Structure and morphology of ultrathin Co/Ru(0001) films

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New Journal of Physics 9 (2007) 80
Received 3 November 2007
Published 30 March 2007
Online at http://www.njp.org/
doi:10.1088/1367-2630/9/3/080

Abstract. We follow the layer by layer growth of cobalt on ruthenium by means of low-energy electron microscopy (LEEM) and diffraction (LEED). Around 500 K each layer forms through the nucleation and growth of triangular islands. Fully dynamical calculations of the diffraction intensities establish that the first monolayer (ML) grows pseudomorphically, i.e. following the Ru hexagonal close packed (hcp) stacking sequence. In films thicker than a ML, the in-plane lattice spacing is relaxed and the resulting superstructures produce satellite spots in the diffraction patterns. Our LEED analysis indicates that in two ML films the first Co layer is stacked in two ways on Ru, but there are no stacking faults between the Co layers themselves. In three ML thick regions, additional stacking faults are located at the topmost Co layer. These stacking faults are associated with distinct island shapes and unique selected-area diffraction spectra. Our study supports the simple picture that island orientation reflects the stacking type.
1. Introduction

An important challenge in the science of thin-film growth is to understand how the atomic structure of film/substrate interfaces comes about during the growth of the films. Bulk crystal structures of substrate- and film-material are in general not identical and therefore, to accommodate mismatch between the materials, defects such as dislocations and stacking faults develop at the film–substrate interfaces.

Understanding how interface structure evolves during the dynamic conditions of film growth can benefit greatly from measuring atomic structure in situ, during film deposition. In this field, electron diffraction techniques, including the analysis of intensity versus voltage low-energy electron diffraction (LEED) spectra IV [1, 2], have supplied much helpful experimental data. However, the fact that only spatially averaged information is accessible to conventional LEED IV measurements is a severe limitation. Interfaces are usually not homogeneous and spatial averaging of heterogeneities induces strong artifacts even in some of the simplest imaginable interfaces. For example, if one considers the Ru(0001) surface as a simple interface between a bulk hcp crystal and the vacuum, an important artifact of spatial averaging is evident. Observing the LEED pattern of Ru(0001), one usually finds a pattern with six-fold symmetry, even though an atomically perfect surface of an hcp crystal has three-fold symmetry. The observed six-fold pattern is a result of spatial averaging over many atomically flat terraces: the apparent change of symmetry happens because the three-fold symmetry of terraces separated by atomic-height steps is rotated by 180°. Using a low-energy electron microscope (LEEM) [3]–[5] for micro-LEED IV measurements, we recently showed that the LEED patterns of individual atomic terraces on Ru(0001) indeed have the correct three-fold symmetry [6]. From analysis of these micro-LEED IV measurements, we were able to determine structural parameters of the relaxed Ru(0001) surface that are in better agreement with theoretical predictions [7, 8] than results from the previous LEED IV analysis, which was based on spatially averaged measurements [9]. The benefit of using micro-LEED IV to resolve heterogeneities was also demonstrated in a recent study of surface alloying during the deposition of Pd onto Cu(100) [10] and in earlier work on CO/NO reaction diffusion fronts on Pt(100) [11].
The central aim of the present paper is to understand how atomic structure evolves near the film/substrate interface during the deposition of the first few atomic monolayers (MLs) of Co on Ru(0001). The system is interesting because many studies have shown unusual magnetic properties, which have already spawned important applications. For example, Ru spacer layers are used to induce an antiferromagnetic coupling between thin films of Co alloys in spin-valves and magnetic-recording media [12]. Basic studies have shown that deposition of Co on Ru can result in the formation of three-dimensional (3D) islands in a Stranski–Krastanov growth mode [13]–[15], and that these 3D islands have interesting magnetic properties. In our recent work on flat, ultrathin Co/Ru(0001) films, we showed that the film magnetization easy-axis changes from an in-plane orientation for ML thick films, to out-of-plane for bilayer islands or films, and back to in-plane again for thicker islands or films [16].

One issue that has not been fully understood up to now is how the interfacial atomic structure in Co/Ru(0001) films evolves to accommodate lattice mismatch. Hexagonally close-packed bulk Ru has a 7.3% larger lattice constant than bulk cobalt. Yet, using LEEM we have seen that under appropriate conditions Co can be grown on Ru(0001) in a layer-by-layer mode up to 10 ML [16]. In this paper we present our detailed micro-LEED IV analysis of the morphology and the structure of Co films grown on Ru(0001) up to 3 ML thick. We employ LEEM to follow in real time the growth of the films. The films grow layer by layer through the nucleation and growth of triangular-shaped islands in large, atomically flat terraces. An earlier conjecture suggested that the orientation of the islands reflects the stacking sequence of the Co layers that form each island [17, 18]. We confirm this hypothesis using LEED IV spectra acquired from individual, microscopic regions on the surface that are essentially free of atomic-scale defects.

2. Experimental

The experiments were performed in LEEM systems with base pressures in the $10^{-11}$ Torr range. The lateral spatial resolution is close to 10 nm. The instruments have facilities for in situ heating (up to 1300 K) and cooling (down to 100 K) of the samples while recording images at up to video rate.

The Co films were grown on Ru(0001) crystals. The substrates were cleaned in situ by repeated cycles of exposure to oxygen followed by heating to at least 1800 K. The crystals contains areas, in some cases over 100 µm wide, with a low density of atomic steps. In these regions, terraces more than 5 µm wide can be found routinely. Co was sublimated from high-purity Co rods heated by electron-beam bombardment. Typical evaporation rates were between 1 ML/2 min and 1 ML/35 min. The chamber pressure always remained below $4 \times 10^{-10}$ Torr.

By placing an aperture in the electron beam path to reduce the illuminating beam diameter on the sample to a few microns, we used the LEEM instrument to measure local-area intensity versus energy (IV) curves [1, 2]. This procedure is described in more detail in [6].

3. IV analysis

Fully dynamical IV calculations were performed with a modified version of the Van Hove–Tong package [2, 19, 20]. The surface was modelled by stacking the required number of Co atomic planes (1, 2 or 3) on top of two Ru atomic planes. These surface layers were then stacked on top of
five atomic planes of bulk Ru(0001) using the renormalized forward scattering (RFS) approach. The resulting 2D slabs thus contained between 8 and 10 atomic layers, depending on the Co film thickness. Relativistic phase-shifts [21] were calculated and subsequently spin-averaged. Well-converged values for both the number of beams and the number of phase shifts ($l_{\text{max}} = 8$) were employed in all cases. We explored the parameter space comprised of the stacking sequence of the Co layers, the topmost three interlayer spacings, $d_{l-3}$, and the interlayer spacing of the bulk Ru atomic planes, $d_{\text{bulk}}$, by calculating the IV curves over fine 3D-grids. The interlayer spacings were swept over wide ranges for all possible stacking sequences of the Co layers. We found that including the parameters $d_3$ and $d_{\text{bulk}}$ in the IV analysis had little effect on the agreement between experiment and theory, but increased significantly the error bars for the other parameters. Therefore, we fixed both to the literature Ru spacing, $d_3 = d_{\text{bulk}} = 2.14$ Å. We also included the in-plane lattice parameter, $a_{\parallel}$, in the structural search. $a_{\parallel}$ was made common to all surface and bulk layers.

All simulations were performed for a temperature $T = 300$ K using an energy increment of 2 eV. The experiment–theory agreement was quantified via Pendry’s $R$-factor ($R_P$) [22], while the error bars for each parameter were obtained from its variance: $\Delta R_P = R_P^{\text{min}} \times \sqrt{8E_i/\Delta E}$, where $E_i$ gives the optical (inner) potential and $\Delta E$ corresponds to the total energy range analysed. Correlations between the structural parameters were taken into account for the error-limits estimation. We note that all structural parameters derived in this work represent well-defined minima in their respective $R$-factor plots. Non-structural parameters such as the muffin-tin radius, the optical potential or the Debye temperatures at the surface planes were varied. We found that these parameters had no impact on the final structural conclusions; therefore, we omitted their systematic optimization.

4. Results and discussion

The growth of the Co films was followed in real time by LEEM imaging. The growth on flat areas of the sample proceeds layer by layer up to at least 10 ML. In figure 1 we show frames from a representative movie of a film grown on terraces larger than 5 µm. Islands are nucleated on the terraces in addition to some material growing from the steps of the substrate. The shape of the islands is triangular. On a given substrate terrace, the islands point in one direction for 1 ML islands on Ru, and in the opposite direction for 2 ML islands on a 1 ML film. For 3 ML islands on a 2 ML film, two orientations can be detected on a single substrate terrace.

To understand the structure of the growing film, we perform selected-area diffraction on areas of uniform thickness. Representative LEED patterns are shown in the right panel of figure 1. There is a clear difference between the LEED patterns of different thickness films. One ML islands and continuous films only produce $1 \times 1$ reflections corresponding to the same reciprocal lattice vectors as the original Ru substrate beams. This clearly indicates that the first Co ML is coherently strained to match the in-plane lattice spacing of the Ru substrate. By contrast, the LEED patterns of 2 ML and thicker islands or films are more complex, featuring satellite beams around the substrate reflections. Both for two- and for 3 ML-thick regions, the satellite beams around the specular beam have hexagonal symmetry with the same orientation as the Ru integer beams (i.e. these superstructure spots are non-rotated relative to the substrate beams). In different regions of 3 ML thick films, two noticeably different LEED patterns can be identified. The two patterns can be correlated with the orientation of the original 3 ML islands that expanded into the film regions.
Figure 1. (a)–(c) Sequence of LEEM images acquired during continuous growth at a rate of 1 ML/120 s. The substrate temperature is 470 K. We observe triangular Co islands 1 ML thick on Ru (a), 2 ML thick on 1 ML film (b) and 3 ML thick on a 2 ML film (c), respectively. The LEEM images are 4.4 µm wide, and were acquired with an electron energy of 5 eV (a) and (b) and 20 eV (c). Only in the case of 3 ML islands (c) we observe two different triangular orientations on the same substrate terrace. (d)–(f) LEED patterns acquired from constant thickness areas in Co films with total coverage close to 1 (d), 2 (e), and 3 ML (f). The LEED patterns were recorded at 60 eV (1 and 3 ML) and 37 eV (2 ML) beam energy. The two LEED patterns for 3 ML areas were acquired on the same substrate terrace, on two different regions that originated from islands with different orientation.
Figure 2. LEEM images from a continuous movie taken while growing approximately 0.9 ML Co/Ru(0001) with a substrate temperature of 523 K and a growth rate of 1 ML/223 s. Co is dark grey and Ru is light grey. Three frames (a, b, c) are shown in chronological order. Field of view is 10 µm and electron energy is 20.6 eV.

4.1. The first ML

For the nucleation and growth of the first ML, good contrast conditions with a high intensity of backscattered electrons can be observed using an electron energy of 5 eV. Under these conditions the ML islands appear dark on a light grey background corresponding to the Ru substrate.

A sequence of images illustrating the growth of the first ML is shown in figure 2. There is no growth of second layer islands until more than 90% of the Ru surface is covered with a single-ML film.

The shape of the growing islands is triangular, as already reported in a previous scanning tunneling microscopy (STM) study [23]–[25]. Within each substrate terrace, the triangular islands are all oriented in the same direction, with their edges following compact directions of the substrate surface. When crossing from one terrace to the next, the islands change their orientation by 180°. This change is explained by the substrate hcp(0001) structure, where a rotation of the terrace structure by 180° occurs when one atomic step is crossed [6, 26], as shown schematically in figure 3(b).

In principle, one might have guessed that the observed island shapes are energetically favoured equilibrium shapes. By considering the atomic structure of a hexagonal island on an hexagonal substrate, as sketched in figure 3(a), one can appreciate the origin of three-fold symmetric island shapes. The sketched hexagonal island has two types of symmetry-in equivalent step edges, each step-type exposing a different type of microfacet [27]. In another system, it was shown that the resulting energetic inequivalence can be sufficient to lead to three-fold symmetric shapes of ML islands [28, 29]. However, from our measurements it is evident that the triangular shapes of the islands are not equilibrium shapes, but are a consequence of kinetic limitations. For example, when islands coalesce during growth, the merged multisided shapes do not readily evolve into compact, equilibrium shapes. This implies that edge diffusion is too slow to equilibrate the island shape. In our system, the fact that edge diffusion rates are different for the two types of steps leads to the observed island shapes. The same conclusion was drawn from the previous STM observations [23]–[25].

The fact that all observed islands point in the same direction within each substrate terrace is a strong hint that the stacking sequence is the same for all the islands [17, 18]. For example, in order to expose equivalent microfacets at its step edges, a stacking-faulted island would be rotated by 180° compared to a pseudomorphic island.
Figure 3. (a) Schematic of an hexagonal island on an hexagonal substrate. There are two kinds of step edges, exposing \{100\}-type and \{111\}-type microfacets. Edge-atom diffusivity along the two different types of steps is different, leading to different growth rates of the two step-types. As a result, islands grow in triangular shapes. (b) Schematic of triangular hcp-islands bounded by \{100\}-type steps. In consecutive terraces (left and right sides of the schematic) triangular islands pointing in opposite directions expose the same step-edge type.

In order to describe the stacking sequence of the films, we will use two notation styles. The first is the classic labelling A, B or C for each possible close-packed layer, with ABC... or BCA... indicating face centred cubic (fcc) structure, and ABAB... indicating hcp structure. In this paper, we use a slash to indicate the interface between the Ru substrate and the Co film (or the vacuum interface when the substrate surface is bare). For example, the notation AB/A stands for 1 ML of Co continuing the bulk hcp sequence in a given substrate terrace. Additionally, for summarizing and understanding our results concerning the orientation of the triangular-shaped islands, it is helpful to employ Frank’s notation [30], indicating the stacking of each layer relative to the one below. Transitions of one layer to the next following the sequence A→B→C→A are denoted by △, while the opposite transitions, namely C→B→A→C are denoted by ▽. An fcc structure is written either △△△ or ▽▽▽. An hcp structure corresponds to △▽△ ▽△ ▽.

To determine the stacking sequences of the films, we use LEED IV analysis in the following way. Selected-area LEED patterns from cobalt-ML covered regions show only integer \(1 \times 1\) spots (figure 4(a)). The Co films were grown at 464 K and LEED IV curves were measured three hours later when the sample was at room temperature. Electron energy was swept in the range...
Figure 4. LEED of 1 ML Co/Ru. (a) LEED pattern at 60 eV. (b) Experimental and best fit calculated IV curves. (c) Pendry’s $R$-factor, $R_P$, versus in-plane lattice parameter of the $(1 \times 1)$ cell, $a_\parallel$, for each of the four possible stacking sequences considered. For each sequence and $a_\parallel$ value, we plot the best $R_P$ value among the rest of the structural parameters. The horizontal grey line corresponds to the $R$-factor variance for the best-fit stacking sequence, hcp, from which errors (vertical grey lines) on this parameter are estimated.

50–350 eV and the intensities of the specular (00) beam, the three (10) beams, the three (01) beams, as well as four of the six (11) beams were measured (the remaining two (11) beams were omitted due to systematic distortions associated with the instrumentation). Symmetry-equivalent spectra were averaged, leading to the four experimental IV-curves shown in figure 4(b) as solid
For the structural analysis we considered both possible terminations for the Ru terrace: ABA or BAB/, together with the hcp and fcc stacking sequences for the Co layer. Thus, we explored four stacking sequences in total: BA/B, BA/C, AB/A and AB/C. (Actually, this represents just two different stacking sequences, plus another two that correspond to the same sequences exchanging the labelling of the experimental beams.) The R-factor analysis yields an acceptable agreement for the BA/B hcp sequence, $R_{P^{BA/B}} = 0.23$, while the other cases can be ruled out given their poor fit to the experimental curves: $R_{P^{BA/C}} = 0.76$, $R_{P^{AB/A}} = 0.66$ and $R_{P^{AB/C}} = 0.59$. In Frank’s notation, the best-fit structure corresponds to $\nabla \triangle / \nabla$.

The associated interlayer spacings are reported in table 1. Given the misfit of 7.3% between the in-plane lattice spacings of bulk-Co and bulk-Ru, the Co film is severely strained. This strain is reflected in the first Co–Ru interlayer spacing, $d_1 = 2.05 \, \AA$, which is 4% smaller than the bulk Ru–Ru out of plane distance, and leads to an interatomic distance $d_{Co-Ru} = 2.58 \, \AA$, which is in nice agreement with the sum of their covalent radii, $r_{Co} + r_{Ru} = 1.25 + 1.34 = 2.59 \, \AA$. Finally, figure 4(c) presents the $R$-factor behaviour versus $a_\parallel$ for all stacking sequences explored. The purpose of this fit is to check the sensitivity of the LEED IV curves to the Ru in-plane lattice constant, $d_{Ru} = 2.70 \, \AA$. The error estimation reveals a reasonably good lateral resolution of $\pm 0.03 \, \AA$. The error level is, nevertheless, large enough that we can disregard the potential errors from assuming a constant inner potential as described in [31].

After resolving the structure of the 1 ML film, we proceed to determine the type of step edge of the islands. To such end we need to orient the diffraction pattern of a 1 ML Co film on a single Ru terrace relative to the triangular orientation of the growing islands, as observed on the same terrace. The magnetic lenses of the LEEM system used for these measurements rotate the image when switching between imaging- and diffraction-mode. Therefore, we experimentally measured the image rotation between both lens settings. With this calibration, comparing the island shape and the LEED pattern on the same substrate terrace shows that the exposed step edges are of type {100}.

Our main conclusion for the 1 ML case is that Co grows pseudomorphic with the Ru substrate, keeping both the in-plane lattice parameter and the hcp stacking sequence. It is important to note that our $R_P$ shows a strong sensitivity to the bulk Ru orientation, which allowed us to establish unambiguously the BABA/ (or $\nabla \triangle$/) termination of the Ru terrace used in the experiment reported here. This fact will become relevant for the analysis of higher Co coverages, discussed in sections 4.3 and 4.4, since for those cases it is otherwise difficult to know the Ru orientation.

Table 1. Optimized structural parameters for the Ru(0001)-p(1 x 1) + Co system and for the three coverages studied in this work: 1, 2 and 3 MLs. For the 3 ML case, we provide the values for each phase. All distances are given in (Å). Input records without error bars were not optimized in the IV analysis. See text for further explanations.

| Coverage | Stacking (ABC) | Stacking (Frank’s) | $a_|$ | $d_1$ | $d_2$ | $d_3$ | $d_{bulk}$ |
|----------|----------------|-------------------|------|------|------|------|-------------|
| 1 ML     | BA/B           | $\nabla \triangle / \nabla$ | 2.70 | 2.05 ± 0.05 | 2.10 ± 0.02 | 2.14 | 2.14 |
| 2 ML     | BA/(CB + BA)   | $\nabla \triangle / (\triangle + \nabla) \triangle$ | 2.56 ± 0.08 | 1.94 ± 0.06 | 2.14 ± 0.08 | 2.14 | 2.14 |
| 3 ML-I   | BA/(CBA + BAC) | $\nabla \triangle / (\triangle + \nabla) \triangle \nabla$ | 2.52 ± 0.06 | 1.97 ± 0.04 | 1.99 ± 0.06 | 2.14 | 2.14 |
| 3 ML-II  | BA/(CBC + BAB) | $\nabla \triangle / (\triangle + \nabla) \nabla \nabla$ | 2.52 ± 0.06 | 1.97 ± 0.04 | 1.99 ± 0.06 | 2.14 | 2.14 |
4.2. Transition from first to second ML

When the first Co-ML nearly covers the substrate but before second layer islands nucleate, a change in contrast is observed within the film (figure 5). We interpret this contrast as the conversion of the pseudomorphic first layer film into another phase. The new phase grows quickly until it covers nearly the entire 1 ML film. Second ML islands nucleate shortly after the appearance of the new phase in the ML areas. As the 2 ML islands grow, the new 1 ML phase starts to disappear around them. If deposition is interrupted, the new phase disappears after half a minute at 523 K.

The transient nature of this phase prevents us from carrying out a meaningful LEED IV analysis. Nevertheless, a reasonable guess about its nature can be made based on what has been observed in other, similar systems. Observations of a similar effect have been reported for Cu/Ru(0001) [32] and Pt/Pt(111) [33] films, where a new phase near 1 ML total coverage corresponds to a metastable network of misfit dislocations in the ML areas, making the film about 5% denser than the pseudomorphic phase seen at lower coverage. In those systems, the network of dislocations is only stable under a high concentration of adatoms on top of the film. Consistent with Frenkel–Kontorova modelling [34], this effect is explained by the difference in the energy required to incorporate an atom into the film at a dislocation versus at a step edge. We propose that the new phase in the Co-ML areas corresponds to a similar network of misfit dislocations. In support of our interpretation, we note that misfit dislocations have been observed by STM in Co-ML islands [35]. Note that this type of dislocation network can be described as a reconstruction composed of a network of stacking transitions; i.e. in our interpretation the observed transient phase contains a mixture of small regions stacked in the BA/B hcp sequence and small regions stacked in the BA/C, fcc-like, sequence.

The reason for the ephemeral nature of this reconstructed phase is, firstly, that the required high concentration of adatoms on the 1 ML islands is only achieved when the islands cover most of the Ru surface (which otherwise acts as an adatom sink). Secondly, once 2 ML islands are nucleated, the adatom concentration falls because the edges of 2 ML islands act as adatom sinks. This explains the appearance and subsequent disappearance of the reconstructed phase during the completion of 1 ML Co and the onset of second layer growth, respectively.

4.3. The second ML

The growth of the second layer is shown in figure 6. There are many similarities with the 1 ML case. Nucleation of the second layer is followed by the growth of triangular islands. The orientation of the triangles is constant within each atomic terrace and rotates by 180° from terrace to terrace. The orientation of 2 ML islands relative to 1 ML islands that grew in the same terrace is also changed by 180° (compare figure 6(a) with figure 2(a)). This observation might be interpreted as an indication that the second layer of Co also grows following the hcp stacking sequence of the underlying Ru substrate. The detailed atomic structure is, however, more intricate. The LEED pattern shows satellite spots around the specular and the Ru integer-beams (figure 7(a)), aligned in the same directions as the Ru beams. This indicates that the in-plane lattice spacing of the 2 ML Co islands differs from the lattice spacing of the Ru substrate. Measuring the spacing of the satellite spots indicates a contraction of 5.4 ± 2%, where the error bar is due in part to distortions of the LEEM imaging optics.
Figure 5. LEEM images near completion of the first Co layer (a) and shortly after nucleation of the second layer (b), showing the appearance of a new phase (growth conditions are indicated). The new phase fills up all the ML areas of the film and disappears when the second cobalt ML proceeds to grow. The time between frames is 66 s. Dashed lines frame the light-grey metastable phase when it coalesces.
Figure 6. LEEM images of 2 ML Co island growth, from a continuation of the experiment described in figure 2. The substrate temperature is 523 K and the growth rate is 1 ML/223 s. 2 ML Co regions are dark grey and 1 ML Co regions are light grey. Three frames (a, b, c) are shown in chronological order. Field of view is 10 µm and electron energy is 20.6 eV.

The LEED pattern confirms previous STM experiments [25] where a periodic superstructure was observed and attributed to different lattice parameters of the Co film and the underlying Ru substrate. The reported size of the unit cell was close to a 13 × 13 Ru unit cell [25, 35]. This kind of LEED pattern is typical for lattice-mismatched, heteroepitaxial systems (for example, Co/Pt(111)) [36] or 4 ML Cu/Ru(0001) [37]). The simplest model for such structures is a moiré pattern formed by the coincidence lattice between substrate and film. In principle, in a moiré pattern all relative positions between film and substrate atoms are present. However, film-substrate interactions normally favour three-fold hollow sites (either fcc or hcp adsorption sites). As a result, films tend to distort such that atoms are displaced towards fcc- or hcp-sites, with only few atoms remaining close to bridge and on-top positions. This effect is easily observed in Frenkel–Kontorova models. For example, in the Frenkel–Kontorova calculations of figure 10 of [34], the commensurate supercell is split into two sections: in one section, atoms are close to hcp positions and in the other section atoms are close to fcc positions. The two sections are separated by a smaller number of atoms in or close to bridge and on-top positions. Thus, most film atoms are very close to either fcc- or hcp-sites relative to the substrate.

Dynamical LEED computation accounting for such large unit cells exceeds the scope of this work. Since we are interested primarily in identifying the stacking sequences of the films, we can simulate the super-structures by starting from a simplified model. We first consider combinations of perfect stacking sequences of atoms (A, B, or C stacking positions, not bridge nor on-top positions), and we model the Co layers plus the bulk Ru by assuming a common p(1×1) cell. We then simulate the structure of the supercell by performing weighted mixtures of the IV-curves corresponding to the different stacking sequences of the two main sections of the unit cell.

We fit only the integer beams (0,0), (1,0) and (0,1) for this exploration, choosing integration boxes around each beam that were large enough to include the satellite spots. We vary the lattice in-plane parameter between the Ru bulk constant ($a_{\text{Ru}} = 2.70 \text{ Å}$) and that of Co-hcp ($a_{\text{Co}} = 2.50 \text{ Å}$). For the case of 2 ML films on an hcp substrate, there are eight possible stacking sequences (BA/BA, BA/BC, BA/CA, BA/CB, and AB/AB, AB/AC, AB/CA, AB/CB). Here
we do not consider the possibility of stacking faults forming between the top several atomic layers of the Ru crystal. The reason for disregarding this possibility is that introducing stacking faults in the Ru substrate is unlikely. To relax the tensile strain in the Co film, the topmost Ru layers would need to become denser. The needed atoms would have to come from the Co film or etching the substrate. From measurements described elsewhere [38] we know that Co/Ru interdiffusion can indeed take place, but only at temperatures well above those used in the preparation of samples described in this paper. Also, we do not observe motion of Ru steps during growth. On the other hand, when the first Co layer is being overgrown by the second, the cobalt layer can readily increase its density by incorporating Co atoms from the growth flux. Detailed analysis also shows that Ru substrates do not reconstruct in the closely related systems of Ag/Ru, Au/Ru [39] or Cu/Ru [37].

Our knowledge of the previous 1 ML analysis, then allows us to eliminate half of the eight possible stacking sequences: having measured the IV-curves for 1 ML coverage on the same terrace where the data for the 2 ML islands was subsequently acquired, we can determine the substrate stacking termination by comparing against the 1 ML curves shown in figure 4. The clear difference between the (1,0) and (0,1) spectra permits unambiguous identification of the substrate stacking termination and shows that the Ru surface ends with a BA/ stacking sequence (see the data set summarized in figure 7). Therefore, we explored all four possible registries for the two Co layers: BA/BA, BA/BC, BA/CA and BA/CB. The first two interlayer spacings, $d_1$ and $d_2$, were optimized for each sequence. We point out that the intensity of the experimental (0,1) beam was found to be strongly attenuated for energies above 100 eV. One problem we detected is that the large integration boxes used in order to include the intensity of the satellite beams decreases the signal to noise ratio in the IV-curves. Also we note that the beam alignment was slightly worse in the 2 ML dataset that in either the 1 ML or the 3 ML films. We therefore chose to suppress this range from the analysis in the 2 ML case.

The analysis shows that the stacking sequences BA/BA and BA/CB match the observed IV-data more reliably than the sequences BA/CA and BA/CB. Therefore, we conjecture that the supercell of 2 ML Co/Ru(0001) films contains two regions, one where atoms are close to the stacking sequence BA/BA, and another where atoms are close to BA/CB. To model this structure, we assume that the two phases cover the supercell with given area fractions, and we set the parameters $d_1$ and $d_2$ common to both phases. Then we optimize these three parameters. The best $R$-factor drops to $R_p = 0.27$ when we assume an area fraction of 70% for the BA/BA stacking sequence (hcp) and 30% for BA/CB (fcc), consistent with the STM observations reported in [25].

The two stacking sequences included in our best fit correspond, in Frank’s notation, to $\nabla \Delta / (\nabla + \Delta) \Delta$. As Frank’s notation indicates the stacking sequence relative to the layer below, the unique Frank’s symbol for the top layer of the film means that all the atoms of the upper Co layer are in equivalent three-fold hollow sites formed by the lower Co layer, i.e. no stacking faults exist between the two Co layers. The reconstruction is composed of a network of stacking faults that are confined to the interface between the Ru substrate and the Co bilayer film. In other words, the atoms of the first Co layer occupy both types of Ru hollow sites. But the second-layer Co atoms occupy only one type of hollow site.

Figure 7(c) also shows the sensitivity of $R_p$ to the value of $a_\parallel$. Our analysis suggests the value $a_\parallel = 2.56 \pm 0.08 \, \text{Å}$, which is quite close to the bulk Co in-plane constant ($a_\parallel^{\text{Co}} = 2.50 \, \text{Å}$) and clearly different from the bulk Ru in-plane spacing (2.70 Å). The unit cell calculated from this value is close to $14 \times 14$ Co atoms (35 Å in length), in good agreement with the STM findings.
Figure 7. LEED of 2 ML Co/Ru. (a) Left panel: pattern at 157 eV showing the integer beams. Right panel: zoom of the specular spot at 132 eV. (b) Experimental and best-fit calculated IV curves. (c) Pendry’s $R$-factor, $R_P$, versus in-plane lattice parameter of the (1 × 1) cell, $a_\parallel$, for each of the four possible stacking sequences considered. For each sequence and $a_\parallel$ value, we plot the best $R_P$ value among the rest of the structural parameters. The horizontal grey line corresponds to the $R$-factor variance for the best-fit stacking sequence, BA/BA or hcp, from which errors on each parameter are estimated.

reported in [25]. We feel the agreement between experimental data and our computed IV spectra is reasonable, given the simplified model employed. The structural parameters corresponding to the best fit are given in table 1.

Summarizing, for 2 ML Co films, we find that they present a moiré pattern composed of two stacking sequences. The stacking transitions are located at the Co/Ru interface, not between the
Figure 8. 3 ML Co island growth. The images shown are from same experiment as those in figures 2 and 6. The substrate temperature is 523 K and the growth rate is 1 ML/223 s. Three ML Co is dark and medium grey and 2 ML Co is light grey (some white regions are 1 ML Co). Three frames (a, b, c) are shown in chronological order. Field of view is 10 µm, and electron energy is 20.6 eV.

two Co atomic layers. This structure of the 2 ML islands can be expressed in Frank’s notation, which reveals more directly the fact that the termination of the Co film is unique: ▽△/(▽△ + △)△.

4.4. The third ML

The third ML also grows by way of triangular islands (figure 8). Unlike in thinner films, we now find populations of triangle-shaped islands with two (opposite) orientations on each terrace (figure 9(a)). One might guess that the presence of both orientations on a given terrace can be explained by associating the two orientations with two different stacking sequences. That is, depending on the stacking sequence, favoured growth of type {100} island edges leads to different orientations of triangular islands (see figures 9(c) and (d). This effect has been used as a fingerprint of stacking faults in other systems such as Co on Cu(111) [18], or Ir/Ir(111) [40]. We use LEED IV analysis to show that this interpretation is correct and to establish exactly at which layer the stacking fault occurs.

We find that at particular electron energies, for example close to 20 eV and to 48 eV, the specular reflectivities of islands with opposite orientations are substantially different. In the images taken at 20 eV all the islands with one orientation appear dark grey, while islands in the opposite orientation appear light grey (figure 9(b)). A similar kind of contrast has been observed previously in the Cu/Ru(0001) system, where we attributed the effect to stacking-sequence domains at the second layer of Cu on Ru(0001) [41]. The difference in contrast between islands oriented in opposite directions allows us to keep track of the stacking type of local regions during growth from isolated islands to continuous films, in which island shapes and orientations became obscured due to coalescence. The contrast also reveals that both types of regions occur in areas where the third layer grows from steps (step-flow, lower part of figures 9(a) and (b)). The contrast difference is stable with respect to mild annealing. The two film types can be also imaged in dark field as well as in bright field, using non-specular integer reflections. At 40 eV the (01) beams are much more intense than the (10) beams in islands of one orientation, while the reverse is true for the islands with opposite orientation. This leads to strong contrast in dark-field images (similar to the contrast observed by transmission electron microscopy between twins in systems such as gold-on-mica [42]). The dark-field contrast reverses when going from one substrate terrace to
Figure 9. (a) and (b): experimental observations of triangular islands with opposite orientation on 3 ML Co. The size is $2.1 \mu m \times 1.7 \mu m$. Electron energy is 5 and 20 eV, respectively. (c) and (d) Schematic of two triangular islands on an hexagonal substrate. (c) The substrate and the island are hcp and the favoured microfacet is {100}. (d) The island has a stacking fault, i.e. the atoms are located at fcc adsorption sites. With the inverted shape relative to (c), step edges expose the same type of microfacet. (e) and (f) Same area observed in bright field (specular beam, $eE = 22$ eV) (e) and in dark-field using one of the first order Co beams (f, $eE = 55$ eV). In dark-field imaging (f) island-orientation reversal matches contrast reversal when crossing a substrate step. In bright field imaging (e) contrast remains constant when crossing substrate steps.
the next, matching the orientation reversal of the island shape at consecutive terraces, as shown in figure 9(f). On the other hand, bright field contrast shows no reversal from terrace to terrace (compare figures 9(e) and (f)).

It is helpful to note that when we assign stacking sequences to films 3 ML thick, the sequences correspond to either fcc or hcp structure within the Co-slab, independent of their registry with the Ru substrate. Not taking into account the presence of a moiré-like structure at the Co/Ru interface, we might naively try to assign the two island populations to hcp and fcc stacking sequences. We might guess that hcp stacking corresponds to the islands whose orientation is inverted relative to 2 ML islands that grew previously on the same terrace, as suggested by Frank’s notation of an hcp stacking sequence $\triangle \nabla$. The other 3 ML islands, aligned in the same orientation as 2 ML islands grown earlier in the same terrace, would be assigned to fcc stacking by this argument. Surprisingly enough, this guess of the stacking sequences within the Co film is confirmed by selected-area LEED IV analysis.

For this analysis, we measured LEED patterns and IV-curves from each type of region when the total coverage is close to three complete MLs. As in the case of 2 ML films, the diffraction patterns show satellite spots, indicating that the 3 ML films are relaxed (reconstructed) within the surface plane. Following the same procedure as in the case of 2 ML films, the integer beam IV-curves were obtained by integrating intensity within boxes that were sufficiently large to include also the satellite beams.

We simulated the IV spectra for a 3 ML thick Co film on top of Ru(0001), again assuming a common $p(1 \times 1)$ cell for all layers. Using our prior knowledge (as discussed in section 4.1) that the Ru substrate termination in our region of interest corresponds to BA/, we explored all eight possible stacking sequences of the three Co layers: BA/BAB, BA/BAC, BA/BCA, BA/BCB, BACAB, BACAC, BA/CBA, and BA/CBC. (Again, as for the 2 ML case, we rule out the possibility of a reconstruction in the last Ru layers.) We varied the in-plane lattice parameter, $a_\parallel$, and the first two interlayer spacings. For the two types of regions we had identified experimentally, $R$-factor analysis was performed independently. The resulting $R$-factors are plotted in figures 10(d) and (f) as a function of $a_\parallel$. Two very similar pairs of minima are substantially more pronounced than all other minima: $R_p^{BA/CBA} = 0.32$ and $R_p^{BA/BAC} = 0.37$ for region I and $R_p^{BA/CBC} = 0.29$ and $R_p^{BA/BAB} = 0.30$ for region II. Using Frank’s notation, these minima correspond to $\nabla \triangle \nabla \triangle$ in region I and to $\triangle \nabla \nabla \triangle \nabla$ in region II. We note that the two minima in region I (figure 10(d)) correspond to fcc stacking within the Co film (/CBA and /BAC) and that both minima share very similar $a_\parallel$ values. The only difference between these two minima is the relative stacking of the film with respect to Ru. In contrast, both minima in region II (figure 10(f)) correspond to hcp stacking within the Co film. Again, both share the same in-plane lattice constant and differ only by their relative stacking with respect to the Ru substrate. This local-area LEED IV analysis confirms the conjecture we proposed at the beginning of this section, stating that the two different orientations of the triangular shapes of 3 ML islands are associated with fcc- versus hcp-stacking. The two types of 3 ML films only differ in how the third Co layer is stacked on the second layer. This stacking difference, a stacking fault, consistently explains our experimental observations. The existence of two minima per region suggests that the two types of 3 ML regions are both reconstructed and that the reconstructions are composed of two stacking sequences relative to the underlying Ru, as expected from the moiré-like LEED pattern. As was done in the case of 2 ML, we tested this model by comparing the experimental spectra with weighted mixtures of the two best-fit pure structures. This led to improvements for both regions: $R_p = 0.31$ for region I (fcc) and $R_p = 0.28$ for region II (hcp).
Figure 10. LEED of 3 ML Co/Ru. (a) 55 eV LEED pattern of a region corresponding to the islands that appear dark grey (region I) in figure 9(a). (b) Zoom of the specular beam of the same region at 132 eV. (c) and (e) Experimental and best-fit calculated IV curves for region I (BA/BCA or fcc stacking) and region II (BA/BAB or hcp stacking), respectively. (d) and (f) Pendry’s $R$-factor, $R_P$, versus in-plane lattice parameter of the $(1 \times 1)$ cell, $a_\parallel$, for region I and region II, respectively. We include in each plot the eight possible stacking sequences. For each sequence and $a_\parallel$ value, we plot the minimal $R_P$ value with respect to all other structural parameters. The horizontal grey line corresponds to the $R$-factor variance for the stacking sequences, BA/CBA and BA/CBC, from which errors on each parameter are estimated.
During mild annealing, or during deposition of additional Co, we do not observe changes in the stacking structure of completed 3 ML thick regions of the films. This stability of the two populations with different third layer stacking sequence is in contrast to other systems such as Cu/Ru(0001) [41], Ir/Ir(111) [43, 44], or Ag/Ru(0001) [45] where stacking faults were observed to heal out either by thermal activation, or during further deposition of additional material (Ag/Ru).

It is interesting to examine the dependence of the area-fraction of fcc- versus hcp-regions on the substrate morphology. The ratio of both type of islands depends very clearly on whether the islands grew from underlying Ru step edges by step-flow, or whether they nucleated within atomically flat terraces. Figure 9 shows both types of areas. At 471 K, roughly half of the Co that grows from steps has fcc structure (lower part of figure 9(b)) and the other half has hcp structure. When deposited at slightly lower temperature, 435 K, all the step-flow Co grows hcp. A suggestion to explain this difference is that the fcc structure is energetically preferred, while the presence of the step replicated from the Ru-substrate in the growing film favours nucleation in an hcp stacking sequence that can match the step-edge without additional dislocations. More experiments will be required to confirm this idea.

The ratio of fcc to hcp islands nucleated away of the substrates steps, on atomically flat terraces, is very sensitive to the overall cleanliness of the experiment. When the Co-deposition and the LEEM measurements are done at total pressures below $5 \times 10^{-11}$ Torr, then the 3 ML islands grow mostly in the hcp stacking sequence. In this case the orientation of 3 ML islands is reversed compared to the orientation of 2 ML islands that appeared earlier on the same terrace. This can be seen by comparing figures 11(c) and (d). With continued deposition (not shown), we find that 4 ML triangular islands point mostly in the same direction as 3 ML islands, indicating fcc stacking. By contrast, when the residual gas pressure during deposition is higher, then the 3 ML islands mostly grow in fcc structure. In this case, the orientation of most 3 ML islands (as well as thicker islands during further deposition) is the same as for 2 ML islands (figures 11(a) and (b)). These findings suggest that a transition from hcp to fcc structure occurs at 3 ML, unless the film is extremely clean, in which case the transition is delayed until 4 ML. This observation highlights the strong effect that even minute amounts of adsorbates can have on the stacking fault density.

We find that the fcc structure is preferred in Co/Ru(0001) films in the thickness range above 3 or 4 ML. This fact might seem surprising, given that the most stable bulk-Co structure below 690 K is hcp. Nevertheless, we note that the same result, i.e. mostly fcc films, was reported for the growth of Co on Pt(111) [36, 46].

5. Conclusions

In summary, we have studied the growth of the first few layers of Co on Ru(0001) by means of LEEM, LEED and dynamical IV calculations. The large terraces found in the Ru substrate allow Co to grow layer by layer despite the large difference in in-plane lattice parameters. We summarize in figure 12(a) the structures derived in the present work. The first layer grows pseudomorphically and continues the hcp stacking sequence of the Ru(0001) substrate. The shape of the islands is triangular, exposing \{100\}-type steps, and the orientation rotates 180° in consecutive terraces, as expected for the hcp substrate. Thicker films reconstruct in order to recover the Co bulk in-plane lattice constant, yielding satellite spots in the diffraction patterns.

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Figure 11. Comparison of triangle orientation with different background pressures and similar conditions (growth rate and temperature are 1 ML/220s and 515 K respectively). Black triangles mark the most common orientation. (a) and (b) Background pressure $4 \times 10^{-10}$ Torr (field of view is 10 µm, $eE = 20$ eV). (c) and (d) Background pressure in the $10^{-11}$ Torr range (field of view is 7 µm, $eE = 7$ eV).

For 2 and 3 ML films, best IV fits are always obtained for weighted mixtures of hcp and fcc stacking sequences between the lower-most Co layer and the top-most Ru layer. Coexistence of two stacking sequences is consistent with STM observations of Co films [25], which have shown the presence of reconstructions with large unit cells that contain regions with different stacking sequences. The second layer of Co also forms triangular islands. Their orientation is inverted with respect to the 1 ML triangular islands on the same terrace, and there are no stacking faults between the two Co layers. The third layer grows again in triangular islands, but this time, islands with two opposite orientations are observed on the same terrace. By selected area LEED IV-analysis, we confirm the correspondence between island orientation and stacking-sequence in the 3 ML islands: the two experimentally detected regions correspond to two possible stacking sequences of the third layer on top of the 2 ML film. The detailed knowledge of the stacking structure and its relation to island shapes revealed here, along with the interesting magnetic properties of these films [16], makes the Co/Ru system an excellent candidate for basic and applied material research studies.
Figure 12. (a) Cross-sections of the stacking sequences, both in ABC and Frank’s notations, as derived from the LEED IV analysis. For coverage above 1 ML, the film is reconstructed and two relative registries between the deepest Co layer and the topmost Ru layer coexist. Note that the orientation of the triangles in Frank’s notation follows that experimentally found for the triangular islands. In 3 ML films, regions I and II differ only in the stacking of the third Co layer.

Acknowledgments

This study was partly supported by the US Department of Energy under contracts no. DE-AC02-05CH11231 and no. DE-AC04-94AL85000, and by the Spanish Ministry of Science and Technology under projects no. MAT2003-08627-C02-02, MAT2003-04278, 2004-HU0010, MAT2004-05348-C04-2, NAN2004-09125-C07-06 and MAT2006-13149-C02-02. FE gratefully acknowledges support from a PhD contract from the Education and Science Spanish Ministry.

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