doses in mammography. Since the first days of XPCI, mammography has been considered as one of the most important candidates for a clinical application [3]. In fact, the imaging of breast can greatly benefit from soft tissue contrast improvements and/or from radiation dose reductions provided by XPCI.

In order to achieve this aim, a proof-of-principle experiment was performed at the European Synchrotron Radiation Facility (ESRF, France), on excised human breast specimens. A photon-counting detector achieving almost 100% efficiency at high X-ray energies was used in order to minimize the image noise. Moreover, a new retrieval algorithm capable of extracting the phase shift from a single EI image was exploited to process the acquired images [4]. This method presents the twofold advantage of being stable with respect to noise (thus allowing further dose reductions) [5] and of needing only one input image, thus significantly simplifying and speeding up the acquisition. Importantly, although this proof-of-principle study was carried out with synchrotron radiation, the method has potential for an application in table-top setups, which represents an essential requirement for any future clinical implementation.

In this talk, we will first introduce the EI technique and its main features. We will then present the recently developed single-image retrieval algorithm and the pilot experiment carried out at the ESRF, and suggest ways to exploit these results for potential future clinical applications.

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Session VI

Tuesday, September 6 - afternoon

I6

SYNCHROTRON-BASED X-RAY STRUCTURAL ANALYSIS OF FUNCTIONAL MATERIALS TOWARDS CATALYTIC STRUCTURE-ACTIVITY RELATIONSHIPS

J. P. Hofmann

Laboratory of Inorganic Materials Chemistry, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600MB Eindhoven, The Netherlands
j.p.hofmann@tue.nl

Heterogeneous catalysis plays a significant role in chemical industry. To arrive at a knowledge-based catalyst design, fundamental insight into relations between structure and catalytic properties, such as activity, selectivity and stability, is needed. During this lecture, examples from recent work at ESRF beamlines ID01 and ID03 will be discussed. Three showcase applications from the field of heterogeneous model catalysis will be highlighted.

1) Zeolites are commonly used as solid acid catalysts in many large scale industrial processes, such as the Methanol-to-Hydrocarbons process. Zeolite H-ZSM-5 is a well-known candidate and has been studied extensively because of its intriguing 3D intergrowth structure. We have applied micro-focused X-ray diffraction imaging at higher order Bragg reflections to unravel the intergrowth pattern of individual large H-ZSM-5 crystals [1]. Additionally, information about aluminium zoning, which sensitively impacts on catalytic properties, could be obtained based on subtle changes of the lattice constants. Recently, we extended the μXRD approach by coupling optical detection of X-ray excited optical fluorescence (XEOF) of labelled H-ZSM-5 crystals [2]. Recording XEOF of styrene oligomers as a Brřnsted acid site specific label together with μXRD response led to the simultaneous characterization of local crystallinity and the presence and nature of catalytically active sites.

2) *Operando* surface X-ray scattering experiments under electrochemical conditions have been carried out to arrive at catalytic structure-activity relationships for single crystal (here Pt(111)) model electrodes [3]. In this experiment, SXRD, XRR and GISAXS have been applied together with On-Line-Electrochemical Mass Spectrometry (OLEMS) to study the influence of surface structural changes on activity of the model electrode in hydrogen and oxygen evolution reactions. OLEMS adds chemical specificity to electrochemically measured currents and plays to its strength when reactions with a selectivity dimension are studied.

3) Most recently, nanocrystal model catalysts have been introduced for *in-situ* studies of individual nanoparticle catalysis. Real space structure and strain distribution is studied by Coherent X-ray Diffraction Imaging (CXDI). *In-situ* cells for both heterogeneous gas phase catalysis and electrocatalysis have been constructed and successfully applied; showcases from both field will be highlighted.

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C18

TRANSMISSION SURFACE DIFFRACTION: A NEW TOOL FOR IN-SITU AND OPERANDO SURFACE SCIENCE

F. Reikowski[1], T. Wiegmann[1], J. Stettner[2], J. Drnec[2], V. Honkimäki[2], F. Maroun[3], O. M. Magnussen[1]

[1]*Institute of Experimental and Applied Physics, Kiel University, Kiel 24098, Germany*
[2]*Experimental division, ESRF, 71 Avenue des Martyrs, 38000 Grenoble, France*
[3]*Physique de la Matière Condensée, Ecole Polytechnique, CNRS, 91128 Palaiseau, France*
drnec@esrf.fr

A new surface diffraction method for in situ studies of buried interfaces which employs synchrotron X-ray radiation of high photon energy is presented. In contrast to the standard geometry with grazing incidence angles [1], in this technique a transmission geometry where the X-ray beam passes through the sample is used (Fig. 1). Transmission surface diffraction (TSD) is a powerful and user-friendly method that enables fast simultaneous imaging of the full in-plane structure of solid surfaces. Furthermore, it allows surface X-ray diffraction studies with micrometer spatial resolution, opening up the way to map the atomic interface structure of spatially inhomogeneous systems or to study the surface properties of small samples. The feasibility of this approach is demonstrated by TSD measurements of Co and Bi electrodeposition on Au(111) electrodes [2], performed at beamline ID 31 of the ESRF. The formation of the crystal truncation rods (CTRs), changes in the Au CTRs due to epitaxial strain, and the disappearance of the rods corresponding to the (22 x 3) phase of the Au surface reconstruction can be directly observed without lengthy searches in reciprocal space. In addition, in situ microscale mapping of the deposit and substrate properties and studies during Co dissolution are discussed.

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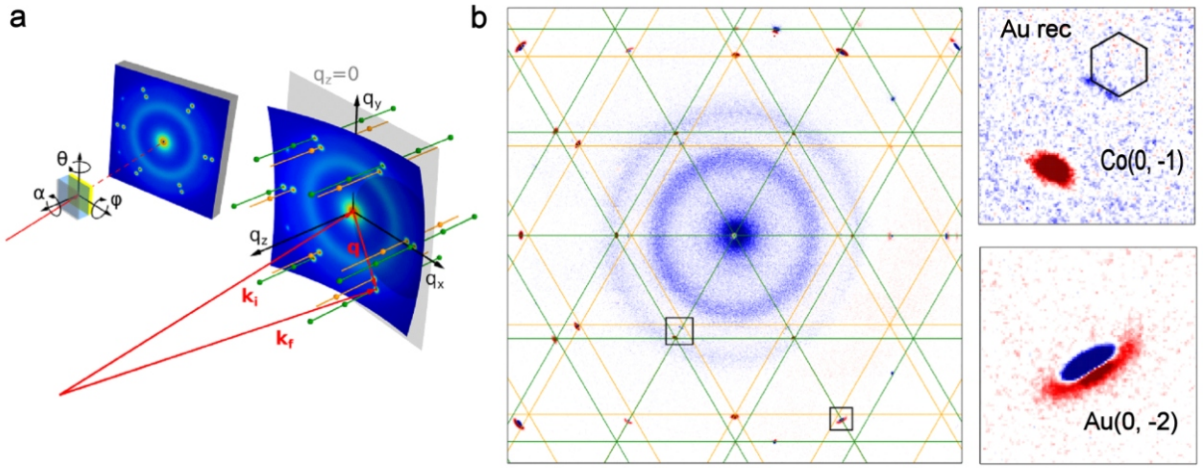

Figure 1. (a) Real space and reciprocal space geometry of TSD. (b) In situ TSD of Au(111) in 0.1 M $NaClO_4$ + 1.3 mM HCl + 1mM $CoCl_2$, recorded at 40 keV. Shown is the intensity difference between detector images of the Au sample at -0.2 $V_{Ag/AgCl}$ and after electrodeposition of a 20 ML thick epitaxial Co(001) film at -1.05 $V_{Ag/AgCl}$.

C19

INTERMIXING IN SINGLE Ge-Si CORE-SHELL NANOWIRES: A COHERENT X-RAY IMAGING STUDY

S. Fernández[1,2], M.-I. Richard[1,2], S. Labat[2] , P. Gentile[3], T. Schülli[2], O. Thomas[1]

[1]Aix-Marseille Université, CNRS, IM2NP UMR 7334, Campus de St-Jérôme, 13397 Marseille, France
[2]ESRF, The European Synchrotron, 71 Avenue des Martyrs, 38043 Grenoble Cedex, France
[3]CEA Grenoble/ INAC/PHELIQS, 17 Avenue des Martyrs, 38054, Grenoble

Characterising the structural properties (strain gradients, chemical composition, crystal orientation and defects) inside nanostructures is a grand challenge in materials science. In this context, the temperature evolution of the interface structure in a core-shell nanostructure is especially interesting to study. It raises fundamental questions about intermixing at the nanoscale where a strong interplay between strain and interfacial energies is expected to play an important role. Coherent diffraction imaging (CDI) in Bragg condition is a promising and attractive method to map the shape, the concentration and deformation fields simultaneously inside *single* nanostructures. It also permits *in situ* experiments owing to its non-destructive nature.

We demonstrate the capabilities of the CDI technique in Bragg condition on single Ge-Si core-shell nanowires (NWs) with a typical diameter of 300 nm and a length of 10 micrometers. NWs are grown by Vapor-Liquid-Solid (VLS) phase epitaxy and then isolated using a SEM/FIB instrument.

High resolution X-ray diffraction experiments have been performed at the ID01 beamline of ESRF (France). A Fresnel Zone Plate focused the beam on a 150 (V) × 400 (H) nm^2 spot. X-ray reciprocal space maps around four different Bragg reflections were recorded, evidencing a Ge core completely relaxed (*i.e.*, at its bulk lattice parameter). Also a lattice tilt in the growth direction of the NW was observed during the measurements. Then, an *in-situ* study as function of temperature was performed on the isolated wire, yielding changes in the recorded diffraction patterns. Phase retrieval analysis and reconstruction of the studied NW are in progress.