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Ultrathin films of body-centered-cubic Co on TiAl(010)

S. K. Kim, F. Jona, and P. M. Marcus
Department of Materials Science and Engineering, State University of New York, Stony Brook, New York 11794-2275

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Slow deposition in ultrahigh vacuum of cobalt onto a clean (010) surface of the ordered alloy TiAl (the bulk structure is tetragonal of the CuAu I type) produces ultrathin films of Co that contain large numbers of steps and defects, but also large regions that are both epitaxial and pseudomorphic. In these regions, the unit mesh of the Co films in the plane of the film is a rhombus with sides equal to 2.855 Å and an angle between the sides of 89.068°. A quantitative low-energy electron-diffraction intensity analysis shows that the bulk interlayer spacing is 1.40±0.03 Å and that the first interlayer spacing is contracted by 8.6%. Strain analysis finds that the equilibrium (i.e., the unstrained) phase of the films is the metastable body-centered-cubic (bcc) modification of Co (lattice parameter 2.83 Å). Thus, the square unit mesh of bcc Co under a tensile strain of 0.9% becomes a rhombus with a consequent contraction of the *bulk* interlayer spacing by about 0.86%. The close match of the unit meshes in side and angle stabilizes the metastable bcc Co structure for about 15–20 layers. This case is a rarely encountered example of pseudomorphic epitaxy in which the unit mesh of the equilibrium phase of the film differs from the unit mesh of the substrate either by the ratio of the lengths of the sides or by the magnitude of the angle between the sides or both.

I. INTRODUCTION

At room temperature, the stable phase of cobalt has the hexagonal-close-packed structure (hcp, $a=2.507$ Å, $c=4.070$ Å). A metastable modification with the face-centered-cubic structure (fcc, $a_0=3.544$ Å) can be prepared at room temperature by very rapid quenching of molten samples[1] or in the form of ultrathin films by pseudomorphic epitaxy on Cu{001} (Refs. 2–4) or Ni{001}.[5] A considerably less stable phase with the body-centered-cubic structure (bcc, $a_0=2.83$ Å, Ref. 6) can also be stabilized by pseudomorphic epitaxy on suitable substrates.

The latter possibility, first demonstrated by Prinz[6] for Co on GaAs{110}, has aroused considerable interest in students of ferromagnetism because bcc Co, not available in bulk form, is a ferromagnetic phase of Co and proof of its stability is a challenge. Photoemission experiments[7] and band-structure calculations[8] have shown that the electronic structure of bcc Co is similar to that of bcc Fe, with a shift due to the addition of one electron; the exchange splitting is approximately 1.6 eV, as in bcc Fe, but in contrast to Fe, the majority-spin *d* bands are fully occupied. On GaAs{110}, with molecular-beam epitaxy Prinz[6] could grow films of bcc Co as thick as 357 Å, and Idzerda *et al.*[9] confirmed the structure to be bcc and determined the lattice constant to be 2.82±0.01 Å.

On metallic substrates, however, the growth of the bcc modification seems to be controversial. On one hand, Scheurer *et al.*[10] reported the growth of 20-layer-thick films of Co on Cr{001}, which were judged to be "probably in a metastable bcc phase." Later, Scheurer *et al.*[11] determined by quantitative low-energy electron diffraction[12] (QLEED) that two-layer films had the same structure as the substrate, i.e., bcc, but contamination of the films by nitrogen prevented the growth of epitaxial films thicker than four or five layers. On the other hand, Donner *et al.*[13] reported the growth of "high-quality single-crystal Co/Cr{001} superlattices with layer thicknesses of 5–50 Å" and showed that "the stable configuration of cobalt on Cr{001} is the hcp(11$\bar{2}$0) plane. . .[and] that the hexagonal symmetry remains for Co layer thicknesses down to 4 Å." Houdy *et al.*,[14] also working on Co/Cr multilayers, reported observing diffusion of Cr into Co and found that below a thickness of about 10 Å cobalt has the bcc structure. The same authors grew Co/Fe multilayers with different thicknesses and found evidence of a bcc Co phase for Co thicknesses up to 20 Å. Li and Tonner[15] grew 3-layer-thick Co films on a 3.5-layer Fe film on top of an Ag{001} substrate and concluded from x-ray excited photoemission and Auger-electron angular distributions that the structure of the Co films was bcc.

It appears, to our knowledge, that a direct *quantitative* determination of the structural parameters of bcc Co films on metallic substrates has not been reported in the literature so far. Wang *et al.*[16] did carry out a QLEED analysis of 13-Å films of Co on FeAl{001}, but their results were ambiguous as to whether the Co films had a strained bcc or a strained fcc structure.

In this paper we report the results of a QLEED and a strain analysis of ultrathin films of Co grown epitaxially on a TiAl(010) substrate. These results are noteworthy on three accounts. First, they constitute a *quantitative* determination of the structure of (strained) bcc Co films on a metallic substrate. Second, they demonstrate the growth of such films on a *noncubic* substrate. Third, they represent a well-documented case of what we call case-2 epitaxy,[17–20] namely, the general case of pseudomorphic epitaxy in which the unit mesh of the equilibrium phase of the film and the unit mesh of the substrate differ from one another in either or both the ratio of the sides and the angle between the sides.

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The substrate used in the present paper is a single crystal of the alloy TiAl, which has the tetragonal structure of AuCu I. In this structure, (001) planes are alternately 100% Ti and 100% Al, whereas (010) planes are all 50% Ti and 50% Al. However, a recent QLEED analysis of TiAl(010) found that the surface is chemically reconstructed: Ti and Al atoms in the first and second layer exchange places, so that the first layer is all Al and the second layer is all Ti.[21] Thus, whereas in the bulk (010) planes have primitive rectangular nets (with a basis), at a (010) surface the first and the second atomic layers have centered rectangular nets with a rhombic primitive unit mesh.

We present experimental details of the growth of Co on TiAl(010) in Sec. II, the QLEED analysis of these films in Sec. III, the strain analysis in Sec. IV, and the conclusions in Sec. V.

II. EXPERIMENTS

The experiments were done in an ultrahigh vacuum chamber capable of reaching a base pressure of about 1×10^{-10} Torr and provided with front-view LEED optics both for crystallographic studies and, in the retarding-field analyzer mode, for AES (Auger-electron spectroscopy) measurements. The TiAl(010) substrate was the same sample used in a recent QLEED study of the surface structure.[21] In the experimental chamber the sample could be heated by electron bombardment of the back surface. Its temperature was measured by means of an infrared radiometer with an accuracy estimated at ±50 °C. The LEED intensity data needed for quantative structure analysis [the so-called $I(V)$ curves] were measured with a video LEED system described elsewhere.[22]

The sample surface was cleaned *in situ* by a series of Ar-ion bombardments and high-temperature anneals, and its chemical state was monitored by AES as described in Ref. 21. The Co source consisted of a thin (0.25 mm diameter) 99.9965% pure Co wire tightly wound on a tungsten spiral that could be electrically heated. During deposition of Co on the substrate surface the source was heated to temperatures between 1050 and 1250 °C. The deposition rates were kept slow at approximately 1 Å/min.

The thickness of the Co films was estimated from the decrease of the Ti and Al AES signals, and the increase of the Co AES signal, as described elsewhere.[16] During deposition the substrate was neither heated nor cooled—its temperature was monitored with an infrared pyrometer and was never at or above the minimum temperature measurable with this instrument (~150 °C). Previous experiments using identical sources and a thermocouple showed that the substrate was not significantly heated by radiation from the source during deposition.

The LEED pattern from the clean TiAl(010) surface, a twofold-symmetric, high-contrast, low-background pattern, worsened upon deposition of Co: the background became notably higher and the diffracted beams broader. With increasing deposition the background increased to the point where the diffracted beams became almost indistinguishable from the background and the whole pattern was almost completely obliterated. This observation suggests that the deposited Co atoms initially agglomerated to form many small islands, which eventually covered the whole substrate surface, but did not produce a distinguishable LEED pattern. With continued deposition of Co a new LEED pattern started to emerge, initially with weak and broad beams, then with sharper beams over a still substantial background when the Co film reached a thickness estimated at 20–30 Å. With such thick Co films, AES scans showed no Ti signal, but still showed a small Al signal, approximately 30–35 times smaller than that observed on the clean substrate surface. On the basis of the experience gained in the study of Co on FeAl(001) (Ref. 16) we assumed that the Al impurities, obviously segregated on or in the surface of the Co film from the substrate, were disordered, and as such contributed only to the background, not to the diffracted beams, of the LEED pattern from the Co film. The results of the QLEED analysis, reported below, indicate that this assumption is good.

Since the LEED pattern of the clean substrate surface was no longer visible, the relation between the new pattern and that of the clean surface, i.e., the relative position of the new beams from the Co film with respect to those from TiAl(010), was not immediately obvious. We resorted to the measurement of the distances on the fluorescent screen between a number of selected substrate spots *before* deposition of Co, and to the comparison of these distances with those measured, at the same incident electron energy, between spots of the new pattern from the Co film. In this way we established that the Co beams coincided with the 11- and 20-type beams from TiAl(010) as depicted in Fig. 1(a). In this figure, the solid circles represent beams from clean TiAl(010) (with some indices written on their right) and the superposed squares represent beams from the Co film (with some of *their* indices written in parentheses). The figure outlines, in reciprocal space, the centered rectangular unit mesh of the substrate surface, in dashed lines, and the rhombic unit mesh of the Co film plane, in dotted lines.

The relation of the Co pattern to the substrate's allows us to determine the size and the shape of the unit mesh in direct space. Since the sides of the rectangular TiAl(010) unit mesh are 4.0707 and 4.005 Å, respectively, the sides of the rhombic unit mesh of the strained Co film are given by $\sqrt{(4.0707/2)^2+(4.005/2)^2}=2.8553$ Å and the angles between the sides are 89.068° [from $2\times\arctan(2.0025/2.03535)$] and 90.932°. The strained Co{001} and TiAl(010) nets are depicted in Fig. 1(b), where the solid squares represent Co atoms and the open circles represent Al atoms [recall that the top layer of TiAl(010) is 100% Al, see Ref. 21]. The figure does *not necessarily* show the correct positions of the Co atoms relative to the Al atoms, positions that are not known at this time, but does show the relative mesh sizes: the centered rectangular unit mesh of the top TiAl(010) layer is drawn with dashed lines, while the primitive rhombic unit mesh of the Co film is drawn with dotted lines.

In order to do a QLEED intensity analysis we needed to measure beam intensities versus incident energy [the $I(V)$ spectra]. In the present case the relatively large size

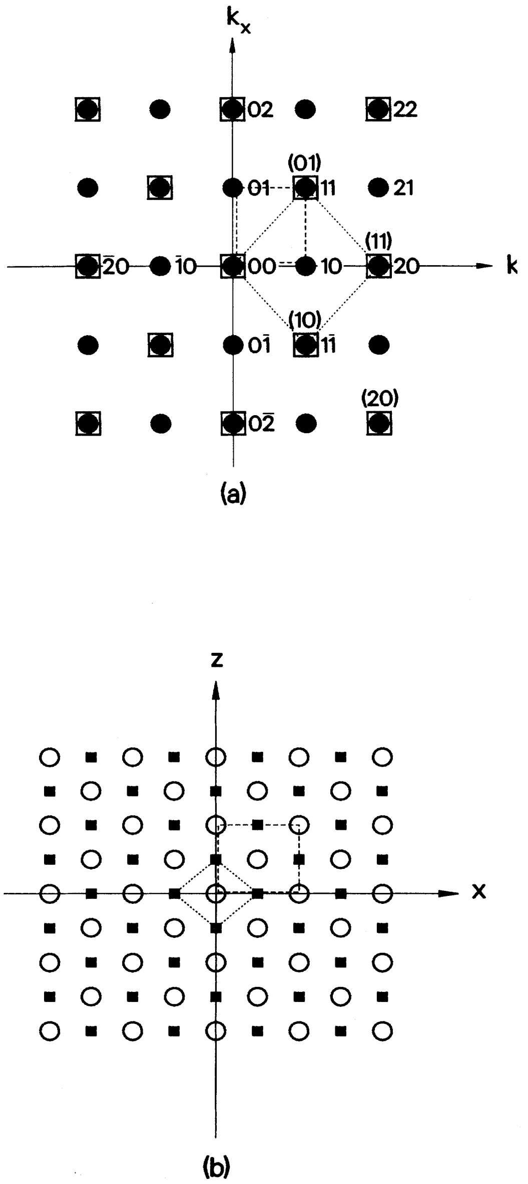

FIG. 1. (a) The LEED pattern from clean TiAl(010) is shown schematically by the solid circles and some of their indices. The unit mesh, drawn with dashed lines, is centered rectangular: the aspect ratio has been intentionally exaggerated to emphasize the fact that the unit mesh is *not* square. The LEED pattern from a 20–30-Å-thick Co film, which is recognizable only after the pattern of the clean substrate has vanished, is shown with the superposed squares and the indices written in parentheses. The unit mesh of the Co pattern is the rhombus drawn with dotted lines. (b) The open circles represent Al atoms on the chemically reconstructed surface of TiAl(010): the net is defined by the centered rectangular unit mesh drawn with dashed lines. The solid squares represent Co atoms: the corresponding net is defined by an *identical* centered rectangular unit mesh or alternatively by the primitive rhombic unit mesh drawn with dotted lines. The figure is intended to show the unit meshes, not necessarily the relative atomic positions, i.e., the registration, which are not known.

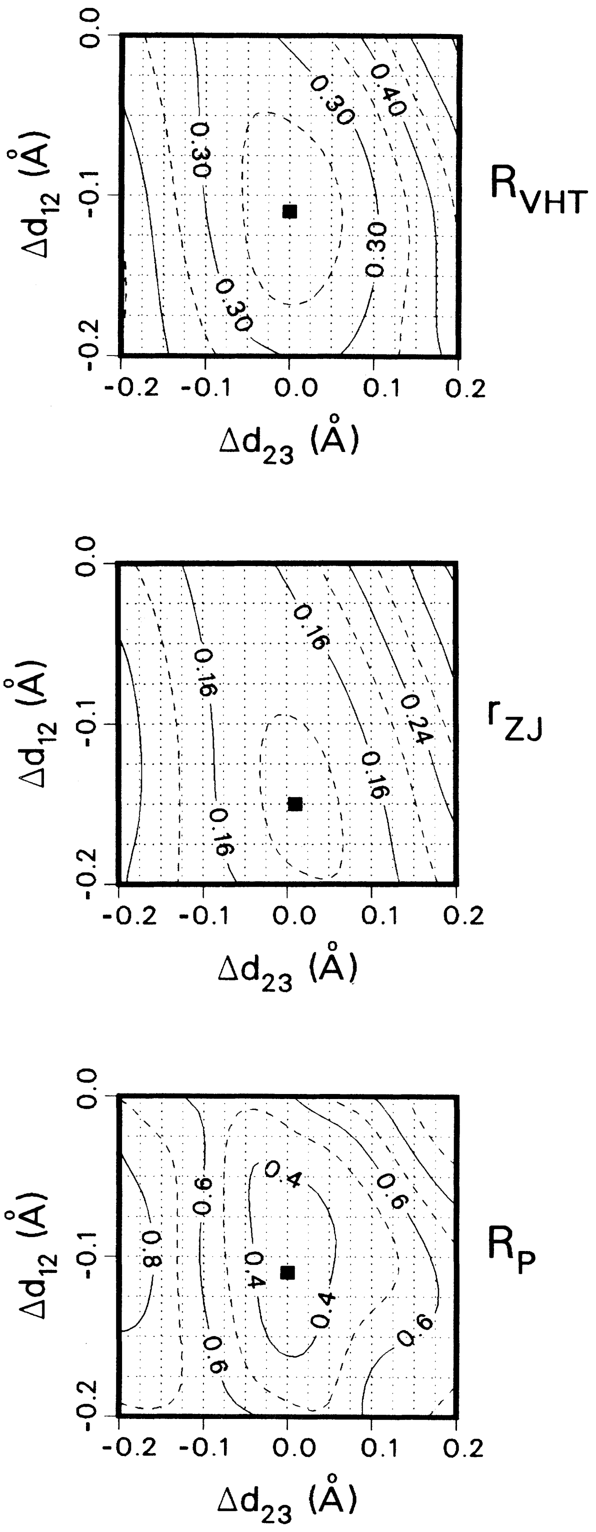

FIG. 2. Epitaxial growth of Co on TiAl(010): contour plots of the Van Hove–Tong R_{VHT} factor, the Zanazzi-Jona r_{ZJ} factor, and the Pendry R_P factor in the plane of Δd_{12} vs Δd_{23} (the changes in interlayer spacings between first and second, and between second and third atomic layers, respectively) for a constant bulk interlayer spacing of 1.40 Å. The plots show that d_{12} is on average contracted by 0.12 Å and d_{23} is at its bulk value.

of the reciprocal net and the high background, particularly at large electron energies, did not allow us to measure more than three spectra, namely, the 10, 11, and 20 spectra at normal incidence of the primary electron beam. Three sets of these three spectra were measured on three newly prepared Co films: the three sets are not identical, but sufficiently similar to one another to give us confidence that they are representative of the same structure.

III. QLEED INTENSITY ANALYSIS

The intensity calculations were performed with Jepsen's full-dynamical CHANGE program[23] and the following nonstructural parameters: Co potential taken from the collection of Moruzzi, Janak, and Williams;[24] 8 phase shifts and 69 beams up to 400 eV; inner potential $V_0 = -(10+4i)$ eV, with the real part adjustable in the fitting process (it became -8 eV after refinement); isotropic root-mean-square amplitude of thermal vibrations of 0.15 Å. Evaluation of the agreement between theoretical and experimental curves was done both by R-factor analysis and visually. Three R factors were used, namely, the Van Hove–Tong $R_{\rm VHT}$ (Ref. 25), the Zanazzi-Jona $r_{\rm ZJ}$ (Ref. 26), and the Pendry R_P (Ref. 27) factors.

The intensity calculations assumed as a model a semi-infinite Co crystal strained in such a way that the normally square primitive unit mesh in the $\{001\}$ planes becomes a rhombus with sides 2.8553 Å and angles 89.068° and 90.932°. In the calculations we varied first both the bulk- and surface-interlayer spacings $d_{\rm bulk}$ and d_{12}, respectively: $d_{\rm bulk}$ from 1.3277 to 1.5277 Å in steps of 0.05 Å, and the change Δd_{12} of d_{12} from -0.2 to $+0.2$ Å in steps of 0.05 Å. We then kept $d_{\rm bulk}$ at its optimum value and varied both Δd_{12} and the change Δd_{23} of the second-to-third interlayer spacing. The analysis was done independently for each one of the three sets of data, although we report here only the results obtained with the set that gave the best fit to the experimental data, i.e., the lowest R factors (the structure results are the same for the other two sets within experimental error). Figure 2 shows the final R factor contour plots in the Δd_{12}-Δd_{23} plane for all three R factors involved.

The best-fit parameters are $d_{\rm bulk} = 1.40 \pm 0.03$ Å, $d_{12} = 1.28 \pm 0.03$ Å ($\Delta d_{12}/d_{\rm bulk} = -8.6\%$), and $d_{23} = 1.40 \pm 0.04$ Å, for the minimum R factor values $R_{\rm VHT} = 0.22$, $r_{\rm ZJ} = 0.11$, and $R_P = 0.32$. The quality of the agreement between experiment and calculations can be gauged visually in Fig. 3.

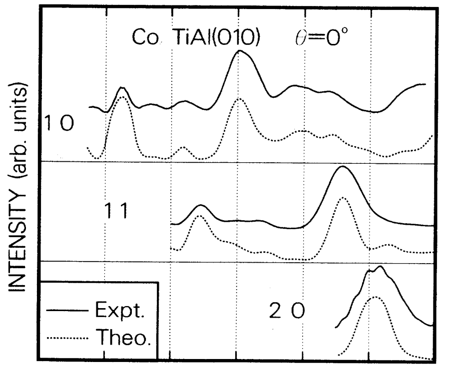

FIG. 3. Comparison between experimental (solid lines) and theoretical (dotted lines) $I(V)$ spectra for strained bcc Co on TiAl(010).

IV. STRAIN ANALYSIS

As mentioned above, the epitaxial system considered in the present study is an example of the most general case of pseudomorphic epitaxy—what we call case-2 epitaxy.[17–20] In case-2 epitaxy, the equilibrium (i.e., the unstrained) phase of the film material has a unit mesh in the plane of the film which differs from the unit mesh of the substrate surface either in the ratio of the mesh sides or in the angle between such sides, or both. If the film grows pseudomorphically, the mismatch produces a strain which in general has three components (called ϵ'_{11}, ϵ'_{22}, and ϵ'_{12}) in the plane of the film. The complete strain tensor in the films will in general have three out-of-plane strain components (called ϵ'_{33}, ϵ'_{13}, and ϵ'_{23}). The problem to be solved in strain analysis is to find these three out-of-plane components. The solution of this problem and a FORTRAN program have been given elsewhere for the calculation of the three out-of-plane components.[17,20]

In order to solve for the out-of-plane strain components we need to know the lattice constant and the elastic constants of the equilibrium phase. In the present case there are two possible choices for the equilibrium phase of Co: one is the metastable fcc phase, for which the elastic constants are known from experiment, and the other is the metastable bcc phase, for which the elastic constants are not known from experiment, but can be estimated theoretically. We will therefore solve the problem of finding the complete strain tensor in the film for both phases, and from this tensor we will calculate the value of the bulk interlayer spacing $d_{\rm bulk}$ for comparison with the experimental value obtained with the QLEED analysis.

Consider first the fcc phase. The lattice constant is $a_0 = 3.5447$ Å (Ref. 28), hence the primitive unit mesh has sides $a_{eq} = a_0/\sqrt{2} = 2.5065$ Å. For pseudomorphic growth the linear strain ϵ'_{11} in the plane of the film is therefore $[(2.855/2.5065) - 1] \times 100 = 13.9\%$ (tension), a rather large value by normal standards of pseudomorphic epitaxy. The elastic constants are $c_{11} = 2.42$, $c_{12} = 1.60$, and $c_{44} = 1.28$ in units of 10^{12} dyn/cm^2 (Ref. 29). The calculation of the complete strain tensor gives the result $\epsilon'_{33} = 0.1838$, indeed a very large value, which requires a compression of the bulk interlayer spacing $d_{\rm bulk}^{\rm equil} = 1.7724$ Å of the equilibrium phase by $-0.1838 \times 1.7724 = -0.3258$ Å. The value of $d_{\rm bulk}$ in the strained Co film would therefore be $1.7724 - 0.3258 = 1.45$ Å, to be compared with the experimental value 1.40 ± 0.03 Å found with QLEED. We conclude that the equilibrium phase of the Co film was very probably *not* the fcc phase.

Now consider the bcc phase. The lattice constant, as determined from thick films of Co on GaAs$\{110\}$ is 2.83 Å (Ref. 6), so that the linear strain along one side of the unit mesh when bcc Co grows on the rhombic unit mesh of TiAl(010) with sides 2.855 Å is $\epsilon'_{11} = -0.008\,83$. The elastic constants are not known from experiment, but can be estimated from first-principles calculations of the shear modulus G (Ref. 30) and the bulk modulus B (Ref. 31): $G = 0.926$, $B = 2.309$, hence $c_{11} = 3.604$ and $c_{12} = 1.752$, all in units of 10^{12}dyn/cm^2. With these data the calculation of the complete strain tensor finds the perpendicular strain $\epsilon'_{33} = -0.0086$ and the strain ratio $\epsilon'_{33}/\epsilon'_{11} = -0.965$, while the shears ϵ'_{13} and ϵ'_{23} vanish because of the symmetry of the square and rhombus. Hence, the bulk interlayer spacing is calculated to be $d_{\text{bulk}} = 1.403$ Å.

Thus, with elastic constants from first-principles calculations we find that a pseudomorphic film of bcc Co on TiAl(010) would be strained to have a bulk interlayer spacing of 1.40 Å. The good agreement between this value and the QLEED result is taken as evidence for the fact that the Co films grown in our experiments have an atomic structure derived from the metastable bcc phase of cobalt, strained to fit on the centered rectangular net of TiAl(010).

V. CONCLUSIONS

It has been established earlier[21] that the top layer of TiAl(010) has only Al atoms, so that the surface net of TiAl(010) is a centered rectangular net with sides 4.0707 Å (the tetragonal c axis) and 4.005 Å (the tetragonal a axis), and hence the primitive unit cell is a rhombus with sides 2.855 Å and angles 89.068° and 90.932°. By slow deposition of Co atoms in an ultrahigh vacuum, ultrathin films of Co can be grown on this surface epitaxially and pseudomorphically, i.e., the Co films assume the same net as the substrate in the plane of the film. In the early stages, the deposit consists very probably of small islands, which then grow in number, with continued deposition, until they cover the whole substrate surface (at this stage, the LEED pattern of the clean substrate surface is almost completely obliterated). In later stages the islands coalesce and a continuous film is formed that has steps and defects, but also sufficiently wide terraces to produce a measurable LEED pattern. This pattern reveals that the Co film has the same primitive unit mesh as the substrate.

A QLEED intensity analysis of the Co pattern finds a bulk interlayer spacing of 1.40±0.03 Å and an 8.6% contracted first interlayer spacing. Strain analysis finds that the equilibrium (i.e., the unstrained) phase of the Co film is the metastable bcc phase (lattice parameter $a_0 = 2.83$ Å), but cannot be the fcc phase. Thus, the epitaxial strain in the plane of the film consists in a distortion of the square net of bcc Co{001} into a rhombus so that the sides are stretched by about 0.9% and the angles between the sides are changed from 90° to 89.068° and 90.932°. As a consequence, the bulk interlayer spacing is contracted by about 0.86%.

This work illustrates the general case of pseudomorphic epitaxy which we call case-2 epitaxy, namely, the pseudomorphic growth of a film whose equilibrium unit mesh differs from that of the substrate on which it is growing by the length of the sides or the angle between the sides, or both.

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