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Reconstructed bcc Co films on the Cr(1 1 0)/W(1 1 0) surface

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Abstract

Ultrathin epitaxial Co films on Cr(1 1 0) are examined by scanning tunneling microscopy and spectroscopy (STM and STS). At room temperature Co grows as pseudomorphic bcc layers for the first two monolayers and forms close-packed Co layers with stacking faults for thicker coverages. A periodic lattice distortion appears in two equivalent (3×1) reconstruction domains in combination with a regular lattice of dislocation lines oriented along the in-plane close-packed row directions bcc$[1\,\bar{1}\,1]$ and bcc$[\bar{1}\,1\,1]$. The reconstruction and the occurrence of dislocation lines are caused by the epitaxial strain. The local density-of-states function is mapped by scanning tunneling spectroscopy. The bcc Co layers show pronounced differences in comparison to close-packed layers in agreement with theoretical predictions.

Keywords: Scanning tunneling microscopy (STM); Scanning tunneling spectroscopy (STS); Growth; Metallic films; Pseudomorphic structure; Cobalt; Chromium; Tungsten

1. Introduction

Ultrathin epitaxial films represent a class of metastable materials providing exceptional electronic and magnetic properties. Of particular interest are ultrathin Co films that are stabilized in a metastable bcc state [1]. Used as ferromagnetic contacts of a tunneling magnetoresistance device (TMR), bcc Co has enabled a remarkable increase of the TMR effect to a value of 410% at room temperature [2]. The exceptional high effective spin polarization of bcc Co in combination with its high potential Curie temperature was made responsible for this progress. In addition Co/Cr superlattices comprising bcc Co interlayers are interesting for perpendicular recording due to the large out-of-plane anisotropy of this interface [3].

The epitaxial stabilization of bcc Co has been a longstanding case of scientific debate [1]. According to theory bcc Co is unstable, but a metastable body-centered-tetragonal (bct) state exists for (1 0 0) oriented films exposed to epitaxial strain [4]. The epitaxial strain depending on the lattice constant of the bcc substrate is minimized in the case of Cr because of the coincidence of nearest neighbor distances ($a_{\mathrm{nn}}(\text{bcc-Cr}) = 2.498$ Å and $a_{\mathrm{nn}}(\mathrm{Co}) = 2.506$ Å).

Textured Co/Cr(1 0 0) [5], Co/Fe(1 1 0) [6] and Co/Cr(1 1 0) [3,7,8] superlattices have been prepared on various substrates. The growth of tetragonally distorted (1 0 0)-oriented Co films has been reported for Co on Pt(1 0 0) [9], GaAs(1 0 0) [10], Ge(1 0 0) [11], Fe(1 0 0) [2,12–14], FeAl(1 0 0) [15], Pd(1 0 0) [16,17], W(1 0 0) [18,19] and Au(1 0 0) [20]. On Cr(1 0 0), Co grows pseudomorphically in a bcc structure for the first few monolayers followed by continuous relaxation towards hcp structure [21,22].

The bct-type of tetragonal distortion observed in (1 0 0)-oriented films is forbidden by symmetry in (1 1 0)-oriented films. Therefore the growth in this orientation is also of great interest. Co films up to 35 nm were grown on GaAs(1 1 0) [1] with a magnetization slightly lower than the bulk value. A recent study showed that Co forms an interfacial alloy at the GaAs(1 1 0) surface followed by

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bcc Co containing 6 at.% Ga [23]. Using Sb as a surfactant partly leads to a removal of lattice distortions and to an improvement of the magnetic properties [24].

Using high-resolution low-energy electron diffraction it was shown that ultrathin epitaxial Co/Cr(110) films can be grown as pseudomorphic bcc films up to 30 ML [25,26]. Electron diffraction also revealed a (3×1) reconstruction at the surface of bcc Co(110) [25]. However, the atomic structure of this superstructure has not been clarified yet.

First principles theory predicted different electronic states for bcc Co [27,28] in comparison to fcc Co [29] or hcp Co [30]. A prominent difference in the density-of-states function is given by the position of the sharp maxima related to minority states, +0.6 eV (+1.2 eV), and majority states, −1.9 eV (−0.7 eV) relative to the Fermi energy for bcc Co (fcc/hcp Co). The calculated Curie temperature turns out to be considerably larger for bcc Co than for hcp Co, suggesting that TMR devices with bcc Co electrodes maintain high magnetoresistance values at elevated temperatures [28]. In experiment it turned out to be difficult to obtain spectroscopic information on bcc Co because of the inhomogeneous character of the thin film samples.

The aim of the present study is to verify the stabilization of bcc Co on Cr(110) and to reveal the atomic positions within the previously observed superstructure. We will further investigate the local density-of-states function on a well-defined bcc Co surface using scanning tunneling spectroscopy. Instead of using a bulk Cr substrate, which is difficult to prepare, we have grown thick Cr buffer layers on W(110). After annealing the Cr has formed large separated islands with lateral dimensions of up to 100 nm and a (110) oriented surface without steps. On this Cr(110) surface Co forms an epitaxial bcc phase up to 2 ML comprising a surface reconstruction and a net of dislocation lines. Thicker films show a close-packed phase with stacking faults. For the bcc films we could identify the atomic positions in the unit cell of the previously reported superstructure [25]. Differential tunneling spectra measured on homogeneous bcc Co areas are compared to the calculated band structure features.

2. Experimental

The experiments were carried out in an ultrahigh vacuum chamber (UHV, $p < 1\times10^{-10}$ Torr) equipped with a 4-grid LEED optics and an omicron ‘Micro-STM’ for measurements at room temperature. The single crystal W(110) surface was cleaned by cycles of annealing in an oxygen atmosphere at 1200 K and subsequent flashing at 2000 K. We deposited Co and Cr (99.99% purity) from BeO crucibles with a rate of 0.1 ML/min at a substrate temperature of 300 K. After the deposition of the Cr buffer layer we annealed the sample at 500 K. Subsequently the Co film was deposited near room temperature in order to avoid interdiffusion. The pressure increases during evaporation to $p = 2\times10^{-10}$ Torr. The evaporation rate for both elements was monitored by a quartz balance which in turn was calibrated by STM images.

Differential conductance $\mathrm{d}I/\mathrm{d}U$ spectra were measured by scanning tunneling spectroscopy (STS), using a lock-in technique with a 8.44 kHz bias voltage modulation of 50 mV. All bias voltages denote sample voltages with respect to the tip. For STM and STS we have used a $\mathrm{Pt}_{80}\mathrm{Ir}_{20}$ tip cut under tensile stress from a thin wire.

3. Morphology and structure

The growth of Cr on W(110) starts with the growth of a pseudomorphic monolayer with a misfit of 10% and proceeds with the formation of a regular net of dislocation lines indicating that the epitaxial strain has already relaxed in the second layer. Thicker Cr films grow in the Stransky–Krastanov growth mode thus forming elongated island structures with steps oriented preferentially along the [001] direction. The growth mode is largely similar to that of Fe on W(110) as expected because of the similar lattice constants and surface free energies of Fe and Cr [31,32]. With increasing annealing temperature the step density of the Cr surface decreases and simultaneously the difference between the thickest and thinnest areas of the Cr film increases. This behavior turns it difficult to obtain flat films in combination with a small step density.

Here we focus on Cr buffer layers annealed at comparatively high temperatures (500 K). At this temperature the previously continuous Cr film forms islands with lateral dimensions of up to 200 nm [31] (see Figs. 1a and 2). A single monolayer of chromium resides at the W(110) surface adopting a flat coincidence lattice [31,32]. In our case the island formation occurs at slightly lower temperature than previous observations [32]. The Cr island surface represents a nearly ideal (110) surface, i.e. the steps on the island surface have completely disappeared. The lateral shape of the Cr islands is no longer influenced by the W(110) substrate steps, which are now hidden below the island. Instead the island shape is marked by straight edges running along the close-packed $\langle 111\rangle$ and $\langle 001\rangle$ atomic row directions of the bcc(110) surface. The underlying step structure of the substrate thus leads to a thickness variation across the island as illustrated by the profile shown in Fig. 1b. In this case the thickness increases from 12 ML at the left side to a maximum of 18 ML at the right side of the island.

Because the islands are much larger than the transfer length of the LEED electron gun the LEED image (Fig. 3a) simply comprises the addition of the diffraction from 1 ML Cr/W(110) surface and from the Cr(110) island surface. The inner (1×1) pattern in Fig. 3a stems from the 1 ML Cr/W(110) surface while the outer set originates from the Cr(110) island surface. The ratio of the distance of corresponding spot positions results in (1.085 ± 0.005) which is in agreement with the different lattice constants of W (3.16 Å) and Cr (2.91 Å). The W(110) and Cr(110) related spots are equally sharp, thus confirming the translation symmetry of the Cr surface. In