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Epitaxy of Co on FeAl{001}. I. 1×1 films

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Ultrathin films of Co have been grown by slow vapor deposition on an FeAl{001} substrate (lattice constant $a_0=2.904$ Å). Up to a thickness of about 13 Å the films are found to be pseudomorphic with the substrate, but contain 5–10 at. % Al. Quantitative low-energy electron diffraction (LEED) finds the best-fit model for the films to be pure Co with body-centered-tetragonal structure, bulk interlayer spacing 1.40±0.03 Å, and first interlayer spacing 1.25±0.03 Å, suggesting that the Al impurities were disordered and contributed only to the background of the LEED pattern. Strain analysis gives ambiguous results with regard to the equilibrium phase, as both fcc and bcc Co (metastable phases) have strain ratios within acceptable limits. The strains themselves are unusually large for fcc Co and fairly small for bcc Co, but the Poisson ratio has normal values for fcc Co and unusually small values for bcc Co. The contraction of the first interlayer spacing is abnormally large (~11%) for magnetic materials.

I. INTRODUCTION

Ultrathin films of cobalt are currently of great interest for both their technological applications in magnetic multilayer systems and for their ability to stabilize, through epitaxy, structures that are not naturally encountered at room temperature, i.e., the metastable face-centered-cubic (fcc) phase and the metastable body-centered-cubic (bcc) phase. Strained fcc films have been grown on metallic substrates (Cu{001}, Ni{001}), and strained bcc films have been grown on metallic (Fe{001}, Cr{001}) and semiconducting substrates (GaAs{110}) (see, e.g., Ref. 1). Generally, the mismatch between the lattice constant of the substrate and the lattice constant of the unstrained (equilibrium) metastable phase plays an important role in determining the structure and hence the strains in the grown film.

This paper reports the results of a study by quantitative low-energy electron diffraction (QLEED) of the growth of ultrathin Co films on an alloy surface, FeAl{001}. FeAl is a cubic alloy with a CsCl-type structure (lattice constant 2.904 Å). The {001} surface of this alloy was recently the object of a QLEED study,[2] which showed the top surface plane to be an Al layer, with a Fe plane as the second layer. The first interlayer spacing, between the Al and the Fe planes, was found to be contracted by 14.4% with respect to the bulk, while the second interlayer spacing (between the second-layer Fe and the third-layer Al) was found to be expanded by 4%. The square mesh of FeAl{001} has a size sufficiently close to that of bcc Co{001} to offer good prospects for growing epitaxial and pseudomorphic films of this metastable modification of cobalt.

The experiments are described in Sec. II, the observations in Sec. III, the QLEED analysis in Sec. IV, and the strain analysis in Sec. V. The results are discussed in Sec. VI and the conclusions are summarized in Sec. VII.

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 low-energy electron-diffraction (LEED) optics both for crystallographic studies and, in the retarding-field analyzer mode, for Auger electron spectroscopy (AES) measurements. The FeAl{001} sample was the same sample used in a recent LEED study of the surface structure.[2] The alloy composition was fixed by x-ray photoelectron spectroscopy at (46±2)% and the lattice constant was determined by x-ray diffraction to be 2.904 Å. 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 quantitative structure analysis [the so-called $I(V)$ curves] were measured with a video-LEED system described elsewhere.[3]

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. 2. The Co source consisted of a thin (0.25-mm-diam) 99.9965%-pure Co wire tightly wound on a tungsten spiral, which could be electrically heated. During deposition of Co on the substrate surface, the source was heated to temperatures between 1050 and 1250 °C. The deposi-

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tion rates were kept slow, varying from about 1.5 Å in 20 min to approximately 20 Å in 30 min.

The experimental procedure consisted typically in sequences of Co deposition, AES analysis, LEED observations, and LEED intensity-data collection. The thickness of the Co films was estimated from the decrease of the Fe and Al AES signals, and the increase of the Co AES signal, as is customary in this kind of work.[4] 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.

III. OBSERVATIONS

At a Co coverage of about 1 Å, the background of the LEED pattern became notably higher and the diffracted beams broader than from the clean substrate surface. The diffracted intensities [the $I(V)$ curves] changed considerably with respect to those from the clean surface. At a coverage of about 3.5 Å the quality of the pattern improved somewhat, i.e., the background decreased. The geometry of the LEED pattern remained 1×1, but the $I(V)$ spectra kept changing with coverage until about 6 Å, whereupon they remained stable up to a thickness of about 13 Å.

With films thicker than 13 Å, new diffracted beams appeared and the LEED pattern became $c(2\times2)$. The $I(V)$ spectra changed again, but were restabilized at a coverage of approximately 20 Å. The fractional-order beams increased gradually in intensity to become comparable to the integral-order beams.

The AES spectra showed a monotonic decrease of the Fe and Al signals with increasing deposition of Co, but while the Fe peak disappeared into the noise at a coverage of about 6 Å, the Al peak persisted, although decreasing in intensity, until a Co coverage of approximately 35 Å. In the coverage range that produced the 1×1 LEED pattern, the Al concentration was estimated to be between 10 and 15 at. %. This concentration was reduced to less than 5 at. % in films thicker than 17 Å, and to less than 2% in films thicker than 26 Å. Above a Co coverage of 35 Å, in the range of the $c(2\times2)$ structure, the Al signal was no longer detectable, and it was established that the aluminum atoms responsible for the AES signal did not affect the LEED $I(V)$ curves of the $c(2\times2)$ structure, because the $I(V)$ curves did not change when the Al AES signal disappeared. The $c(2\times2)$ structure appeared to be very stable, with all beams intense, up to Co-film thicknesses of about 200 Å, the largest thickness attained in this work.

Thus, the observations revealed the formation of two structures with increasing Co coverage: a 1×1 structure (different from the substrate's) up to about 13 Å, and a $c(2\times2)$ structure in thicker films. The persistence of a 1×1 LEED pattern from Co films thinner than 13 Å indicates that these films were pseudomorphic with the FeAl{001} substrate, at least within the experimental resolution of about 1%. The AES tests showed that these films contained no Fe, but did contain a detectable amount of Al estimated to be between 10 and 15 at. %.

In the present paper, called Paper I, we describe a LEED intensity analysis and a strain analysis of the 1×1 films. [A corresponding study of the thicker films with the $c(2\times2)$ structure is described in the following paper, Paper II.] We collected a number of diffracted degenerate spectra at normal incidence of the primary beam from a Co film estimated to be about 8-Å thick, then appropriately averaged these intensities to obtain six nondegenerate $I(V)$ spectra, namely, 10, 11, 20, 21, 22, and 30 for energies between 40 and 400 eV.

IV. LEED INTENSITY ANALYSIS OF 1×1 Co FILMS

The intensity calculations were performed with Jepsen's full-dynamical CHANGE program[5] and the following nonstructural parameters: Co and Al potentials taken from the collection of Moruzzi, Janak, and Williams[6]; 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_{VHT},[7] the Zanazzi-Jona r_{ZJ},[8] and the Pendry R_P (Ref. 9) factors.

Having established that the $I(V)$ spectra from 8-Å films were stable with respect to small thickness changes, we concluded that the film-substrate interface and the substrate itself no longer contributed to the diffracted intensities from those films. We therefore carried out intensity calculations assuming as a model a semi-infinite Co crystal with 2.904 Å in-plane lattice constant (equal to that of the FeAl{001} substrate) and with variable bulk and surface interlayer spacings. Initially, we ignored the Al impurities that were revealed in these films by AES—the results in this case are described in Sec. IV A. Thereafter we attempted to determine the location of the Al atoms in the films–the results are described in Sec. IV B.

A. Pure Co films

The variables in the calculations were the bulk interlayer spacing d_{bulk}, the first interlayer spacing d_{12}, and eventually, the second interlayer spacing d_{23}. Initially, d_{bulk} was varied from 1.60 to 1.81 Å in steps of 0.04 Å (the expected range for a strained fcc model) and from 0.8 to 1.40 Å in steps of 0.2 Å (the expected range for a strained bcc model). When both the R-factor analysis and the visual evaluation of the fit disqualified the first range of values, the refinement involved variations of d_{bulk} from 1.25 to 1.45 Å in steps of 0.05 Å. For each value of d_{bulk} the *change* Δd_{12} of the first interlayer spacing d_{12} was varied from a contraction of 0.2 Å to an expansion of 0.2 Å in steps of 0.05 Å. The contour plots of the three R factors in the d_{bulk}-Δd_{12} plane are depicted in Fig. 1, and yield the following minima; $R_{\rm VHT}=0.28$ for $d_{\rm bulk}=1.40$ Å, $\Delta d_{12}=-0.15$ Å; $r_{\rm ZJ}=0.11$ for $d_{\rm bulk}=1.41$ Å, $\Delta d_{12}=-0.18$ Å; and $R_P=0.41$ for $d_{\rm bulk}=1.39$ Å, $\Delta d_{12}=-0.13$ Å.

The effect of changes in the second interlayer spacing d_{23} was then investigated by keeping $d_{\rm bulk}$ fixed at 1.40 Å and varying Δd_{12} from -0.11 to -0.19 Å in steps of 0.02 Å, in each case varying Δd_{23} from -0.2 $+0.2$ Å in steps of 0.05 Å. All three R factors were minimized for Δd_{12} values within 0.02 Å of -0.15 Å, and for Δd_{23} values within 0.03 Å of 0.

Averaging the parameter values that minimize the three R factors, we therefore quote the results of the LEED intensity analysis as follows: $d_{\rm bulk}=1.40\pm0.03$ Å, $\Delta d_{12}=-0.15\pm0.03$ Å, and $\Delta d_{23}=0\pm0.03$ Å. The $I(V)$ spectra calculated with these parameters are compared with experiment in Fig. 2 (see the top two curves in each panel). The fit is mediocre for the 10 beam, quite satisfactory for the 11, 20, 21, and 22 beams, and very poor for the 30 beam. (We note, however, that in general, high-order spectra are more difficult to fit than low-order spectra and that in the present case the high background made the measurement of high-order spectra especially uncertain.)

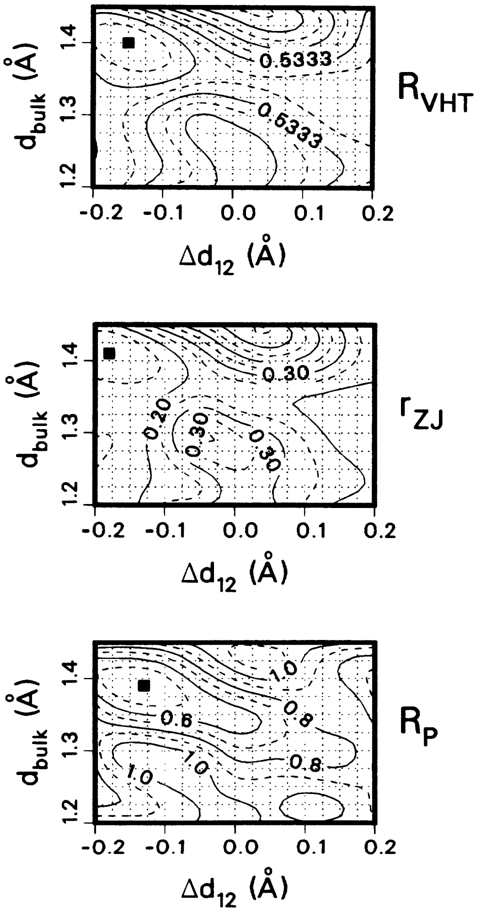

FIG. 1. Contour plots of the Van Hove–Tong ($R_{\rm VHT}$), the Zanazzi-Jona ($r_{\rm ZJ}$), and the Pendry (R_P) R-factors in the plane of bulk interlayer spacing $d_{\rm bulk}$ and change in first interlayer spacing Δd_{12}. The black squares indicate the minima (values given in the text).

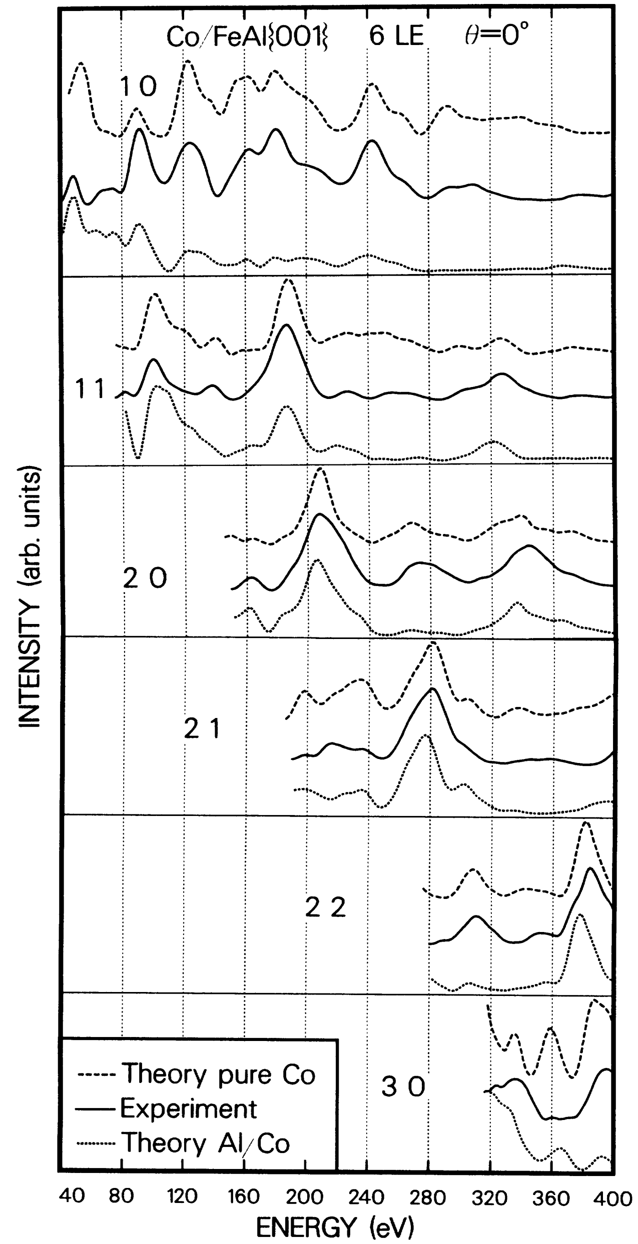

FIG. 2. Comparison between theoretical and experimental LEED $I(V)$ spectra for an 8-Å (about six layer equivalents) Co film. The solid curves (middle curves in each panel) are experimental; the dashed curves (top curves in each panel) are calculated for a pure Co film with the parameters given in the text; the dotted curves (bottom curves in each panel) are calculated for an overlayer of Al on the surface of a pure Co film with the parameters given in the text.

B. Co films with Al impurities

The magnitude of the Al signal that was detected in the AES scans from 1×1 Co films suggest the presence in the films of 10–15 at. % Al. Several attempts were made at the identification of the location of the Al atoms in the films. At the outset, we did not know where the Al atoms are located, and whether they were ordered or disordered. We note that Al atoms either randomly incorporated in the bulk at interstitial sites or randomly chemisorbed on the surface of the Co films would affect only the background of the LEED patterns, so that models based on these assumptions could not be tested with the techniques used in the present study. However, Al atoms randomly distributed on substitutional sites *would* affect the LEED $I(V)$ curves and hence the corresponding models could be tested. Thus, we concentrated on trying to find models for either ordered or substitutional distributions of Al atoms in the Co films that would give a better fit to experiment (lower R factors) than the model of pure Co described in the preceding section.

We assumed at first that the chemical composition of the films was $Co_{85}Al_{15}$ throughout, i.e., that the film was a compositionally disordered alloy with 15 at. % Al. The intensity calculations were done by replacing both the Co and the Al atoms with a "weighted-average" atom whose scattering amplitude was calculated from a suitable weighted average of the scattering amplitudes of Co and Al. We searched again for minima of the R factors in the $d_{\text{bulk}}-\Delta d_{12}$ plane. It turns out that these minima were all notably higher than those reported above for pure Co films: for example, the best R_{VHT} factor was 0.31 for $d_{\text{bulk}}=1.40$ Å and $\Delta d_{12}=-0.15$ Å. The visual evaluation found the fit to experiment unacceptably poor.

Next we assumed that the Al atoms were segregated into the top layer only, forming a monolayer of a compositionally disordered CoAl alloy whose composition we varied over the range from 0 to 75% Al. The R-factor minima were found by interpolation at the 5% and 10% Al composition (depending on the R factor considered) with R factor values about the same or somewhat higher than for the pure Co films, with less good visual fit but with still a very contracted first interlayer spacing ($\Delta d_{12}=-0.16$ Å). We also kept the surface composition fixed at 90% Co–10% Al and searched again for minima in the $d_{\text{bulk}}\Delta d_{12}$ plane, but the results were not satisfactory (e.g., best $R_{\text{VHT}}=0.35$ for $d_{\text{bulk}}=1.35$ Å and $\Delta d_{12}=-0.15$ Å).

Finally, we tried a model of a single *ordered* overlayer of Al onto a pure Co film. This model is attractive because it makes the first two atomic layers of the film identical to those on a {001} surface of CoAl, an alloy with the CsCl structure and lattice constant $a_0=2.86$ Å.[10] In this case the best-fit structure was found to be $d_{\text{bulk}}=1.40\pm0.03$ Å, $d_{\text{Al-Co}}=1.45$ Å, and the first interlayer spacing in the Co film $d_{\text{Co-Co}}=1.35$ Å, but all R factors are somewhat higher ($R_{\text{VHT}}=0.33$ $r_{\text{ZJ}}=0.14$, and $R_P=0.47$) and the visual fit to experiment somewhat worse than in the case of pure Co films, as can be seen in Fig. 2 (bottom curves in each panel).

We conclude therefore that none of the obvious models tested, featuring substitutional Al atoms in the bulk or in the surface, or ordered Al atoms on the surface of the Co films, fit the experimental data better than the pure Co film with strongly contracted first interlayer spacing.

V. STRAIN ANALYSIS

The goal of strain analysis is the determination of the equilibrium (i.e., the unstrained) phase of the Co films and the strains in the films. For the structure of these films we accept the result obtained in Sec. IV A for a pure Co film, namely, a body-centered-tetragonal structure with lattice parameters $a=2.904$ Å and $c=2d_{\text{bulk}}=2.80$ Å.

We are interested in the ratio between the strain ϵ_3 in the direction perpendicular to the film and the strain ϵ_1 in the plane of the film—the so-called strain ratio. We write this strain ratio as

$$\frac{\epsilon_3}{\epsilon_1}=r_s=\frac{(c-c_{\text{eq}})/c_{\text{eq}}}{(a-a_{\text{eq}})/a_{eq}}\ , \tag{1}$$

where c_{eq} and a_{eq} are the lattice parameters of the equilibrium phase (the denominator is the misfit between the substrate and the equilibrium phase). The LEED results (the a and c values) allow us to calculate the experimental value r_s^{exp} of the strain ratio if the equilibrium phase is known. Linear elasticity theory allows us to calculate the theoretical value r_s^{th} of the strain ratio[11] if the elastic constants c_{ik} of the equilibrium phase are known: for a cubic {001} film, $r_s^{\text{th}}=-2c_{12}/c_{11}$. Comparison between r_s^{exp} and r_s^{th} usually determines the equilibrium phase.

In the present case we have two choices for the equilibrium phase, both metastable: either fcc Co or bcc Co. If the equilibrium phase is fcc Co [$a_0=3.544$ Å (Ref. 10)], then $a_{\text{eq}}=a_0/\sqrt{2}=2.506$ Å and $c_{\text{eq}}=3.544$ Å, and therefore $r_s^{\text{exp}}=-1.32$. If the equilibrium phase is bcc Co [$a_0=2.83$ Å (Ref. 12)], then $a_{\text{eq}}=c_{\text{eq}}=2.83$ Å, and therefore $r_s^{\text{exp}}=-0.405$.

The theoretical strain ratio can unfortunately be calculated only for the case of fcc Co—the elastic constants of bcc Co are not known at this time. For fcc Co, $c_{11}=2.42$, $c_{12}=1.6$, and $c_{44}=1.28$ in units of 10^{12} dyn/cm^2.[13] Hence, $r_s^{\text{th}}=-1.32$ for the case of fcc Co. The agreement between theoretical and experimental strain ratio is obviously very good, but since the value of r_s^{th} for bcc Co cannot be calculated, a decision between fcc and bcc Co cannot be made on this ground alone.

Another approach is to relate the strain ratio directly to Poisson's ratio ν, as $r_s=-2\nu/(1-\nu)$, so that we can rewrite Eq. (1) in the form[11]

$$a_{\text{eq}}=\frac{2\nu}{1+\nu}a+\frac{1-\nu}{1+\nu}c\ . \tag{2}$$

With known a and c we can calculate the expression on the right-hand side for several assumed values of ν and plot it on a graph of a_{eq} versus ν, as in Fig. 3.

Thus we get an fcc-Co line by using $a=2.904\times\sqrt{2}=4.107$ Å and $c=2.80$ Å. This line intersects the horizontal line drawn at the ordinate 3.544 Å (the lattice constant of fcc Co) at the point that corresponds to $\nu=0.4$. This value of Poisson's ratio is in fact, as expected, the value calculated from the elastic constants of fcc Co [$\nu=c_{12}/(c_{12}+c_{12})$] so that this approach reproduces the result obtained above.

We can also draw a bcc-Co line by using $a=2.904$ Å and $c=2.80$ Å. This line intersects the horizontal line with ordinate 2.83 Å (the lattice constant of bcc Co) at $\nu=0.16$. This value of Poisson's ratio is unusually small, but physically possible.

The conclusion is that in the present case strain analysis alone is not sufficient to identify the equilibrium phase.

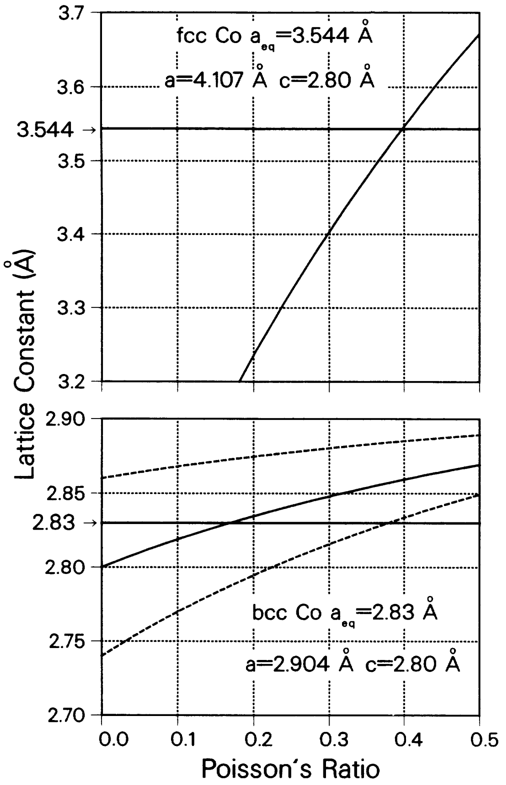

FIG. 3. Graphic solutions of Eq. (2): lattice constant vs Poisson ratio (solid curves). The bottom plot pertains to bcc Co (equilibrium lattice constant $a_{\mathrm{eq}}=2.83$ Å): the dashed lines delineate the upper and the lower bounds of the experimental error ($c=2.80\pm0.06$ Å). The top plot pertains to fcc Co (equilibrium lattice constant $a_{\mathrm{eq}}=3.544$ Å).

VI. DISCUSSION

The present study of an 8-Å-thick 1×1 film of Co on FeAl{001} shows it to have a body-centered-tetragonal structure with lattice parameters $a=2.904$ Å and $c=2d_{\mathrm{bulk}}=2.80$ Å (i.e., $c/a=0.96$), and a strongly contracted first interlayer spacing ($\Delta d_{12}=-0.15$ Å, or -10.7% of the bulk interlayer spacing). There are three major problems with the interpretation of this result, none of which can be fully solved with confidence at the present time.

(1) The AES experiments showed that the 1×1 Co films grown in this work contained between 10 and 15 at. % of Al, undoubtedly diffused out from the substrate. We were unable to find a satisfactory fit between the experimental LEED intensities and those calculated for models involving random substitutional Al atoms either in the first layer or throughout the bulk of the Co film. Only a model involving an ordered monolayer of Al chemisorbed on the first Co layer came close to matching the experimental data, but the fit is less good than the one obtained by ignoring the presence of the Al impurities (which is equivalent to assuming that those impurities were distributed at random either on the surface or on interstitial sites, so that they did not affect the intensities of the LEED beams). This result is surprising because Co and Al are known to form a stable intermetallic alloy CoAl with the CsCl structure—very similar, in fact, to the substrate FeAl used in the present work. Nevertheless, we are forced to conclude that the Al impurities were somehow disordered, or else that they were ordered in structures which we have not tested.

(2) The analysis of the strains in the Co films gave ambiguous results. If we assume that the equilibrium phase of the grown films was the metastable fcc modifiction of Co, we obtain very good agreement between the experimental and the theoretical strain ratios (the ratios between perpendicular and parallel strains). But the strains themselves are very large. The in-plane strain (the so-called misfit) is $+16\%$ and the perpendicular strain is -21%. With present-day experience, both these strains seem much too large to allow the growth of films as thick as six or eight layers. By contrast, if we assume that the equilibrium phase was the metastable bcc modification of Co, then the misfit is $+2.6\%$, and the strain in the perpendicular direction is -1.1%, both reasonable for the growth of ultrathin films of six or eight atomic layers. But in this case, the strain analysis reveals an unusually large stiffness of the films—the Poisson ratio ν is 0.16. This value of ν is small for epitaxial films: compare this value on one hand with the Poisson ratio of ultrathin films of fcc Cu on Pd{001} ($\nu=0.41$) or of fcc Fe on Cu{001} ($\nu=0.45$), and, on the other hand, with the Poisson ratio of bulk diamond ($\nu=0.10$) as calculated from the elastic constants published in the literature.[14]

The choice for the equilibrium phase is therefore limited to either the bcc structure and films with unusually large stiffness, or the fcc structure and films with enormous parallel and perpendicular strains. The main argument against the bcc phase at this time is the abnormally small value of the Poisson ratio ν found in Fig. 3. But we note that, first, the bcc line drawn in Fig. 3 is tagged with an experimental error of ±2%, so that the uncertainty in the value of ν extends from 0 to 0.38 and second, the lattice constant of bcc Co (taken here to be 2.83 Å) is not known with high precision. If this lattice constant were only about 1% larger (2.85 or 2.86 Å), the Poisson ratio would assume much more acceptable values (0.32 or 0.4, respectively). These facts, combined with the relatively small strains found in the films, could make the bcc modification a more likely candidate for the equilibrium phase than the fcc modification.

(3) The contraction of the first interlayer spacing (about 11% of the bulk spacing) is surprisingly large. Indeed, surface relaxations on nonmagnetic bcc {001} surfaces are generally large [$\Delta d_{12}/d_{\mathrm{bulk}}$ is -11% for Ta, -9.5% for Mo, -7% for V (Ref. 15)], but on ferromagnetic metals they are notably smaller (-5% for bcc Fe).

Both fcc and bcc Co are reportedly ferromagnetic. Metastable bcc Co has been shown to be ferromagnetic both experimentally[16] and theoretically,[12] although the calculated moment ($1.66\mu_B$) was found to be 16% larger than the experimental one ($1.4\mu_B$). In general, atoms with a magnetic moment are larger than if they were nonmagnetic, and atoms in the first atomic layer on the surface of magnetic crystals are expected to have a substantially larger moment than those in the deeper layers, owing to their lower coordination number. These factors tend to expand the first interlayer spacing, acting against the usual electrostatic forces, which tend to contract the surface spacing. The balance between these two forces produces in general expansions or small contractions of the first interlayer spacing on {001} surfaces of cubic magnetic crystals.

In the present case, the volume per atom in the bulk of unstrained bcc Co is 11.33 $Å^3$, and the volume per atom in the bulk of unstrained fcc Co is 11.13 $Å^3$, while in the bulk of the strained Co films grown in the present experiments it is 11.81 $Å^3$—hence the magnetic moment is expected to be larger in the strained films than in unstrained crystals. Thus, the 11% *contraction* of d_{12} found in this work is surprising, as it suggests that the surface is either nonmagnetic or less magnetic than the bulk. It is possible that the presence of Al impurities, discussed above, may have been responsible for the observed anomaly, but the data gathered in the present study cannot prove it.

VII. CONCLUSION

Ultrathin films of Co grown by slow vapor deposition on a FeAl{001} substrate (lattice constant $a_0=2.904$ Å) were found to be pseudomorphic with the substrate up to thicknesses of the order of 8–10 Å. Chemical analysis by AES revealed the presence of 10–15 at. % Al in or on the films, but the location of the Al atoms could not be determined. Ignoring the contribution of Al to the LEED signal, QLEED intensity analysis determined the bulk interlayer spacing to be $d_{\text{bulk}}=1.40\pm0.03$ Å and the first interlayer spacing to be strongly contracted by about 11%.

Strain analysis cannot identify with confidence the equilibrium phase of the grown films. The choice is between fcc Co and bcc Co, both metastable phases. The fcc phase seems unlikely because the in-plane strain would be a stretch of almost 16% and the perpendicular strain a compression of 21%, both unusually large for the growth of 8–10-Å pseudomorphic films. The bcc phase involves acceptable strains, +2.6% in the plane of the surface and −1.1% in the perpendicular direction, but in this case the films would be unusually stiff (Poisson ratio $\nu=0.16$).

At this time we feel that the choice of the equilibrium structure for Co on FeAl{001} is still open and awaits more evidence. An important clue would be a theoretical calculation of the relaxation of strained Co slabs from first principles. Such a calculation is now possible, e.g., both bulk and surface relaxations in an 11-layer slab of fcc Fe on Cu{001} have been calculated and *found in agreement* with QLEED values.[17]

ACKNOWLEDGMENTS

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