ESRF	**Experiment title:** Diffusion of iron atoms studied with grazing incidence nuclear resonant scattering	**Experiment number**: HS1616
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Report:

Method

Nuclear resonant scattering (NRS) is a well established method to study structural and magnetic properties of materials as well as dynamics on an atomistic scale. This method combines the high brilliance of a third generation synchrotron source and the excellent characteristics of Mössbauer Spectroscopy (MS). The unique feature of the NRS method, i.e. the selectivity for Mössbauer isotopes, was used to receive information on the dynamics in a monolayer of iron in our experiment. The grazing-incidence geometry was used to enhance the signal from the iron layer.

There are two features of NRS, which predestine NRS for the presented investigations:

- First, NRS is sensitive to the atomic jump diffusion mechanism in different measurement geometry (transmission [1, 2], Bragg reflection [3], grazing-incidence [4]).
- Second, NRS is a technique for the investigation of hyperfine parameters, especially in thin films [5].

Experiment

The substrate was polished ex-situ and cleaned in situ by multiple flashing up to 2300 K. Detailed preparation conditions and sample characterisation techniques are published in [7]. The iron film was deposited using Molecular Beam Epitaxy (MBE) at room temperature onto a polished tungsten substrate. The orientation and structure of the substrate and the iron film were confirmed by LEED measurements of a clean substrate and checked again after the deposition of a 1 ML of iron.

All NRS spectra have been taken at the ID18 beamline of ESRF operating in 16-bunch timing mode. A UHV chamber with a load lock system was constructed in co-operation between the Institut für Materialphysik der Universität Wien, the Institute of Solid State Physics and the Institute of Catalysis and Surface Chemistry in Cracow. This chamber allows to store and to study sensitive thin film samples under UHV conditions and their investigation in grazing incidence geometry in the temperature region -150°C up to 2000°C. The chamber was mounted on a HUBER goniometer to adjust the grazing incidence conditions. A silicon bent crystal was used for sagittal and compound refractive lenses for vertical focusing. The dimensions of the synchrotron beam, monochromatised to an energy bandwidth of 6meV, were 800x100 μm^2. Details about the beamline set-up may be found in [8].

Preliminary results

The main aim of the experiment was to test the sensitivity of NRS in grazing incidence geometry and to gain information about the structure and dynamics of an iron monolayer on a tungsten substrate W(110). The total reflection angle of tungsten and iron for the used 14.4 keV radiation is 5.5 mrad and 3.8 mrad, respectively. The total reflection angle of a single monolayer of iron on tungsten was experimentally found as α_C= (4.9±0.2) mrad , i.e betweeen the value for tungsten (5.5 mrad) and iron (3.8 mrad). The normalised electronic and nuclear reflectivity near the critical angle is shown in Figure 1. .

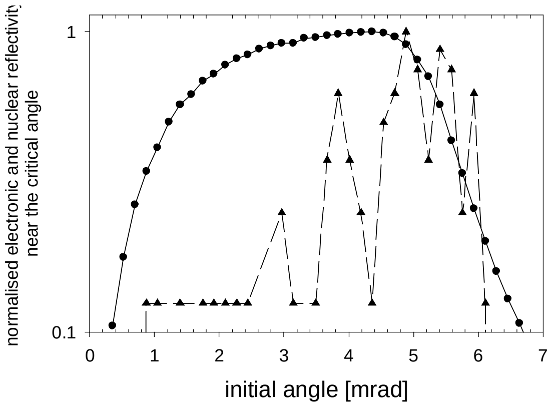

Fig.1:Normalised electronic (circles) and nuclear reflectivity (triangles) around the critical angle.

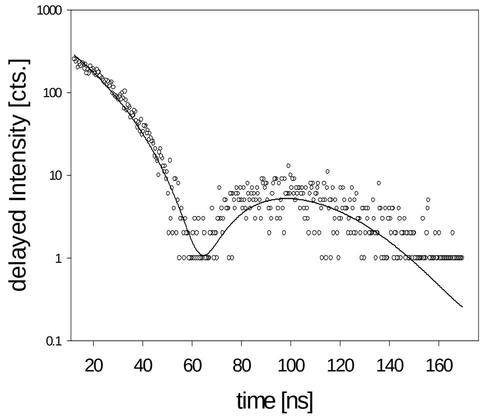

Fig. 2: NRS spectrum of a monolayer of iron on tungsten. The quantum beat is an indication of a tilt of the tilt of the main axis of the EFG out of the position perpendicular to the surface.

All spectra were accumulated at the critical angle. The room temperature spectrum shows a quantum beat corresponding to a quadrupole splitting of 0.68 mm s^{-1}. This value is in excellent agreement with the value 0.66 mm s^{-1} measured by Przybylski with Mössbauer spectroscopy [9]. The expected direction of the electric field gradient (EFG) main axis for a perfect monolayer is perpendicular to the surface due to the broken translational symmetry at the surface. In this case the nuclear resonant spectrum should have the shape of a simple exponential decay due to the perpendicular orientation of the EFG main axis relative to the polarisation plane of the synchrotron radiation. The appearance of the quantum beat in Fig. 2 is an indication of a tilt of the EFG main axis [6]. The tilt angle fitted in the room temperature spectrum is 61 degrees relative to the surface normal. The reason for this tilt is probably the influence of island structure (attoms at edges) and steps.

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