a unified interface to other codes supported by ASE (*e.g.* density functionnal theory programs) that could eventually interact with MsSpec.

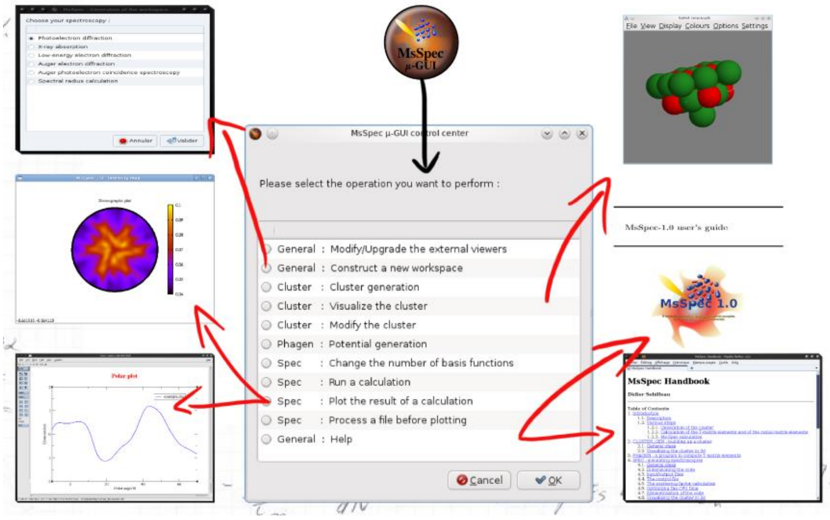

Fig. 1: *An overview of the MsSpec µ-GUI (without the integration within ASE)*

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Bibliography

[1] D. Sébilleau R. Gunnella, Z.Y. Wu, S. Di Matteo, and C.R. Natoli, J. Phys.: Condens. Matter, topical review, **18**, 175-230 (2006).
[2] D. Sébilleau, C. R. Natoli, G. M. Gavaza, H. Zhao, F. Da Pieve and K. Hatada, Comp. Phys. Comm., **182**, 2567-2579 (2011).

Germanène sur Al(111) : étude de la structure électronique

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La découverte du graphène a fortement stimulé la recherche sur les matériaux 2D. Récemment, le silicene, cousin du graphène pour le silicium, a été synthétisé sur un substrat métallique d'argent (111). Ces dernières années, le silicène a également été observé sur des surfaces de dibore de zirconium (0001) ou d'iridium (111). Le germanène, un autre cousin du graphène mais à base de germanium, a été prédit en 2009 comme étant une phase stable du germanium et observé en multiphase sur un substrat d'or (111) en 2014 [1]. La synthèse et l'étude d'une couche de germanène sur d'autres substrats permettrait de comprendre comment se forme ce type de couche 2D.

Dans ce travail, nous avons élaboré et caractérisé une couche de germanène déposée sur un substrat d'aluminium orienté dans la direction (111) [2]. La structure électronique de germanène a été étudiée par photoémission haute résolution et par des calculs DFT [3]. Les niveaux de cœur Al 2p et Ge 3d ont été mesurés sur le système germanène/Al(111) en par rayonnement synchrotron (SOLEIL, ligne ANTARES). Le niveau Ge 3d est déplacé vers les faibles énergies de liaison par rapport au germanium volumique et montre trois composantes qui reflètent la multiplicité des sites atomiques dans le germanène. Les calculs révèlent la présence d'une densité de charge à l'interface germanène/Al(111) ainsi qu'un transfert de charge des atomes d'aluminium de surface vers le germanène. L'existence de trois sites atomiques non équivalents dans la couche de germanène est associée à trois charges de Bader différentes, pouvant ainsi expliquer les mesures de photoémission présentant trois composantes.

En conclusion, les résultats obtenus montrent qu'il y a un transfert de charge entre l'aluminium et le germanium, conduisant à une interaction électrostatique entre le substrat d'aluminium et le germanène. De plus, la présence d'une densité de charge à l'interface indique l'existence d'une interaction chimique faible entre la surface d'aluminium et la couche de germanène. Ainsi, l'interaction du germanène avec le substrat Al(111) présente des similarités avec celle du silicène/Ag(111) [4]. La structure électronique de ces deux systèmes semble être une caractéristique des éléments du groupe IV en couche 2D déposés sur des métaux simples ou nobles.

Bibliography

[1] M. Davila, L.Xian, S. Cahangirov, A. Rubio, G. Le Lay, *New J. Phys.* **16**, 095002 (2014).
[2] M. Derivaz, D. Dentel, R. Stephan, M.-C. Hanf, A. Mehdaoui, Ph. Sonnet, C. Pirri, *Nano Lett.* **15**, 2510 (2015).
[3] R. Stephan, M.C. Hanf, M. Derivaz, D. Dentel, M. C. Asensio, J. Avila, A. Mehdaoui, Ph. Sonnet, C. Pirri, *J. Phys. Chem. C* **120**, 1580 (2016).
[4] R. Stephan, M-C. Hanf, Ph. Sonnet, *J. Phys.: Condens. Matter* **27**, 015002 (2015).

Moduler les interactions germanène-substrat au moyen de l'hydrogénation

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Le germanène, un cousin du graphène mais à base de germanium, a été prédit en 2009 comme étant une phase stable du germanium, et observé en multiphase sur un substrat d'or (111) en 2014 [1]. Récemment, une couche de germanène déposée sur un substrat d'aluminium a pu être obtenue et caractérisée dans notre laboratoire [2]. Nos études DFT ont montré qu'il y avait un transfert de charge entre l'aluminium et le germanium conduisant à une interaction électrostatique entre le substrat d'aluminium et le germanène. De plus, la présence d'une densité de charge à l'interface indiquait l'existence d'une interaction chimique faible entre la surface d'aluminium et la couche de germanène [3]. Cependant pour des applications futures, il serait intéressant d'exfolier une couche de germanène de son substrat. Pour cette raison, nous avons étudié l'hydrogénation du système germanène/Al au moyen de calculs DFT [4].

Nous montrons que les atomes de germanium portant un atome d'hydrogène sont plus éloignés de la surface d'aluminium que les autres atomes de germanium. Ainsi, la distance Ge-Al augmente lorsque que le recouvrement en hydrogène augmente, tandis que l'énergie d'interaction diminue. De plus, le transfert de charge des atomes d'aluminium vers la couche de germanium diminue également, conduisant à réduire les interactions électrostatiques entre le germanène et le substrat d'aluminium. Les calculs de densité de charge et de différence de densité de charge indiquent que la densité électronique localisée à l'interface est fortement réduite sous hydrogénation. Tous ces résultats montrent clairement que les interactions entre le germanium et le substrat d'aluminium diminuent en présence d'hydrogène. Cependant l'hydrogénation représente seulement la première étape pour une éventuelle exfoliation d'une couche de germanène. Une autre étape est nécessaire pour finaliser la séparation entre la couche 2D et le substrat. Ainsi, l'augmentation de la distance entre le germanène et les atomes d'Al pourrait faciliter l'intercalation de différentes espèces atomiques permettant ainsi une séparation définitive.

Bibliography

[1] M. Davila, L.Xian, S. Cahangirov, A. Rubio, G. Le Lay, *New J. Phys.* **16**, 095002 (2014).
[2] M. Derivaz, D. Dentel, R. Stephan, M.-C. Hanf, A. Mehdaoui, Ph. Sonnet, C. Pirri, *Nano Lett.* **15**, 2510 (2015).
[3] R. Stephan, M.C. Hanf, M. Derivaz, D. Dentel, M. C. Asensio, J. Avila, A. Mehdaoui, Ph. Sonnet, C. Pirri, *J. Phys. Chem. C* **120**, 1580 (2016).
[4] A. Marjaoui, R. Stephan, M-C. Hanf, M.Diani, Ph. Sonnet, *Phys.Chem.Chem.Phys.* **18**, 15667 (2016).

Molecular simulation study of the influence of alkali cations on the adsorption properties of chlorinated aromatics in zeolites

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Molecular simulations have been employed in order to explore at the microscopic scale the adsorption of bis-chlorinated aromatics (1,2- and 1,3-dichlorobenzene) in two zeolitic structures with large pore openings: EMT and FAU. Both, the purely siliceous and the sodium cation exchanged forms of zeolite structures have been considered respectively, aiming to clearly determine the role of the charge compensating cation in the adsorption of investigated aromatics. A suited combination of classical and electronic structure simulation tools provided a clear overall picture of the adsorption process, from both, local and global points of view.

From the Density Functional Theory (DFT) level calculations we could extract the local geometry of the interaction between the molecule and the considered zeolite surfaces as well as the associated enthalpy of adsorption. Furthermore, the study of the charge transfer between the molecule and the charge compensating cation provided precious information concerning the nature of the interaction between the molecule and the zeolite.

On the basis of classical forcefields available from the literature [1], the Gibbs ensemble Monte Carlo simulations were realized to predict the adsorption properties such as adsorption isotherms and enthalpies for the investigated molecules in the EMT and FAU zeolitic structures, within the purely siliceous and Na^+ exchanged forms, with mobile extra-framework cations upon the aromatics adsorption. Then, we accomplished a detailed analysis of the microscopic mechanism in play along the whole adsorption process, with a special highlight to the understanding of the geometry of interaction of the molecule with the sodium cation, in function of its crystallographic site [2]. Location of the charge compensating cation has been found to influence the adsorption properties and the preferential adsorption sites have been identified.

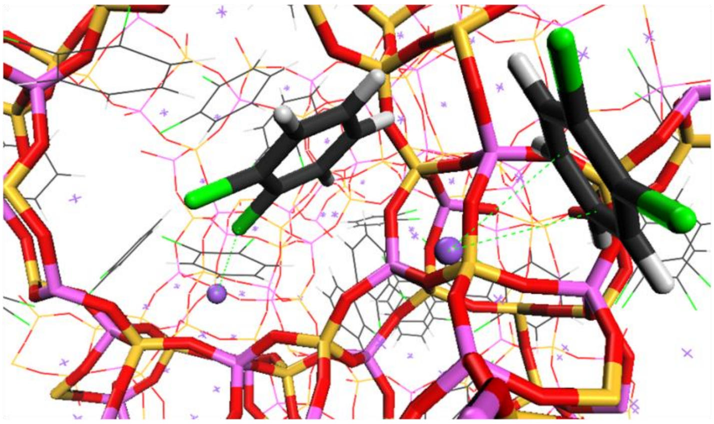

Fig. 1*: Typical arrangement of 1.2-dichlorobenzene molecules at the high loading issued from the Gibbs ensemble Monte Carlo simulation at 298K. Molecules are preferentially arranged to the Na^+ cations situated in the SIII' crystallographic sites.*

Bibliography

1. I.J. Siepman et al., *J. Phys. Chem. B* **117**, 273 (2012).
2. Z. Nour et al., *J. Phys. Chem. C.***116**, 24512 (2012)

Imaging and analysis of graphene nanoribbons using scanning probe microscopies

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One of the major hurdles in the implementation of graphene in present day electronics is its lack of bandgap. One way to overcome this challenge is the creation of graphene nanoribbons (GNRs). Since the magnitude of the bandgap strongly depends on the width and the edge structure of such ribbons, the 'bottom-up' synthesis of structurally well-defined GNRs is being actively pursued [1]. In this contribution, we present structural characterization of monolayer thick films of bottom-up synthesized GNRs on solid substrates using scanning probe methods, namely AFM and STM. We show that STM and AFM can be efficiently employed as complementary analytical tools for characterization of GNR together with conventional spectroscopic tools [1,2]. The highly controlled synthesis and liquid phase processability opens the way to GNR-based devices [2].

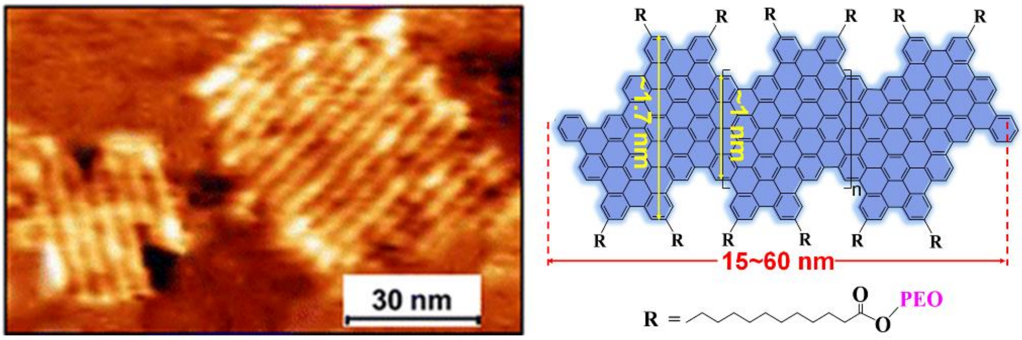

Fig. 1: *AFM image of a self-assembled monolayer of GNRs on graphite (dry film). The structure of the corresponding poly(ethylene oxide) functionalized GNR is shown on the right.*

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FWO, K.U. Leuven (GOA 11/003), BELSPO (IAP–P7/05) and the ERC under the EU's Seventh Framework Programme (FP7/ 2007-2013)/ERC grant agreement no. 340324.

Bibliography

[1] A. Narita *et al.*, *Nature Chemistry* **6**, 126 (2014).
[2] Y. Huang *et al.*, *Journal of the American Chemical Society* **138**, 10136 (2016).

Tunable doping of graphene using physisorbed self-assembled networks

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One current key challenge in graphene research is to tune its charge carrier concentration, *i.e.*, *p*- and *n*-type doping graphene. Adsorption of molecules result in more controlled and uniform doping if they self-assemble in organized networks compared to a random distribution on the graphene surface [1]. To demonstrate controlled doping of graphene using physisorbed organic molecules, we investigated the self-assembly and doping effect of two aliphatic amines, octadecylamine (ODA, $CH_3(CH_2)_{17}NH_2$) and nonacosanamine (NCA, $CH_3(CH_2)_{28}NH_2$). The length of the alkyl chains determines the density of the amine groups at the graphene interface by acting as a spacer and thus, the doping effect can be precisely controlled.

The organization of these two compounds on the graphite and graphene surface was characterized with scanning tunneling microscopy (STM) and atomic force microscopy (AFM), showing that both molecules organize in lamellar films where the difference in periodicity, 5 nm for ODA and 8 nm for NCA, reflects the difference in alkyl chain length. Electrical measurements, performed on graphene field-effect transistors (GFETs) before and after functionalization with ODA and NCA, evidenced the injection of 1.1×10^{13} cm^{-2} and 0.7×10^{13} cm^{-2} electrons, respectively. This difference in doping effect is in agreement with the difference in amine group density, which demonstrates a method for tunable doping of graphene using self-assembled networks by rational design of the self-assembling species.

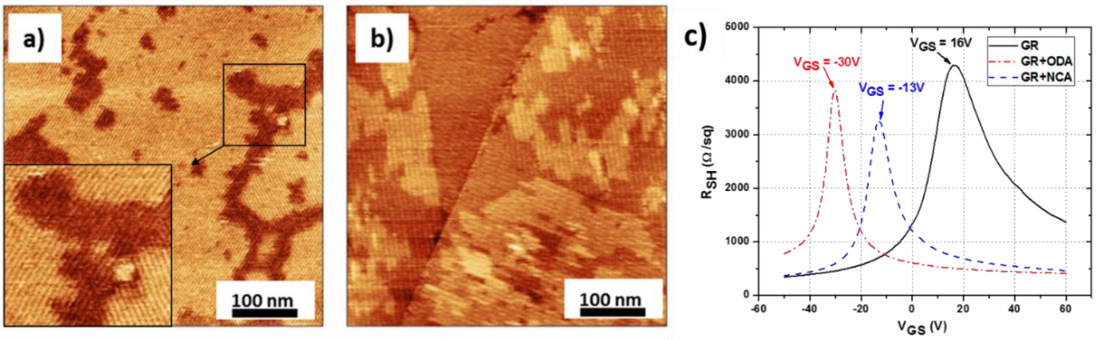

Fig. 1: *AFM images of graphite after functionalization with ODA (a) and NCA (b) via drop casting. (c) GFET transfer curves before and after functionalization with ODA or NCA.*

Acknowledgements

FWO (Belgium), Beyond CMOS program at imec and ERC under the European Union's Seventh Framework Programme (FP7/2007-2013) ERC Grant Agreement No. 340324.

Bibliography

[1] K.S. Mali *et al.*, *Nanoscale* **7**, 1566 (2015).

Poster 32

Indium content impact on structural and optical properties of (In,Ga)As/GaP quantum dots

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Despite many efforts undertaken by the semiconductor scientific community, the demonstration of room-temperature laser source electrically pumped monolithically grown on silicon substrate is still an importante challenge [1]. Amongt III-V semidonductors, GaP appaers as a promising candidate thanks to its small lattice mismatch with Si [2]. Nevertheless, devices based on GaP materials need to deal with the difficulty to obtain efficient active area due to its indirect character. To overcome this, (In,Ga)As quantum dots(QDs) [3] were proposed. In this contribution, Influence of indium content on structural and optical properties is investigated in order to promote the direct optical transition of QDs. Four nominal In content: 10, 25, 35 and 50% of (In,Ga)As/GaP QDs grown by solid source molecular beam epitaxy (SS-MBE) on GaP substrate are analyzed by photoluminesence and atomic force microscopy (AFM) experiments. Significant redshift is reported in comparison between QDs with 10% to 35% of In content due to the valence band modification [4]. Moreover, it is shown that, while for low In contents a monomodal QDs distribution is observed [Fig1.a], a bimodal one appears for In contents reaching 35% and beyond [Fig1.b]. Controlling this distribution is a great challenge for obtaining a direct bandgap emission with GaP-based materials.

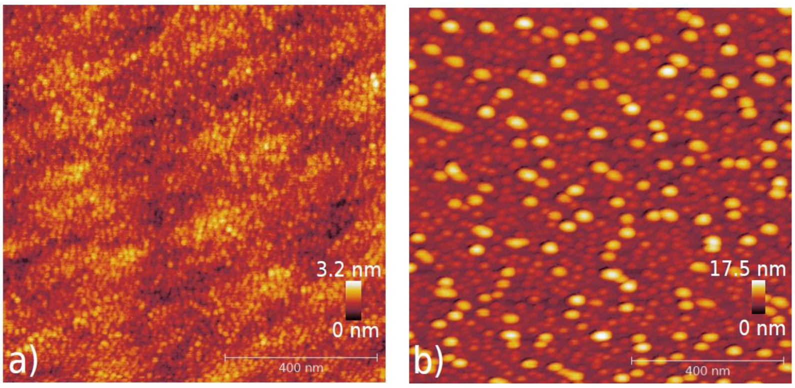

Fig. 1: *1 x 1 μm^2 AFM image of monomodal (a) and bimodal (b) distribution of (In,Ga)As/GaP QDs grown by SS-MBE on GaP substrate*

Acknowledgements

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Bibliography

[1] C. Cornet, Y. Léger, et C. Robert, *Integrated Lasers on Silicon*. ISTE-Elsevier, 2016.

[2] Y. Furukawa, H. Yonezu, A. Wakahara, S. Ishiji, S. Y. Moon, et Y. Morisaki, « Growth of Si/III–V-N/Si structure with two-chamber molecular beam epitaxy system for optoelectronic integrated circuits », *J. Cryst. Growth*, vol. 300, nº 1, p. 172-176, mars 2007.

[3] M. Heidemann, S. Höfling, et M. Kamp, « (In,Ga)As/GaP electrical injection quantum dot laser », *Appl. Phys. Lett.*, vol. 104, nº 1, p. 11113, janv. 2014.

[4] C. Robert *et al.*, « Electronic, optical, and structural properties of (In,Ga)As/GaP quantum dots », *Phys. Rev. B*, vol. 86, nº 20, p. 205316, nov. 2012.

Poster 33

Influence of Grain Boundaries and surface segregation phenomena on Thin-film Solar Cell Efficiencies

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As planar defects, Grain Boundaries (GBs) are often detrimental to physical properties. On the contrary, thin-film solar cells based on polycrystalline $CuIn_{1-x}Ga_xSe_2$ (CIGSe) absorber layer offer a better efficiency than its monocrystalline counterpart. Unfortunately, they may also be responsible for the suboptimal efficiency value when compared to the theoretical efficiency-x curve[1].

For a while the beneficial effect of GBs was thought to only come down to an electrical shunt[2]. Now the composition and structure of these GBs may also be of some influence, so that the structure and composition of these interfaces at the atomic-scale is under question.

By coupling XRD, EDX and Raman techniques for different CIGSe stoichiometries we first illustrate that the texture and grain sizes depend on x, but also on the Cu composition and the possible presence of Na diffusing from the soda-lime substrate. We also show that in the case of x=1, Cu_xSe clusters are located along precise surface orientations [Fig. 1]. We then focus on the reason why these clusters do not form for In-rich (x<0.4) samples and their dependence on the CIGSe deposition process.

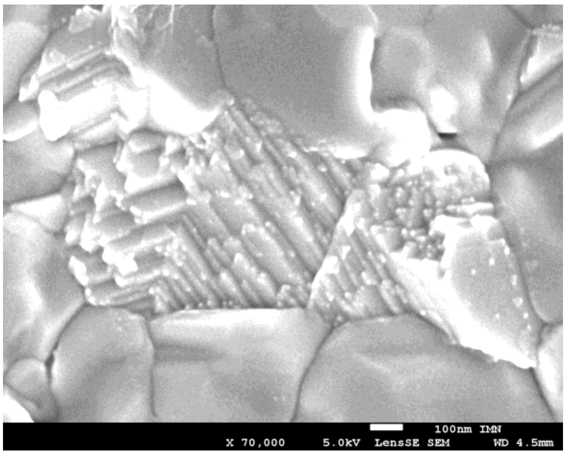

Fig. 1: SEM surface image of $CuGaSe_2$ absorber layer

Bibliography

[1] M. Raghuwanshi, E. Cadel, P. Pareige, S. Duguay, F. Couzinie-Devy, L. Arzel, N. Barreau, *Applied Physics Letters* **105**, 013902 (2014)

[2] C. Persson, A. Zunger, *Phys. Rev. Lett.* **91**, 266401, (2003)

X-ray Nano Coherent Scattering on GaP/Si for III-V Monolithic Integration on Silicon

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GaP/Si is an ideal pseudo-substrate for the defect-free IIIV semiconductor material epitaxy, because of the low lattice mismatch between them[1]. But, defects, such as Micro-Twins(MT) and Anti-Phase Boundaries(APB), must be avoided. In this context, XRD has been performed as non-destructive technique for quantitation and local characterization of these defects[2]. We developed software tools for faster lab setup analysis[3]. Different GaP/Si nanolayers were also studied at ID01/ESRF with an 8keV X-ray nano-beam. Here a 140nm thick GaP presents annihilated APB (less than $3/\mu m$ emerging APB). Two-dimensional fast mapping (k-map)[4] have been carried out for different Bragg condition and region of interest integration (ROI) of the camera(defined Fig. 2a). As shown Fig. 1b), the weak scattered intensity in ROI1, exhibits contrast lines oriented along both [1 1 0] and [-1 1 0] crystallographic directions. This contrast likely corresponds to regions of high tilt, surrounding misfit dislocations[4]. Strong scattering conditions performed on the *002* (Fig. 2c) and the *002* Bragg reflections present a quite different contrast with large spotty regions. This anisotropic contrast is believed to be due to the weak tilt/strain, associated to the APD annihilation process. These preliminary analyses through the peak structure and k-map indicates the potentiality of a new method of fine structure detection of III/V semiconductor material.

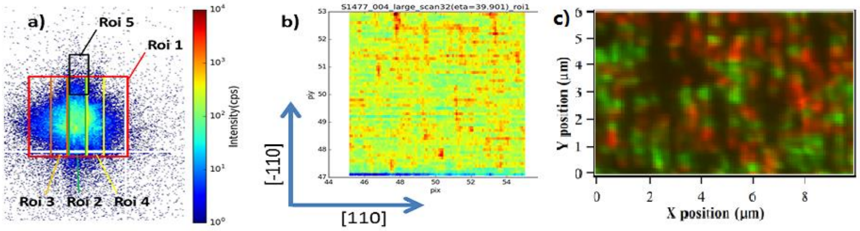

Fig. 2 *a) ROI definition b) ROI1 weak beam (-0.5° on rocking angle) 10x6 μm^2 k-map on GaP 004. c) Combination of ROI3&ROI4 for strong beam k-map on GaP 002.*

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Bibliography

1. Y. P. Wang et al., Appl. Phys. Lett. **107**, 191603 (2015).
2. S. Labat et al., ACS Nano **9**, 9210 (2015).
3. RSM_Plot_Fit. (2016). from Github: https://github.com/Naluen/RSM_Plot_Fit

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4. M. H. Zoellner et al., ACS Appl. Mater. Interfaces **7**, 9031 (2015).

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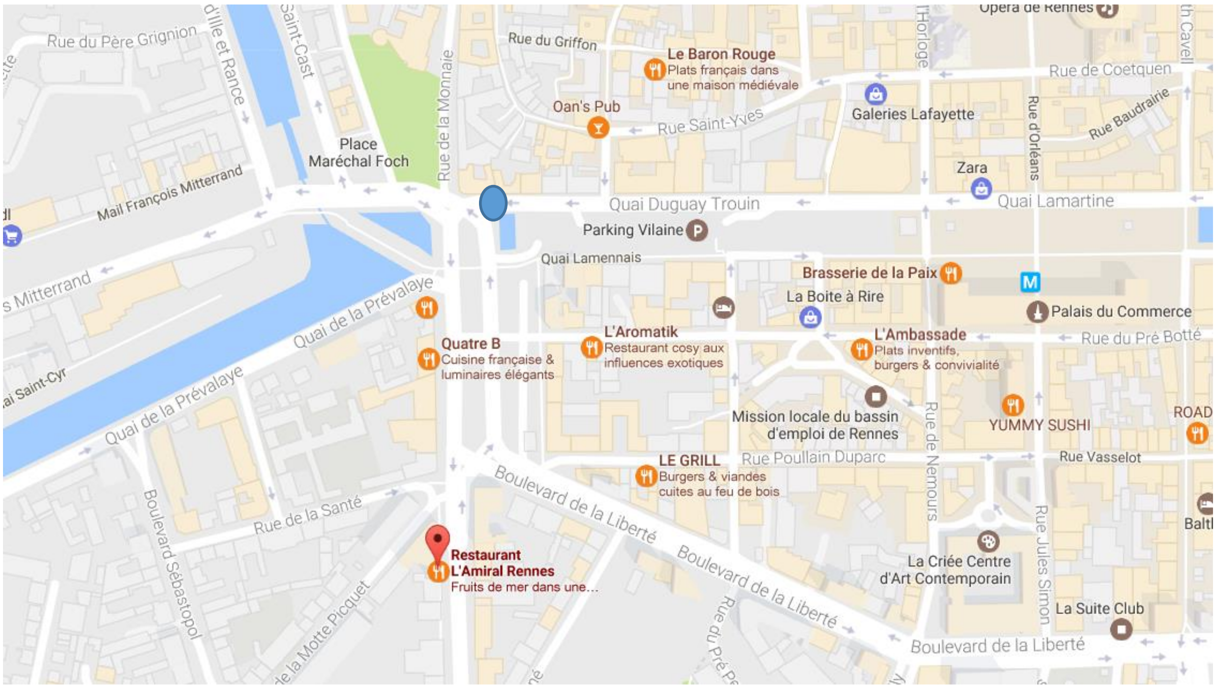

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Pour information

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Sciences Chimiques de Rennes (ISCR)

Heure	Mercredi 25	Heure	Jeudi 26	Heure	Vendredi 27
			Session 2 **9h-12h30**		**Session 4** **9h-12h30**
		09:00	**Tao ZHOU** ESRF	09:00	**Anne-Laure BIANCE** ILM
		09:45	**Anny MICHEL** Institut P’	09:45	**Matthieu BUGNET** MATEIS
		10:30	**Pause-café** **10h30-11h**	10:30	**Pause-café** **10h30-11h**
		11:00	**Thomas JAOUEN** IPR et Univ. Fribourg	11:00	**Fabrice COUSIN** LLB
		11:45	**Jacek GONIAKOWSKI** INSP	11:45	**Véronique VIE** IPR
12:00	**Accueil** **12h-14h** *Hall PNRB* **Buffet de bienvenue** 2ème étage Espace co-working	12:30	**Buffet** **12h30-14h** 2ème étage PNRB Espace co-working	12:30	**Buffet** **12h30-14h** 2ème étage Espace co-working
	Session 1 **14h-18h15**		**Session 3** **14h-16h15**		
14:00	**Xavier MARIE** LPCNO	14:00	**Elena SAVINOVA** ICPEES		
14:45	**Jérôme LAGOUTE** MPQ	14:45	**Samy BOUKARI** IPCMS		
15:30	**Pause-café** **15h30-16h**	15:30	**Mikaël KEPENEKIAN** ISCR		
16:00	**Christophe BRUN** INSP	16:15	**Session Posters** **16h15-19h30**		
16:45	**Franck PALMINO** FEMSTO-ST				
17:30	**Laurence MASSON** CINaM				
		20:30	**Dîner de Gala**		