Epitaxy of Co on FeAl{001}. II. $c(2\times 2)$ films

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The $c(2\times 2)$ low-energy electron-diffraction (LEED) pattern observed on Co films thicker than about 13 Å on FeAl{001} is shown to be caused by a strained hexagonal Co($11\bar{2}0$) film. The film is strained differently in the two orthogonal directions within the plane of the interface: it is expanded by 0.91% in one and compressed by 5.4% in the other direction. As a consequence, the bulk interlayer spacing, as determined by quantitative LEED, is expanded by 2.9% with respect to the spacing in the unstrained hexagonal-close-packed phase (1.2535 Å). This is a more general case of pseudomorphic epitaxy than when film and substrate have similar unit meshes, and requires a more elaborate strain analysis. Such strain analysis finds an interlayer strain of 3.35%, in satisfactory agreement with the quantitative LEED result. It is noted that the strained Co($11\bar{2}0$) film does not grow directly onto the FeAl{001} substrate, but rather on a strained Co{001} film, 8–10 layers thick, which grows first on the substrate and is analyzed in a previous paper.

I. INTRODUCTION

Slow deposition of cobalt, in ultrahigh vacuum, on a clean {001} surface of the binary alloy FeAl produces epitaxial and pseudomorphic films. The structure of these films depends on their thickness: in the early stages of growth, when the thickness is less than about 13 Å, the in-plane lattice constants of the films are equal to those of the FeAl substrate (2.904 Å) and hence the corresponding low-energy electron-diffraction (LEED) pattern is geometrically identical to that of the substrate (1×1 pattern); in the later stages of growth, the in-plane lattice constants are $\sqrt{2}$ times larger than and rotated 45° with respect to those of the FeAl substrate [$c(2\times 2)$ pattern].

In an earlier paper, hereafter referred to as paper I,[1] we have reported the results of a study by quantitative LEED (QLEED) of the 1×1 Co films. The atomic structure of such films was found to be body-centered-tetragonal with in-plane periodicities of 2.904 Å and bulk interlayer spacing of 1.40 Å, with a strongly compressed first interlayer spacing.

In the present paper we report the results of a QLEED study of the $c(2\times 2)$ films, which show the structure to consist of four domains of a strained hcp ($11\bar{2}0$) phase, and of a related strain analysis. We summarize the experimental information and observations in Sec. II; we discuss the possible structure models in Sec. III; we describe the QLEED analysis in Sec. IV, the strain analysis in Sec. V; and we present a discussion of the results and the conclusions in Secs. VI and VII, respectively.

II. EXPERIMENT AND OBSERVATIONS

Details of the experiment were given in Paper I.[1] Here we give only a brief summary of the procedures and the observations.

Cobalt was vaporized in ultrahigh vacuum from a 99.9965% pure wire wound on an electrically heated tungsten basket. The substrate surface was a clean unheated {001} surface of the binary alloy FeAl.[2] The deposition rates were kept in the range between 0.08 and 0.7 Å/min. The thickness of the Co films was estimated from the relative magnitudes of Auger electron spectroscopy (AES) signals of Fe, Al, and Co. The crystallinity and the structure of the Co films were studied by LEED.

The LEED pattern remained 1×1, albeit with enhanced background, up to a thickness of about 13 Å, whereupon it changed into an initially weak $c(2\times 2)$, which became stronger with increasing deposition. This structure persisted, above a notable background, up to a thickness of about 200 Å, the largest attained in these experiments. Above a thickness of about 20 Å the fractional-order beams were on the average as intense as the integral-order beams, and all $I(V)$ spectra were independent of film thickness. In the earlier stages of film growth (for thicknesses smaller than about 35 Å), the AES spectra revealed the presence of decreasing amounts of Al in the films, but the stability of the $I(V)$ curves for all thicknesses larger than 20 Å showed that the Al impurities did not contribute to the coherent LEED signal.

The structure of the 1×1 Co films was determined by

QLEED to be pseudomorphic to the FeAl{001} substrate. The present paper concerns only the structure of the $c(2\times2)$ films and the strains produced in them by the epitaxy.

Several $I(V)$ spectra from the $c(2\times2)$ structure were measured for normal incidence of the primary electron beam and for energies between 40 and 400 eV from a Co film 40 Å thick. The spectra were then normalized to constant incident current, modified by background subtraction, and appropriately averaged to produce eight nondegenerate (four integral-order and four fractional-order) $I(V)$ curves, namely, 10, 11, 20, 21, $\frac{1}{2}\frac{1}{2}$, $\frac{3}{2}\frac{1}{2}$, $\frac{3}{2}\frac{3}{2}$, and $\frac{5}{2}\frac{1}{2}$. However, the $\frac{1}{2}\frac{1}{2}$ spectrum was not used in the analysis because the high background in its vicinity made the background subtraction, and hence its intensity, uncertain, and also limited the photometrically accessible energy range to energies between 40 and 140 eV.

III. MODELS FOR THE $c(2\times2)$ STRUCTURE

At the outset, the occurrence of a $c(2\times2)$ structure on top of a 1×1 structure of the same material (in this case, Co) appears puzzling. The first explanation that comes to mind is one involving impurities: with prolonged slow deposition, impurities may accumulate on and in the film, and if ordered they can produce a $c(2\times2)$ structure. However, the AES scans gave no indication of impurities in the films, and in particular no indication of impurity concentrations increasing with the appearance of the $c(2\times2)$ pattern, so that any impurity model must be rejected. Another possible explanation may be some spontaneous rearrangement of the Co atoms in the surface of the films. But this explanation appears unlikely, primarily because a $c(2\times2)$ structure limited to the surface layer of an otherwise 1×1 film would hardly be consistent with the observed almost-equal strengths of fractional- and integral-order beams. A third possibility, a $c(2\times2)$ structure extending throughout the bulk, is difficult to conceive, although a few intensity calculations were made for models involving, e.g., buckling of both the surface and/or the bulk layers in the Co films.

The model that appears to make the most sense is one involving the growth of a *strained* Co($11\bar{2}0$) film on top of a 1×1 Co film with the in-plane lattice constant of FeAl{001}. The 1×1 Co film itself was found to have a body-centered-tetragonal structure in the study already reported in Paper I.[1] But the stable phase of Co is of course hexagonal-close-packed (hcp), and it is worthwhile examining the relative sizes of the unit meshes involved in order to see whether pseudomorphic epitaxial growth of Co($11\bar{2}0$) onto a FeAl{001} geometry is probable.

The unit mesh of (unstrained) Co($11\bar{2}0$) is depicted schematically in Fig. 1(a). The dimensions are 4.342 Å in the $[10\bar{1}0]$ direction (within the basal plane) and 4.070 Å in the [0001] (or c) direction, hence the shape of the unit mesh is rectangular, but not far from square. The rectangular lattice has a basis of two atoms, one at the corners of the unit mesh and one inside. The second basis atom is located midway along the c direction and $\frac{1}{3}$ of the way from the left edge of Fig. 1 in the $[10\bar{1}0]$ direction (1.447 Å).
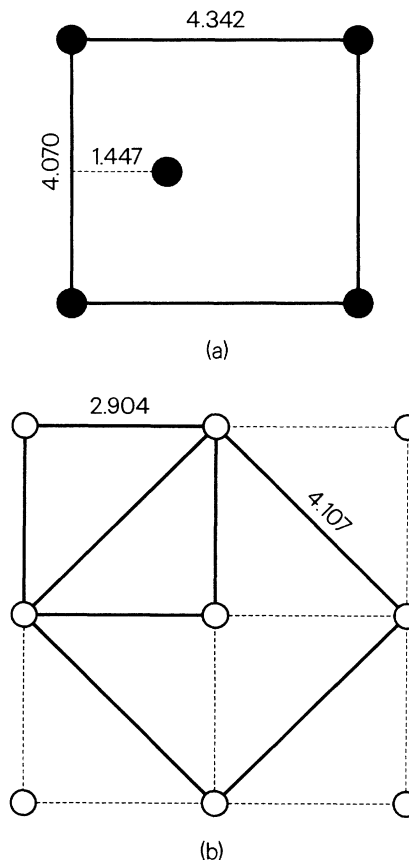

FIG. 1. (a) Unit mesh of Co($11\bar{2}0$), distances given in Å. (b) Primitive square unit mesh (2.904 Å) and centered square unit mesh of FeAl{001} (4.107 Å). The figures are drawn to scale.

The geometry of a FeAl{001} plane is shown in Fig. 1(b). The primitive unit mesh is a square with sides 2.904 Å, but the diagonal of the unit mesh is 4.107 Å long. If we compare the centered square on FeAl{001}, sides 4.107 Å [Fig. 1(b)], with the almost-square unit mesh of Co($11\bar{2}0$) [Fig. 1(a)], we see that the misfit amounts to +0.91% for the short side (the [0001] direction) and −5.4% for the long side ($[10\bar{1}0]$ direction). Hence, the unit mesh of Co($11\bar{2}0$) could be made to fit onto the net of FeAl{001} by rotating it 45° from the orientation given in Fig. 1(a) and straining the sides appropriately.

The interesting point is that if such a fit were to occur, the resulting structure would indeed appear to be a $c(2\times2)$. Figure 2 shows the relative orientations in direct space. In this figure, the empty circles represent Co atoms on the {001} 1×1 film while the full circles represent Co atoms in the stained Co($11\bar{2}0$) plane (omitting the second basis atoms). It is obvious that the black net is a $c(2\times2)$ superstructure of the white net. Note that in its equilibrium state, a Co($11\bar{2}0$) net is twofold symmetric, but in the present model there are four possible orientations of the strained unit mesh onto the square net of Co{001} when the second basis atom is taken into account, hence there are on the surface four rotationally related domains: in the LEED experiment the scatterings from the four domains add to restore fourfold symmetry

FIG. 2. Relative arrangement of the strained hcp Co(11$\bar{2}$0) net (black circles) onto the strained bcc Co{001} net (white circles). The black net is a $c(2\times2)$ superstructure of the white net. The second basis atom present in the Co(11$\bar{2}$0) plane is not shown.

FIG. 3. Schematic experimental $c(2\times2)$ LEED pattern from a 40-Å-thick film of Co on FeAl{001}. In (a) the pattern is indexed as a $c(2\times2)$ structure on cubic {001}. In (b) the same pattern is indexed as a 1×1 structure on strained hexagonal (11$\bar{2}$0). The (a) indexing is conveniently used in the experimental pattern, while the (b) indexing is normally used in intensity calculations of the theoretical pattern.

to the pattern.

In reciprocal space the resulting LEED pattern can be indexed in two ways, one way as a $c(2\times2)$ pattern of cubic Co{001} and another way as a 1×1 pattern of hcp Co(11$\bar{2}$0). It is useful to examine the connection between these two indexing schemes, because the experimental data are naturally indexed on the cubic {001} $c(2\times2)$ pattern, whereas the theoretical calculations (described below) are more conveniently indexed on the hcp (11$\bar{2}$0) 1×1 pattern.

Figure 3(a) shows the $c(2\times2)$ indexing [the axes are labeled $(k_x)_C$ and $(k_y)_C$, C for cubic]. Figure 3(b) shows the 1×1 indexing [axes $(k_x)_H$ and $(k_y)_H$, H for hexagonal]. It is obvious from the figure that, e.g., $(10)_H \equiv (\frac{1}{2}\frac{\bar{1}}{2})_C$, $(01)_H \equiv (\frac{1}{2}\frac{1}{2})_C$, $(02)_H \equiv (11)_C$, $(03)_H \equiv (\frac{3}{2}\frac{3}{2})_C$, etc.

The arguments presented above make it appear reasonable, but do not prove, that a Co(11$\bar{2}$0) film could grow pseudomorphically on a strained Co{001} film with the in-plane geometry of FeAl{001}. To prove the point, we must carry out a QLEED intensity analysis. The purpose of the analysis is to test whether the model produces $I(V)$ spectra in agreement with experiment, and if so, to determine the bulk interlayer spacing d_{bulk} of the film, and the first and second interlayer spacings d_{12} and d_{23}. The exact position of the second basis atom is also unknown at the outset.

IV. LEED INTENSITY ANALYSIS OF $c(2\times2)$ Co FILMS

The model to be tested, as described above, is one of a Co(11$\bar{2}$0) film with its rectangular unit mesh with sides 4.342×4.070 Å^2 strained to fit onto a square mesh with sides 4.107 Å. The presence of a two-atom basis makes the calculations more involved than for a 1×1 film, and requires more beams and more computer time, as was shown in the structure analyses of hcp (11$\bar{2}$0) surfaces.[3,4] Also, the intensity calculations are made for one particular orientation of the strained film, i.e., for a single domain, but before comparison with the experiment, the

calculation results must be averaged to take into account the four possible orientations, i.e., the four domains.

The intensity calculations were performed with Jepsen's full-dynamical CHANGE program.[5] The Co potential was taken from the collection of Moruzzi, Janak, and Williams.[6] Six phase shifts and a different number of beams were used in different energy ranges, namely, 93 beams from 40 to 248 eV, 129 beams up to 348 eV, and 151 beams up to 400 eV. The inner potential was taken as $V_0 = -(10+4i)$ eV, with the real part adjustable in the fitting process (it became 8±2 eV after refinement); and

isotropic root-mean-square amplitude of thermal vibrations of 0.15 Å. As usual in our work, the evaluation of the agreement between theoretical and experimental curves was done both visually and by R-factor analysis using three R factors, namely, the Van Hove–Tong R_{VHT},[7] the Zanazzi-Jona r_{ZJ},[8] and the Pendry R_P (Ref. 9) factors.

In the first stages of the analysis, attention was directed exclusively to the structural parameters which are expected to have the largest effect on the diffracted intensities, namely, d_{bulk} and d_{12}. The position of the second basis atom was fixed in accordance with its relative position in the equilibrium phase, namely, midway between the bottom and top of the unit mesh in the c direction, and $\frac{1}{3}$ of the way between the left and right edges of the unit mesh [cf. Fig. 1(a)]. The bulk spacing d_{bulk} was varied from 1.21 to 1.37 Å in steps of 0.02 Å [the bulk spacing of equilibrium Co($11\bar{2}0$) is 1.2535 Å], all the while varying Δd_{12} (the change in d_{12} with respect to the bulk value) from -0.2 to $+0.2$ Å in steps of 0.05 Å. When all R factors indicated the presence of a minimum in the vicinity of $d_{bulk} = 1.29$ Å for Δd_{12} between -0.12 and -0.14 Å, calculations were made for $d_{bulk} = 1.288$, 1.290, and 1.292 Å, with Δd_{12} varying between -0.2 and 0 Å in steps of 0.025 Å. The R-factor minima were confirmed at $d_{bulk} = 1.29$ Å for Δd_{12} between -0.15 and -0.10 Å.

Attention was then directed toward a possible parallel relaxation of the top atomic layer, similar to the relaxation found, e.g., in Gd($11\bar{2}0$),[4] whereby the two inequivalent atoms in the first layer translate parallel to the surface by equal and opposite amounts ΔX (in order to preserve the glide-line symmetry present in the equilibrium phase). Calculations done with $\Delta X = 0.1, 0.2,$ and 0.3 Å produced a very slight improvement of the fit for $\Delta X = 0.1$ Å, the other parameters remaining fixed at the optimum values found above. The registry of the top atomic layer for $\Delta X = 0.1$ Å is shown to scale in Fig. 4.

Further attempts were made at improving the fit by changing the position of the second basis atom. This atom was moved out of the plane (by 0.05 and 0.1 Å) and along the mirror line (by ± 0.1 Å), but in all cases the fit worsened.

The best-fit structure is then summarized as follows: in-plane square unit mesh with sides 4.107 Å; $d_{bulk} = 1.29 \pm 0.02$ Å; $\Delta d_{12} = -0.125 \pm 0.03$ Å; $\Delta d_{23} = 0 \pm 0.05$ Å; and $\Delta X = 0.1 \pm 0.05$ Å. The second basis atom is located at position (1.369 Å, 2.0535 Å) with respect to the atom at the lowest left corner of the unit mesh as shown for the unstrained structure in Fig. 1(a). The R-factor values are $R_{VHT} = 0.27$ (for $\Delta d_{12} = -0.125$), $r_{ZJ} = 0.07$ (for $\Delta d_{12} = -0.150$), $R_P = 0.47$ (for $\Delta d_{12} = -0.100$). The $I(V)$ spectra calculated with the parameters quoted above are compared to the experimental curves in Fig. 5. We recall that the $(\frac{1}{2}\frac{1}{2})_C \equiv (01)_H$ beam was not taken into account in the analysis because, as mentioned above, the high background in its vicinity made its intensity uncertain (which may be the reason why the experimental peak observed in this spectrum at about 70 eV could not be reproduced in the calculations
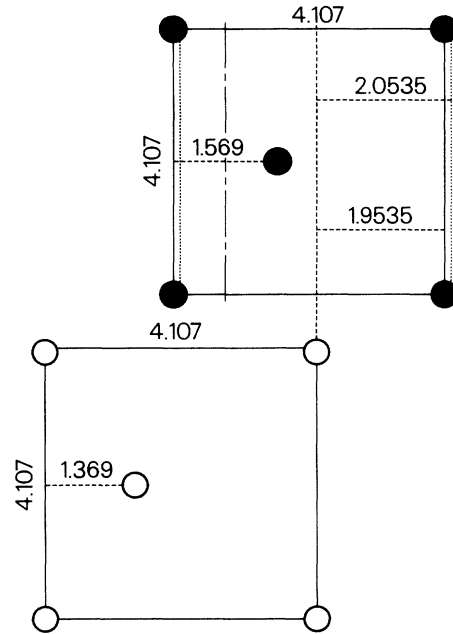

FIG. 4. Schematic drawing of the strained Co($11\bar{2}0$) unit mesh with parallel relaxation of the top atomic layer. For clarity, the unit mesh of the second layer (lower square, atoms shown as open circles) has been translated below the unit mesh of the first layer (upper square, atoms shown as full circles), but all other dimensions are to scale. Before parallel relaxation, the top unit mesh is bisected by the central vertical dashed line; after parallel relaxation, the top unit mesh is translated toward the left by $\Delta X = 0.1$ Å (solid square) and the second basis atom is shifted to the right by $2\Delta X$ to preserve the glide plane (vertical chain-dotted line).

by any of the models tested). The remaining spectra are in satisfactory agreement with the experimental counterparts.

V. STRAIN ANALYSIS

The case under study here is an example of pseudomorphic epitaxy more general than when film and susbtrate have similar unit meshes that differ only in scale. We know which set of net rows on the substrate surface is matched to which set of net rows in the epitaxial film. The substrate in this case is the strained 10–12-Å Co film grown on a FeAl{001} surface,[1] but since the geometries of the film and the substrate are the same, we will refer to the substrate simply as the FeAl{001} surface. To get the smallest overall misfit of this surface to a Co($11\bar{2}0$) plane, we must orient the two nets in such a way that the [0001] direction on Co($11\bar{2}0$) is parallel to the $\langle 110 \rangle$ direction on FeAl{001}. Then, the substrate rows to be matched are the diagonals of the basic square mesh on FeAl{001}, i.e., the $\langle 11 \rangle$ rows, which we will call the $\langle 11 \rangle_C$ rows (subscript C for cubic). We have already mentioned that it is therefore convenient to take as the unit mesh of the substrate the larger (centered) square with sides 4.107 Å ($= 2.904 \times \sqrt{2}$).
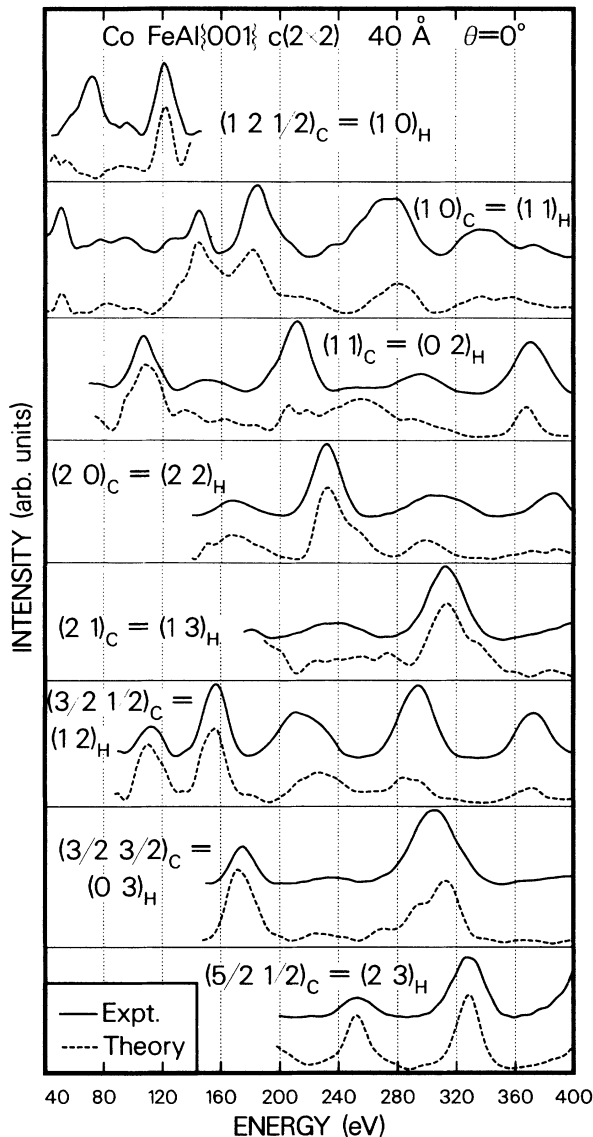
FIG. 5. Experimental (solid) and theoretical (dashed) LEED $I(V)$ spectra from a 40-Å film of Co on FeAl{001} for normal incidence of the primary electron beam. The film being a strained Co($11\bar{2}0$) film, both the cubic [subscript C, see Fig. 3(a)] and the hexagonal [subscript H, see Fig. 3(b)] indices of the spectra are given.

Recall (Fig. 1) that the unit mesh of unstrained Co($11\bar{2}0$) is a rectangle with sides 4.070 and 4.342 Å, so that the film rows to be matched are the [10] and the [01] rows of the Co($11\bar{2}0$) net, which we will refer to as the $[10]_H$ and the $[01]_H$, respectively, (H for hexagonal). These rows are matched to the $\langle 11 \rangle_C$ rows of the FeAl{001} net. We know therefore that the in-plane strains are a 0.91% compression in one direction ($\epsilon_{11} = +0.0091$ referred to surface axes) and a 5.4% expansion in the perpendicular direction ($\epsilon_{22} = -0.054$ referred to surface axes). What we want to determine with strain analysis is the whole strain tensor ϵ_{ik} and in particular the strain component ϵ_{33} in the direction perpendicular to the surface of the film, so that we can compare it

with the value determined by QLEED.

We split the problem into two separate problems, each concerned with matching one set of rows in one direction only, i.e., first matching every $[10]_H$ row with every $\langle 11 \rangle_C$ row and then matching every $[01]_H$ row with every $\langle 11 \rangle_C$ row. At the end we superpose the solutions of the two problems.

Thus, the first problem to solve is the fundamental one of calculating the complete strain tensor produced by the forced matching of a given set of film rows with a given set of substrate rows with no stress imposed along the rows—a row-matching problem. The procedure to follow in order to solve this problem is described in detail in Ref. 10. We only mention here that the method of solution requires transformation of the stress and strain tensors to crystal axes, where the elastic constants are known, and then transformation of the tensors back into the surface axes, where the strain component ϵ_{33} in the direction perpendicular to the surface is the desired quantity. This row-matching problem is solved separately for the two sides of the unit meshes, and the two solutions are superposed to give the total ϵ_{33}. We refer the reader to Ref. 10 for the formulas and their derivations. The tensor transformation formula is given in Ref. 10 and in books on crystal physics such as Ref. 11.

The resulting perpendicular component ϵ_{33} turns out to be $\epsilon_{33} = +0.0335$. Experimentally, we find the perpendicular strain from $(d_{bulk} - d_{eq})/d_{eq}$ (d_{eq} is the bulk spacing in the equilibrium phase), hence $\epsilon_{33}^{exp} = +0.0291 \pm 0.016$. Thus, the agreement between the result of the elastic strain analysis and the QLEED result is acceptably good.

VI. DISCUSSION

The QLEED analysis has shown, and the strain analysis has confirmed, that the $c(2 \times 2)$ LEED pattern observed on Co films thicker than about 13 Å is due to a Co($11\bar{2}0$) film strained to fit onto the in-plane unit mesh of FeAl{001}. We find this result remarkable for a number of reasons.

First, we note that the strained Co($11\bar{2}0$) films grow onto strained Co{001}1×1 only after the latter have reached a thickness of about eight or ten layers—they do not grown directly onto the clean FeAl{001} surface, although the geometrical parameters are exactly the same. This behavior is not new. For example, on a clean Ru(001) surface, films of iron were found to grow with the bcc structure and the {110} orientation, but not directly on the Ru(0001) surface, rather on a strained pseudomorphic monolayer of Fe that covers the substrate surface as soon as a sufficient amount of Fe is deposited.[12] Similarly, Fe on Cu{111} and on Pd{111} first grows pseudomorphically to form six- to eight-layer films with a strained fcc structure and {111} orientation, and only then grows epitaxially to form rotationally related domains of bcc Fe{110}.[13,14]

Second, we note that the Co($11\bar{2}0$) films could be grown to be very thick by ultrathin-film standards (~ 200 Å) despite the relatively large epitaxial strains involved. In fact, with a uniform *planar* strain of -5.4%, we would expect to be able to grow at best two- or three-

layer-thick pseudomorphic films before misfit dislocations set in and destroy the long-range order; whereas in this work, we have learned that with a *linear* strain of -5.4% (and a much smaller linear strain in the in-plane orthogonal direction) much thicker films can be grown.

Third, we note that the present study of the pseudomorphic growth of a rectangular unit mesh on a square net with different lattice constant may be the first reported QLEED analysis of what in Ref. 10 we call "case-2" epitaxy, namely, epitaxy in which the unit meshes of film and substrate are not similar, differing only in scale, but close enough in lengths of sides and in angles between the sides to make pseudomorphism possible.

Fourth, we note that it would be interesting to test the magnetic properties of the strained $Co(11\bar{2}0)$ films and to see how different they may be from those of the corresponding equilibrium phase. Comparison between the atomic volumes (11.076 Å^3 in the equilibrium phase and 10.880 Å^3 in the strained films) would lead us to expect a decreased magnetic moment.

Fifth, we note that, as shown many times before,[10] elastic strain analysis explains well the experimental findings in pseudomorphic epitaxy and is helpful in determining the equilibrium phase of epitaxial films.

Finally, we renew the observation that QLEED is almost uniquely useful in the study of the atomic structure and the elastic properties of ultrathin films because it not only determines the atomic positions in surface layers, but also determines the strained bulk structure required to carry out the elastic strain analysis.

VII. CONCLUSION

The epitaxy of Co on $FeAl\{001\}$ produces sequentially two different, though both pseudomorphic, phases and orientations of crystalline cobalt: first, body-centered-tetragonal $Co\{001\}$ to a thickness of eight–ten atomic layers (determined and discussed in Paper I), and then strained $Co(11\bar{2}0)$ to thicknesses of at least 200 Å (determined and discussed here). The $Co(11\bar{2}0)$ films have in-plane strains of $+0.91\%$ in one direction and -5.4% in the orthogonal direction. QLEED finds the bulk interlayer spacing to be 2.9% expanded with respect to the bulk interlayer spacing in the unstrained hcp structure of cobalt (1.2535 Å), in satisfactory agreement with elastic-strain analysis prediction of 3.35%.

We recently became aware of a paper by Donner *et al.*[15] which describes a study, by x-ray scattering techniques, of single-crystal $Co/Cr\{001\}$ superlattices with various Co thicknesses. The results show that the Co films are hcp with the $(11\bar{2}0)$ plane parallel to $Cr\{001\}$, and that the hexagonal symmetry persists for Co layer thicknesses from about 50 Å down to 4 Å. In this case, the misfits are quoted as -0.2% and $+6\%$ along the two in-plane directions, respectively, but the bulk interlayer spacing is found to be 1.26 Å [very close to that of unstrained $Co(11\bar{2}0)$] for Co multilayer thicknesses of 48.5 Å, and to increase to 1.32 Å for thicknesses of 10 Å. No strain analysis is reported.

[1]C. P. Wang, S. C. Wu, F. Jona, and P. M. Marcus, preceding paper, Phys. Rev. B **49**, 17 385 (1994).

[2]C. P. Wang, F. Jona, N. R. Gleason, D. R. Strongin, and P. M. Marcus, Surf. Sci. **298**, 114 (1993).

[3]M. Welz, W. Moritz, and D. Wolf, Surf. Sci. **125**, 473 (1983).

[4]J. Quinn, C. P. Wang, F. Jona, and P. M. Marcus, J. Phys. Condens. Matter **5**, 541 (1993) for $Gd(11\bar{2}0)$; Y. S. Li, J. Quinn, F. Jona, and P. M. Marcus, Phys. Rev. B **46**, 4830 (1992) for $Tb(11\bar{2}0)$.

[5]D. W. Jepsen, Phys. Rev. B **22**, 5701 (1980); **22**, 814 (1980).

[6]V. L. Moruzzi, J. F. Janak, and A. R. Williams, *Calculated Electronic Properties of Metals* (Pergamon, New York, 1978).

[7]M. A. Van Hove, S. Y. Tong, and M. H. Elconin, Surf. Sci. **64**, 85 (1977).

[8]E. Zanazzi and F. Jona, Surf. Sci. **62**, 61 (1977).

[9]J. B. Pendry, J. Phys. C **13**, 937 (1980).

[10]F. Jona and P. M. Marcus (unpublished).

[11]See, e.g., J. F. Nye, *Physical Properties of Crystals* (Clarendon Oxford, 1957).

[12]D. Tian, H. Li, F. Jona, and P. M. Marcus, Solid State Commun. **80**, 783 (1991).

[13]D. Tian, F. Jona, and P. M. Marcus, Phys. Rev. B **45**, 11 216 (1992).

[14]A. M. Begley, D. Tian, F. Jona, and P. M. Marcus, Surf. Sci. **280**, 289 (1993).

[15]W. Donner, N. Metoki, A. Abromeit, and H. Zabel, Phys. Rev. B **48**, 14 475 (1993).