ESRF	**Experiment title:** Structural origin of an unusual magnetic behavior of Cr on Au(111)	**Experiment number:** SI-888
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The crystallographic structure of Cr, deposited on the herringbone reconstruction of Au(111), has been studied as a function of Cr coverage by means of Grazing Incidence X-ray Diffraction.
The single crystalline Au substrate was of (111) orientation within ± 0.1°. It was prepared *in situ* by Ar^+ sputtering and annealing cycles, up to 1000 K. The Cr was evaporated from a Mo crucible containing high-purity polycrystalline chromium, heated by electron bombardment. The growth was made with the substrate held at room temperature. The thickness of the deposit was controlled by both fitting the specular reflectivity Kiessig fringes and Auger Electron Spectroscopy (AES). The surface and Cr deposits cleanliness were controlled by AES. The (111) single crystalline surface is described by the classical triangular unit cell [1] defined by the surface in-plane basis vectors $\vec{a}_1$, $\vec{a}_2$, making a 120° angle (a_1=a_2=$a_0/\sqrt{2}$, where a_0= 2.88 Å is the fcc bulk parameter of gold) and $\vec{a}_3$, perpendicular to the surface ($a_3 = \sqrt{3}a_0$). In this way the reciprocal space indices H and K describe the in-surface plane momentum transfer (Fig. 1), and L the momentum transfer perpendicular to the surface . The photon energy was set to 17.1319 keV (λ =0.7237 Å). The angular resolution for in-plane scans was 0.03 mdeg and the incidence angle was tuned close to the value for total external reflection of the X-rays (∼0.3 ° at 17.1319 kev).
Twenty six thicknesses have been analyzed, from 0 to 10 Cr monolayers. A particular attention has been paid to the lower coverages (from 0 to 1 ML), where an organized growth of Cr clusters is observed at the kinks of the reconstruction and where the most interesting magnetic phenomena are observed (see experimental report HE 1231). Different scans have been performed for each situation to fully characterize the structure :

- **Quantitative measurements of the (10L), (20L), and (30L) Crystal Truncation Rods**, in order to check if there are pseudomorphic Cr atoms on Au(111) or diffusion and formation of an interfacial compound,
- **k-scans along the** [0 k 0.12] **direction** (fig. 2-(a)) to determine the in-plane lattice parameter of Cr (direction (i) in fig. 1),
- **hk-scans along the** [$2h$ $\bar{h}$ 0] **direction** (fig. 2-(b)) to determine the evolution of the gold reconstruction during the growth (direction (ii) in fig. 1),
- **l-scans along the** [0 1+ξ l] **directions** to determine the out-of-plane lattice parameter of Cr (ξ corresponds to the position of the Cr associated peaks determined from kscans for each situation),
- **Angular maps around the (01L) and (02L)** to determine the precise orientation of the Cr in the case of the non-pseudomorphic bcc(110) Cr planes that have been observed for higher coverages (map (iii) in fig. 1),
- **Reflectivity scans** in order to fit the specular reflectivity Kiessig fringes for coverage measurements.

*[1] A. R. Sandy, S. G. J. Mochrie, D. M. Zehner, K. G. Huang, and D. Gibbs, Phys. Rev. B **43** 4667 (1991).*
[2] H. Bulou, F. Scheurer, P. Ohresser, A. Barbier, S. Stanescu, and C. Quirós, submitted to Physical Review B.

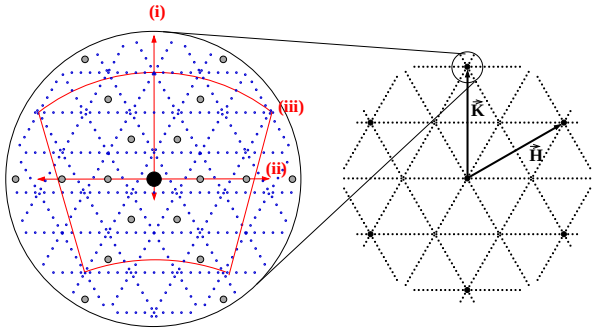

Figure 1: *Reciprocal lattice of the reconstructed Au(111) (right) with enlargements around the (0,1)(left) reflections. The intersection of the crystal truncation rods with the surface plane are represented by the dark disks, the* $22 \times \sqrt{3}$ *reconstruction by smaller grey disks and the reflections due to the kink lattice by dots (for sake of clarity, the contribution of the kinks are only represented in the enlarged regions). Different types of GIXD scans have been recorded in the present study. The arrows labeled (i), (ii) and (iii) indicate the scans displayed in fig.2 and fig.3.*

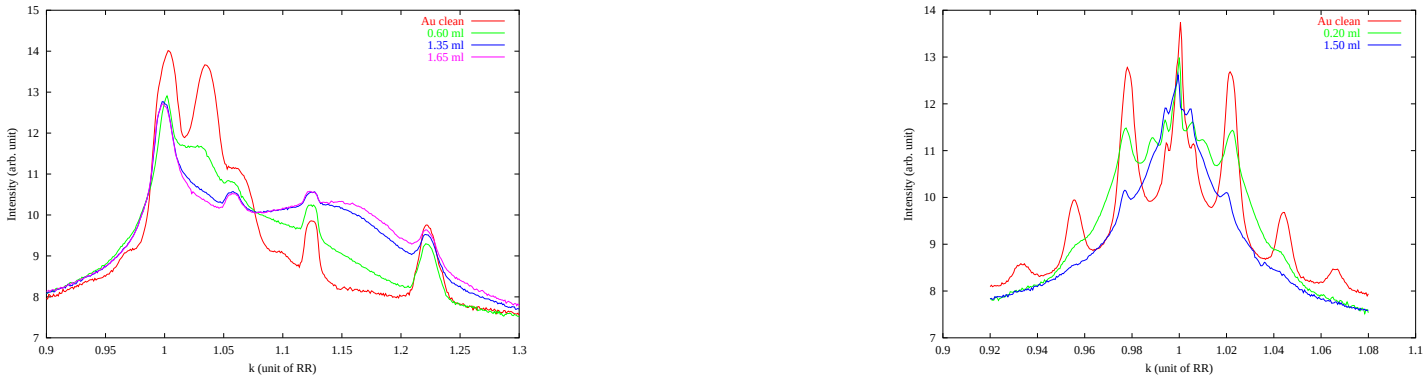

Figure 2: *[left] k-scans along the (0 k 0.1) direction with respect to the Cr thickness. Note that the small bumps at* $k \sim 1.060$, *1.125 and 1.225 are always present on clean gold and likely belongs to residual disoriented crystallites. [right] hkscans around the (0 1 l) rod at l=0.12 for different Cr deposits.*

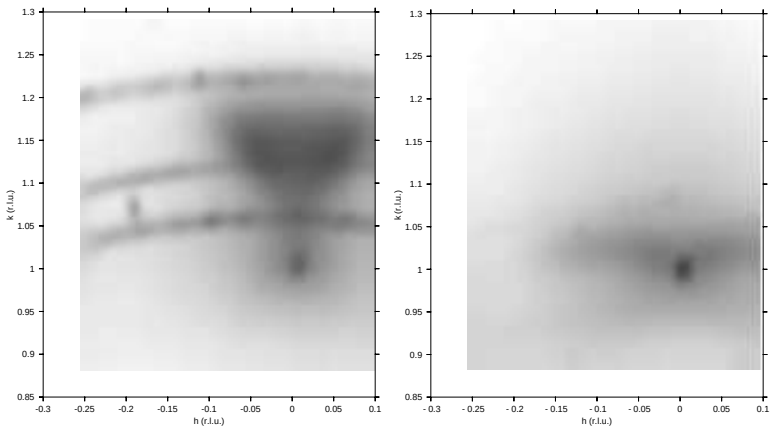

Figure 3: *Maps around the (0 1 0.12) [left] and (0 1 1.7) [right] regions of the reciprocal space for 5 monolayers of chromium. Such maps are characteristic of a bcc(110) structure on an fcc(111) substrate [2]. (The rings are typical of a powder-like diffraction pattern - see figure 2)*