

# Pseudomorphic Co films stabilized on the Cr (1 1 0) surface

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## Abstract

Epitaxial Co films on Cr (1 1 0) are examined by high-resolution electron diffraction. Co is stabilized in pseudomorphic structure over the entire coverage range investigated (up to  $\sim 60$  Å in film thickness). As a structural peculiarity, the overlayer exhibits a  $(3 \times 1)$  reconstruction which exists in two equivalent domains. Each of these domains implies uniaxial threefold superperiodicity along one of the two in-plane close-packed row directions respectively. It is suggested that the reconstruction observed here is a consequence of pseudomorphic stress. © 1999 Elsevier Science B.V. All rights reserved.

**Keywords:** Epitaxial growth; Thin films; Pseudomorphic structure

The fabrication of metallic superlattices provides artificial materials with exceptional magnetic and electronic properties [1]. If one aims at heterostructures with stacking periods down to the atomic scale it is indispensable to achieve a definite crystallographic relationship between particular constituents of the multilayer. For some metal combinations, however, mutual epitaxy is complicated by the mismatched equilibrium structures involved. Such a situation occurs when Co (hcp,  $a = 2.51$  Å,  $c/a = 1.62$ ) and Cr (bcc,  $a_0 = 2.88$  Å) are combined. Despite repeated attempts [2,13,14] the stabilization of pseudomorphic Co within (1 0 0)-oriented Co/Cr superlattices has not succeeded so far. For Co/Cr (1 0 0) films it has been reported that pseudomorphic Co is stable only for the first few monolayers prior to continuous relaxation towards intrinsic hcp structure [3]. In contrast, a quite different behavior occurs when Co is grown on Cr (1 1 0); here, we provide evidence that Cr (1 1 0) serves as a suitable template to stabilize pseudomorphic Co films up to several nm in thickness.

A polished Cr (1 1 0) crystal was cleaned in UHV by  $\text{Ne}^+$  sputtering at  $\sim 900$  K (for further details see Ref.

[4]). After repeated sputtering cycles no residual nitrogen was detectable by X-ray photoelectron spectroscopy (XPS) and a sharp  $(1 \times 1)$  LEED pattern was observed. At this stage a mean defect-free terrace size of  $\sim 600$  Å was deduced from the halfwidth of the specular beam. Co was deposited from an electron beam evaporator at a rate of  $\sim 0.5$  Å/min.

The Co films grown were investigated by high-resolution LEED which allows a quantitative determination of surface roughness [5] by analyzing beam profiles as a function of the scattering phase  $S = |\mathbf{K}_\perp|d/2\pi$  ( $d =$  layer spacing). In the present case, no broadening of the specular beam is observed for films grown at 500 K, while it does occur at lower growth temperatures. Hence, deposition at 500 K essentially leads to a flat growth front. It was confirmed by complementary XPS measurements that significant interdiffusion does not take place under the present growth conditions. For this purpose, the coverage dependence of the Cr2p- and Co2p emission intensities were measured at 500 K growth temperature. Since Cr2p- and Co2p photoelectrons excited by Al  $K_\alpha$  radiation have similar kinetic energies (i.e., their escape depths  $\lambda$  are comparable) the simplified relation  $s/\lambda \cong \ln[1 + (I_{\text{Co}2\text{p}}/I_{\text{Cr}2\text{p}})(S_{\text{Cr}2\text{p}}/S_{\text{Co}2\text{p}})]$  (Ref. [6]) holds if the substrate is attenuated by a film of uniform thickness  $s$ . Here,  $I_{\text{Co}2\text{p}}$  and  $I_{\text{Cr}2\text{p}}$  are the coverage-dependent intensities while the quantity  $(S_{\text{Cr}2\text{p}}/S_{\text{Co}2\text{p}})$  is the atomic

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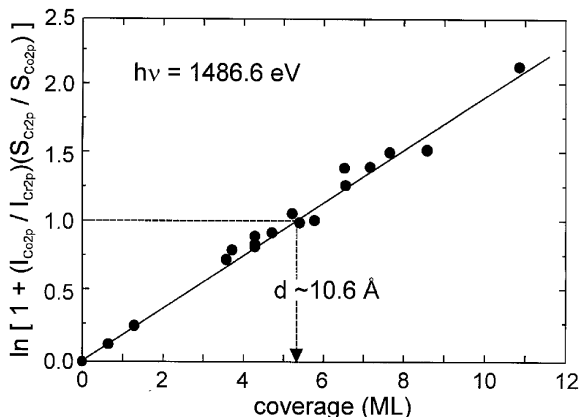


Fig. 1. Quantity  $\ln[1 + (I_{\text{Co}2p}/I_{\text{Cr}2p})(S_{\text{Cr}2p}/S_{\text{Co}2p})]$  vs. coverage with  $I_{\text{Co}2p}$  and  $I_{\text{Cr}2p}$  the coverage-dependent Co2p- and Cr2p XP emission intensities.

sensitivity factor ratio which equals 0.377 [7]. Fig. 1 shows that the quantity  $\ln[1 + (I_{\text{Co}2p}/I_{\text{Cr}2p})(S_{\text{Cr}2p}/S_{\text{Co}2p})]$  extracted from the measured XP intensities indeed depends linearly on the coverage (the latter was calibrated by damped spot intensity oscillations observable at reduced growth temperatures of  $\sim 320$  K). The data yield an escape depth of  $\sim 5.3$  ML for Co2p and Cr2p photoelectrons (equivalent to  $\sim 10.6$  Å, see below) which is in accordance with the generally observed mean free path of electrons as a function of kinetic energy [6].

The structural analysis shows that Co adopts pseudomorphic structure with a superimposed reconstruction. Fig. 2(a) illustrates an exemplary LEED pattern of a 5 ML-thick Co film growth at 500 K. Equivalent diffraction patterns were observed over the entire thickness- and growth temperature range investigated (up to 60 Å and between 250 and 500 K). The integral-order spot positions of the overlayer (denoted by indices) coincide with those of the substrate, i.e., the crystallographic orientation of the epitaxial Co film corresponds to that of the Cr (1 1 0) surface. Additionally, the diffraction pattern exhibits a  $(3 \times 1)$  superstructure in two equivalent domains. Related unit meshes are marked by full and dashed lines in Fig. 2(a). In real space [Fig. 2(b)] each of these domains implies uniaxial threefold superperiodicity along one of the two in-plane close-packed row directions. Suggestively, the  $(3 \times 1)$  superstructure indicates an overlayer reconstruction which serves as an effective pathway for partial relief of epitaxial stress. Such a behavior is not unique: forced structures like e.g. fcc Fe films on Cu (1 0 0) [8] are known to reconstruct in response to the constraint to adopt pseudomorphic structure. Furthermore, several intrinsic d metal surfaces undergo stress-driven reconstructions [9]. At present, we can only speculate whether the observed superstructure is due to periodic lattice distortions [as in the case of fcc

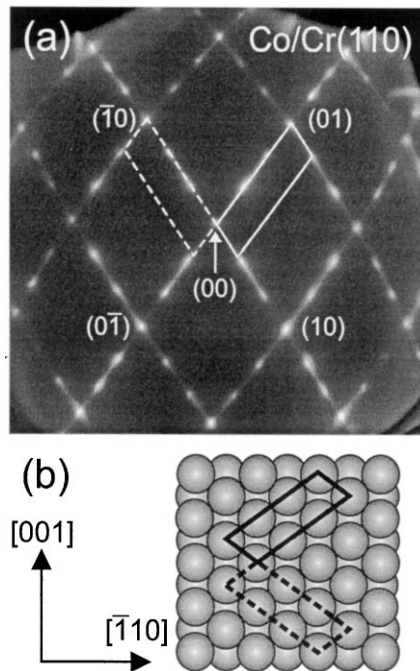


Fig. 2. LEED pattern of a 5 ML-thick Co/Cr (1 1 0) film at 125 eV with  $(3 \times 1)$  superstructure (a), and scheme of related surface arrangement (b); unit meshes of equivalent reconstruction domains in reciprocal (a) and real space (b) are indicated by full and dashed lines.

Fe on Cu (1 0 0)] or whether it is caused e.g. by a missing-row reconstruction of the film surface. Complementary structural information is required to determine the actual atomic structure of the reconstruction found here.

Finally, the lattice parameters of the Co overlayer are discussed. The lateral lattice constants are directly deduced from the integral-order spot spacing in the diffraction pattern. Within an experimental error of  $\pm 1\%$  they retain the pseudomorphic values of 2.88 Å along  $[0 0 1]$  and 4.08 Å along  $[\bar{1} 1 0]$  over the entire coverage range investigated. An estimate for the layer spacing may be extracted from the energy-dependent variation of the specular beam intensity, as illustrated in Fig. 3 for a 5 ML-thick Co film. In the present case, the magnitude of diffracted intensity is predominantly determined by kinematic (i.e. single) electron scattering since the intensity curve is dominated by sharp primary Bragg peaks whose energetic positions (full dots) scale with  $n^2$  (right hand side axis), with  $n$  the order of Bragg reflection. According to the third Laue condition [10] due to layer periodicity normal to the surface a layer spacing of  $d \sim 2$  Å ( $\pm 5\%$ ) is estimated from the slope of the linear regression line in Fig. 3. This value is consistent with (1 1 0)-oriented metastable Co in body-centered cubic structure, which was suggested earlier by experiment

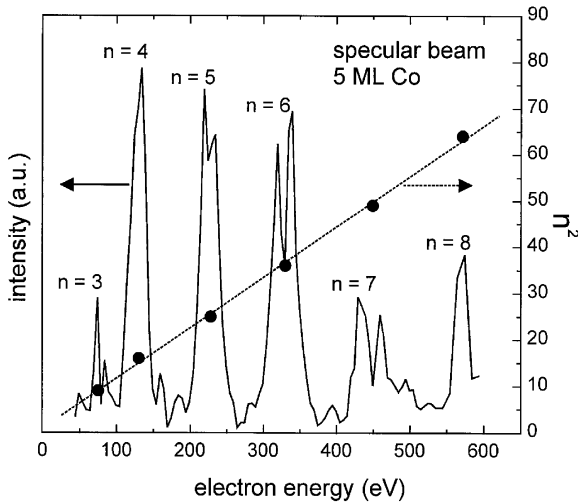


Fig. 3. Specular beam intensity vs. electron energy for 5 ML Co/Cr (1 1 0) [full line]; energetic peak positions (dots) scale with  $n^2$ , where  $n$  is the order of Bragg reflection (right axis).

[11] (bcc:  $a_0 = 2.83 \text{ \AA}$ ,  $d = 2.00 \text{ \AA}$ ) or predicted recently by theory [12] (bct:  $a = 2.91 \text{ \AA}$ ,  $c/a = 0.92$ ,  $d = 2.06 \text{ \AA}$ , or  $1.97 \text{ \AA}$  due to the tetragonal distortion). In addition, we find a systematic correlation between kinematic energy values and measured intensity maxima also for the first-order LEED spots [4], which suggests that Co indeed adopts body-centered cubic structure in the presents case. In conclusion, the presently observed stabilization of smooth pseudomorphic Co films several

nm in thickness meets an essential precondition for potential future fabrication of crystalline Co/Cr (1 1 0) superlattices.

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