

Growth of Cr on Ir(111) studied by scanning tunneling microscopy

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Abstract

We have studied the room-temperature growth of Cr on Ir(111) by scanning tunneling microscopy. Even in the low-coverage regime, up to a total coverage of 2 monolayers (ML), Cr does not grow in the layer-by-layer mode. Instead, we observe islands with local coverages θ between 1 ML and 5 ML. While the 1st layer growth is pseudomorphic, sporadic defect lines are observed in the 2nd layer. For $\theta \geq 3$ ML periodic one-dimensional dislocation lines appear indicating the onset of strain relief. Scanning tunneling spectroscopy reveals that islands with $\theta = 1$ ML exist in two modifications. Though their tunneling spectra are qualitatively rather similar, direct comparison shows that the main peak is shifted by about 15 mV, resulting in peak positions of -0.255 V and -0.270 V. We interpret these two modifications as regular fcc Cr and Cr which exhibits a faulted hcp stacking on Ir(111), respectively. The assignment of fcc to areas directly attached to substrate steps together with the evolution of the ratio of the different ML-areas with coverage leads to the conclusion that hcp is the more favorable stacking.

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1. Introduction

The magnetic properties of ultrathin films continue to be a topic of great interest. Especially non-collinear magnetic configurations open a new exciting field of research and a two-dimensional model system has been established for theoretical investigations: when an antiferromagnetic material is stabilized on a triangular lattice there must be magnetic frustration which can induce non-collinear magnetic structures. Already ab initio electronic structure calculations for several *collinear* magnetic phases of hexagonal 3d transition metal monolayers (ML) predicted interesting relative magnetic energies and exchange coupling constants [1]. From these calculations it is expected that a Cr ML on Ag(111) and probably also on Cu(111) does not have a collinear magnetic structure. In an advanced approach also *non-collinear* arrangements can be considered with ab initio

methods [2–4]. Within this framework a non-collinear, coplanar 120° spin configuration in a $(\sqrt{3} \times \sqrt{3})R30^\circ$ unit cell, the so-called Néel-state, was found for a Cr ML adsorbed pseudomorphically on Cu(111) [2] and Ag(111) [3]. It was demonstrated within the Tersoff–Hamann model that this magnetic structure should be detectable performing spin-polarized scanning tunneling microscopy (SP-STM) measurements [3]. This technique has proven to be a very powerful tool to investigate not only ferromagnetic domain structures but also to resolve periodic spin structures down to the atomic scale [5–7].

Unfortunately the preparation of pseudomorphic 3d transition metal monolayers on the substrates chosen for the calculations, i.e. Cu(111) and Ag(111), is a quite impractical task due to a strong tendency of these surfaces to intermix [8,9]. Therefore other surfaces with a triangular lattice are considered in the search of a suitable realistic system to induce the hexagonal geometry for a monolayer of the antiferromagnetic Cr. The surface energy, defined as the work required to form a unit area of surface, is a good measure for the probability of intermixing with other

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materials. Out of the non-magnetic 3d, 4d and 5d elements of the late transition metals (i.e. Rh, Ir, Pd, Pt, Cu, Ag and Au) ab initio calculations for the fcc(111) surfaces predict that Ir has the highest surface energy of 3.41 J/m^2 , followed by Rh with 2.78 J/m^2 and Ag having the lowest surface energy of 1.12 J/m^2 [10]. Consequently the system of Cr on Ir(111) was chosen as the most promising realistic system for a pseudomorphic monolayer growth without intermixing at room temperature. In addition to the growth of material in the regular stacking onto a fcc(111) surface, the incorporation of a stacking fault resulting in faulted (i.e. hcp) growth, has been observed for various homo- and heteroepitaxial systems [11,12]. Thus to investigate whether this is a suitable realistic system for further investigations of the magnetic ground state with SP-STM and detailed theoretical calculations, a careful analysis of the growth mode of Cr on Ir(111) is essential.

2. Experimental details

The experiments were performed in an ultra-high vacuum (UHV) system with separate chambers for substrate preparation, molecular beam epitaxy (MBE) and room-temperature STM measurements, surface analysis, and low temperature STM measurements. The base pressure in each chamber is in the low 10^{-11} mbar range. For sample preparation the system includes an Ar^+ ion gun, an electron-bombardment heater, as well as evaporation sources for metal deposition. To monitor the cleanliness of the sample a LEED/AES (low energy electron diffraction/Auger electron spectroscopy) unit is used. The STM measurements were performed in two different microscopes. One is operating at room-temperature and is specifically designed for growth studies [13]: it allows subsequent steps of metal deposition onto the sample surface in between STM measurements without taking the sample out of the microscope. The other STM is a low temperature microscope with tip and sample held at 15 K [14]. It has a tip-exchange mechanism and W-tips are used which are flashed to high temperature in vacuo. This STM has been used for the more delicate full dI/dU spectroscopy measurements because of the higher stability. To obtain topographic images, the STM is operated in constant-current mode with a feedback regulation circuit keeping the tunneling current I_t at a given setpoint by adjusting the tip-sample distance. Simultaneously to topographic images, maps of differential conductance dI/dU can be obtained by adding a small oscillating signal U_{mod} to the bias voltage U_B and measuring $dI/dU(U_B)$ by means of lock-in technique, with the feedback loop active. For full $dI/dU(U)$ spectroscopy measurements the tip is first stabilized at I and U as indicated. Then the feedback circuit is deactivated, the voltage is ramped and $dI/dU(U)$ is recorded. For spatially resolved measurements, full spectroscopy is performed for each image point.

The Ir(111) single crystal was prepared by Ar^+ -ion etching with $E = 800 \text{ V}$ for 1 h with subsequent annealing at

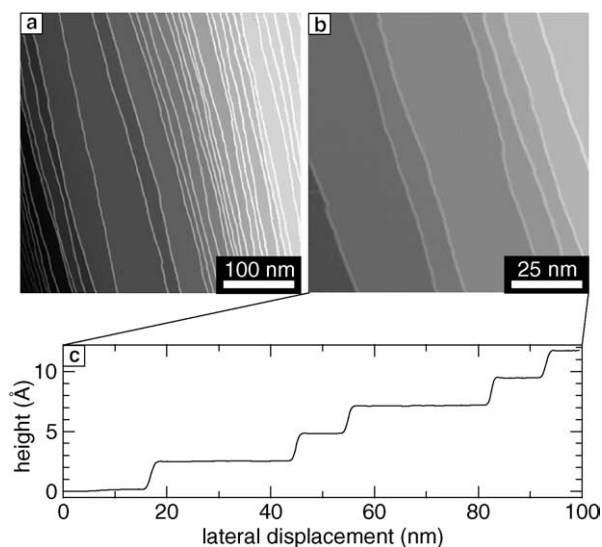


Fig. 1. (a), (b) Topography images of the bare Ir(111) surface ($U_B = +0.5 \text{ V}$, $I_t = 0.5 \text{ nA}$) and (c) height profile along the bottom of (b).

1350 K for 8 min. As-prepared samples showed no major impurities (C, O, N) in AES measurements and a sharp $p(1 \times 1)$ LEED pattern was observed. Typical topography measurements of the bare Ir(111) surface are shown in Fig. 1(a) and (b). The surface is atomically flat with some monatomic steps separating terraces. A height profile along the bottom of Fig. 1(b) is shown in (c) and the measured step height is $2.25 \pm 0.05 \text{ \AA}$, in good agreement with the theoretical value of 2.22 \AA for bulk Ir. Locally, the steps run almost straight and in parallel, while collectively meandering on a larger scale. The adsorbate density is below one per 100 nm^2 or 0.06% of the surface atoms. Cr was evaporated from a tungsten crucible, heated by electron bombardment. The evaporate had previously been cleaned by repeated and prolonged heating. Cr was deposited at a rate of 0.3–0.4 monolayers (ML) per minute with the Ir substrate held at room-temperature. The coverage θ always refers to pseudomorphic monolayers. During deposition, the chamber pressure stayed below 5×10^{-10} mbar. The cleanliness of the material was checked by AES measurements which showed no appreciable contamination (e.g. S, N, C, and O) in a 20 ML thick Cr film.

3. Results and discussion

An overview of the room-temperature growth of Cr on Ir(111) up to a coverage of 1.8 ML is presented in Fig. 2. The bare Ir(111) sample surface is shown in (a). As can be seen in Fig. 2(b) and (c), Cr mainly grows in the step-flow growth mode below 0.5 ML. The few free-standing islands of Cr monolayer have triangular shape, with edges along close-packed rows of the substrate. The surface of the Cr monolayer is smooth without any reconstruction pattern. Together with the appearance of a $p(1 \times 1)$ LEED pattern (not shown) in the submonolayer regime we conclude that the Cr monolayer grows in-plane

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