Monitoring the atomic layer deposition of TiO_2 on InAs(100) with real-time ambient pressure XPS

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Atomic layer deposition (ALD) is a thin film deposition technique for depositing uniform and conformal layers on complex three-dimensional topographies. ALD is highly used in different fields of technology, e.g. in microelectronics for metal–oxide–semiconductor field-effect transistors, in the formation of catalyst materials and in solar cell technology. The understanding of the atomic and molecular surface processes underlying the ALD growth are, however, far from complete, which implies difficulties in further advancing the technology. A thorough investigation for the identification and role of surface species, surfaces defects, impurities and vapour phase reactions is therefore very much needed [1].

Here we have applied ambient pressure x-ray photoelectron spectroscopy (APXPS) to study the ALD growth of TiO_2 on the clean native oxide-covered InAs(100) surface. As precursors we have chosen tetrakis(dimethylamido)titanium (TDMAT) and water. APXPS has the advantage that it can be carried out during thin film growth, i.e. under *operando* conditions. Our investigation focuses on the dynamic nature of the ALD process, and it is for the first time that APXPS has been applied to this subject with millisecond time resolution.

The time resolution is illustrated in Fig. 1, which shows As3d spectra with the native oxide signal at around 44.5 eV binding energy and the bulk As signal at around 41 eV. The spectra were measured with a time resolution of 0.058 s during exposure to TDMAT. Here we can follow in detail how the native oxide is removed by the interaction with the precursor [2].

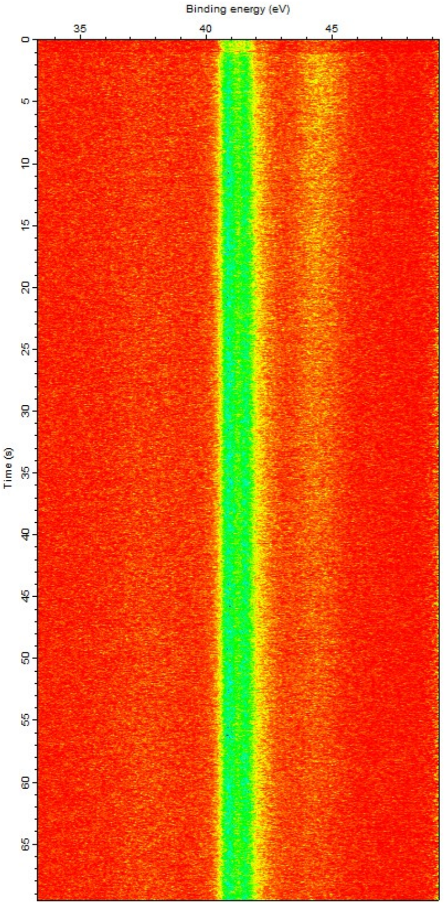

Fig. 1. As 3d spectra taken during the exposure of a native oxide-covered InAs(100) surface during expousre to TDMAT (pressure ca. 10^{-2} mbar). In total 1200 spectra were taken in around 70 s.

We have also used other spectral regions to identify the nature of surface chemical species during the TDMAT half-cycle. In particular, from the N 1s region we can identify methyl methyleneimine as well as the surface-bonded Ti-amido complex. APXPS thus offers the prospect of following the chemical evolution of the surface during ALD growth at unprecedented time resolution.

References:
[1] F. Zaera, Coord. Chem. Rev. **257**, 3177 (2013).
[2] R. Timm, A. R. Head, S. Yngman, J. V. Knutsson, M. Hjort, S. R. McKibbin, A. Troian, O. Persson, S. Urpelainen, J. Knudsen, J. Schnadt, A.Mikkelsen, Nature Commun., in press (2018).