ESRF	**Experiment title:** **Structure of Atomic Gold Chains on Ge(001) by X-Ray Standing Waves**	**Experiment number:** SI2081
Beamline: ID32	**Date of experiment:** from: May 7, 2010 to: May 18, 2010	**Date of report:** October 4, 2010
Shifts: 18	**Local contact(s):** B. Detlefs, P. Rajput	*Received at ESRF:*

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Report:

The aim of the performed experiment was to determine the structure of self-organized atomic Au nanowires on Ge(001) surface by the X-ray standing wave (XSW) technique in flourescence detection. The experiment has been preceded by a test sample preparation time (in March 2010) in order to optimize sample growth conditions. Problems encountered during this preparation time have been identified and solved such that the sample preparation prior to the experiment (May 7th – May 11th) was successful. The commercial substrates we had needed to be repolished in the Optics Lab of the ESRF to meet the required surface quality. During this time, prepared samples were characterized by LEED and STM, showing well organized gold chains with atomic resolution on relatively small terasses (compared to home lab results).

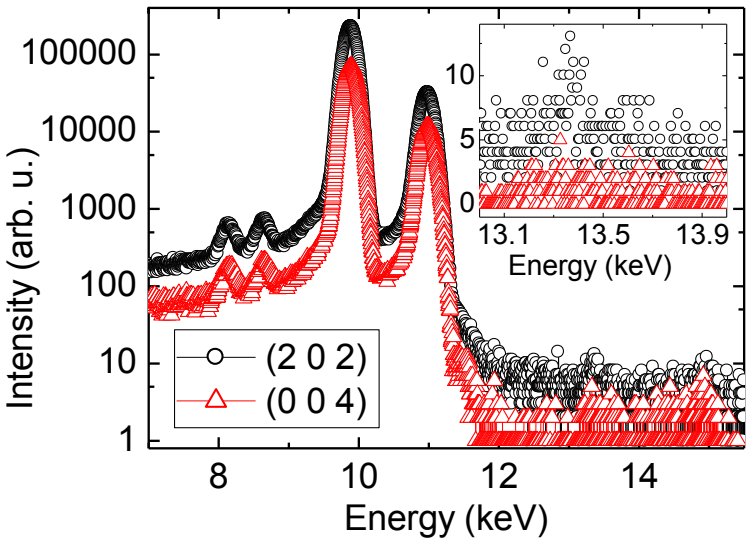

Fig. 1 Fluorescence spectrum of Au chains on Ge(001) taken at an angle close to XSW Bragg condition at Q = (202) (black circles) and Q = (0 0 4) (red triangles). The other available Au L fluorescence line overlaps with Ge K-fluorescence; careful analysis shows it as a shoulder of the strong Ge K line just above 11 keV but the available energy resolution is not sufficient to separate them. The insert shows the energy region used for XSW yield extraction.

The beamtime started with the proposed strategy – to do the XSW experiment with photon energy tuned to 8 keV (to avoid excitation of Ge K fluorescence) using Au M fluorescence lines (Au $M_{\alpha 1,2}$ at ~ 2.1 keV) for XSW yield data. This strategy proved impossible even after careful optimization (Vortex detector settings, geometry changes etc.): as tested with a sample exposed to air (thus fluorescence not passing through the Be window) we were getting far too low intensity to permit XSW imaging. Neglecting possible contamination from air of the air-exposed sample (which is

clearly a simplification), we estimated the transmission of the beryllium window to be in the order of only 0.01% in this energy range.

Hence, the excitation was tuned to 15 keV to probe the Au *L* fluorescence. Since the Au $L_{\beta 1,2}$ lines around ~ 11.5 keV lines are masked by the intense Ge K-fluorescence, only the Au $L_{\gamma 1}$ at 13.382 keV could be analyzed, see **Fig. 1**. However, this line is very weak compared to the Ge *K* fluorescence background, which saturated the SDD detector.The inset of Fig. 1 shows the energy region in the fluorescence scan that was used for XSW yield extraction. As can be seen, the data quality is insufficient for peak fitting so only background has been fitted and the peak integrated intensity was done by numerical integration after background subtraction. The situation was even more complex in the case of off-specular reflection, when the Ge fluorescence could not be partially attenuated by mounting the SSD detector in grazing geometry, which resulted in an even longer tail from the Ge K line. A linear background must have been thus fitted for off-specular reflection instead of a constant one for the specular reflections.

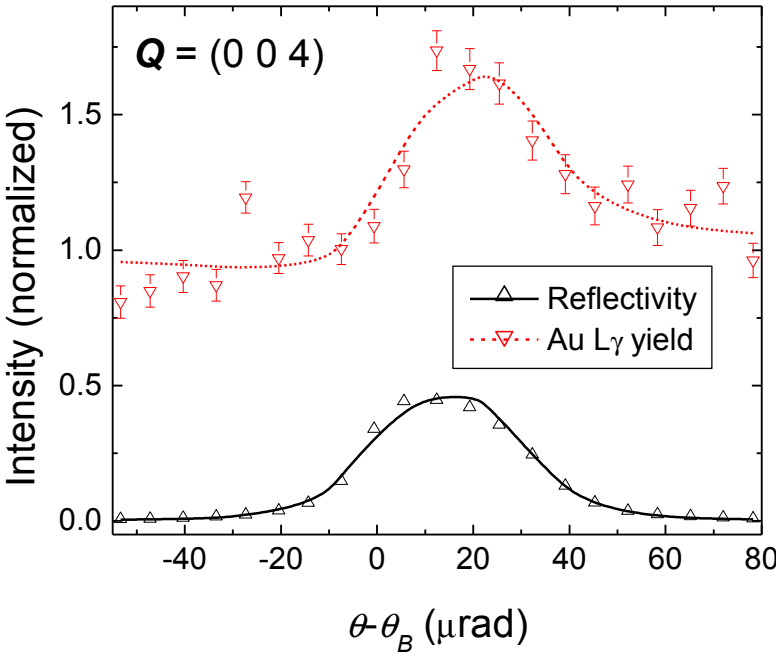

Fig. 2 Reflectivity and Au Lγ fluorescence yield at the ***Q*** = (004) Bragg reflection. High error bars of the fluorescence yield reflect the low intensities. The fit of the XSW signal gives a coherent fraction $F = 0.396(50)$ and coherent position $P = 0.089(25)$.

Two specular reflection (004) and (008) and three off-specular ones: (220), (202) and (1-13) have been studied. A high-resolution channel-cut post-monochromator has been used to match the photon beam energy resolution to the angular width of the studied reflection. This has been necessary because of the high crystalline quality of Ge substrates.

Despite the above-mentioned data acquisition problems related to spectral line composition, a limited XSW data set has been recorded, see **Tab. 1**. Notwithstanding the high quality of the sample (as proven by STM) the determined coherent fractions were much smaller than unity which is indicative of many different Au bonding configurations in the large supercell.

Fig. 2 illustrates the XSW data from the (004) reflection. The rather large error bars on the XSW yield reflect the low intensity of the Au $L_{\gamma 1}$ fluorescence line at 13.382 keV.

We conclude that the fluorescence detection is not a suitable mode for the XSW data acquisition because of the proximity of the spectral lines of adsorbate layer (Au) and substrate (Ge) that challenges the XFS signal detection and analysis. Either a fluorescence detection using a diffraction analyzer crystal or a different yield detection mode, such as photoelectron spectroscopy, must be used in a future attempt to realize this experiment.

Reflection	d_{hkl} *(Å)*	*coh. fraction* F_{hkl}	*coh. position* P_{hkl}	$z_{hkl} = P_{hkl} \cdot d_{hkl}$ *(Å)*
(0 0 4)	1.412	0.396 ± 0.05	0.089 ± 0.025	0.126 ± 0.035
(2 0 2)	1.996	0.263 ± 0.09	0.665 ± 0.06	1.327 ± 0.120
(1 -1 3)	1.702	0.38 ± 0.28	0.21 ± 0.10	0.357 ± 0.170

Tab. 1 Review of the analysis of the XSW data from (004), (202) and (1-13) reflections.