Ultrathin films of Mn on V{001}: γ- or δ-Mn?

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Ultrathin films of Mn grow pseudomorphically on V{001} up to thicknesses of about 15 Å. A quantitative low-energy electron analysis finds the structure of the films to be body-centered tetragonal with $a=3.023$ Å (forced by the V{001} substrate) and $c=2.92\pm0.06$ Å, with a slightly expanded first-interlayer spacing. Strain analysis (necessary in order to find the equilibrium phase of the films) requires knowledge of the crystallographic and elastic properties of the possible equilibrium phases, which are known only approximately and with large uncertainties, particularly for (bcc) δ-Mn. The available crystallographic data do not allow a confident choice between γ-Mn and δ-Mn as the equilibrium phase of Mn films grown on V{001} (this work) or on Pd{001} or Fe{001} as reported elsewhere. [S0163-1829(99)05519-8]

I. INTRODUCTION

Body-centered-cubic (bcc) manganese (δ-Mn) is stable only at high temperatures, between 1133 and 1244 °C, with a lattice parameter (at 1134 °C) $a=3.0806$ Å.[1] There has been great interest in stabilizing δ-Mn at room temperature because the proximity of Mn to Fe in the Periodic Table suggests possible similarities of the magnetic properties of δ-Mn to bcc Fe.

In contrast to its lower-temperature modification (γ-Mn), which has been stabilized at room temperature in dilute alloys with Fe and Ni,[2–4] δ-Mn has not been stabilized by alloying with other metals. Attempts have been made to stabilize it at room temperature by pseudomorphic epitaxy of thin Mn films on selected substrates. In fact, claims of success have been made in print by several authors,[5–8] but none has been proven, since it is necessary to prove that the grown films are not strained γ-Mn.

Heinrich and co-workers[5] write that bcc Mn "can be stabilized by epitaxial growth on the (100) face of bcc Fe," but give no details or supporting evidence. Pohl et al.[6] claim to have grown δ-Mn in Fe-Mn superlattices and give its lattice parameters, as determined by reflection high-energy electron diffraction, as $a=2.86\pm0.008$ Å and $c=2.79\pm0.01$ Å. These numbers show that the *actual* structure of the Mn layers in the superlattice was body-centered tetragonal (bct), as would be expected, but do not prove that the *equilibrium* structure was δ-Mn. In a subsequent paper, Pohl et al.[7] also claim to have grown δ-Mn in Cr-Mn multilayers, but again provide no proof. The lattice parameter of δ-Mn extrapolated from high temperatures is given as 2.86 Å, a value that is more than 7% lower than the high-temperature value. If the equilibrium value of the lattice parameter of δ-Mn at room temperature were in fact 2.86 Å, then it would be almost identical to the lattice parameter of Fe (2.866 Å) and therefore, a film grown on Fe{001} would be expected to be almost perfectly bcc, rather than bct, as observed.[6] Furthermore, a film of δ-Mn with $a=2.86$ Å on Cr{001} ($a=2.884$ Å) would be expanded within the plane and hence, would be expected to contract in the perpendicular c direction, in contrast to the authors' finding[7] that "the lattice parameter c exceeds that of the Cr lattice and is even distinctly larger than the one expected for δ-Mn."

In a later paper on x-ray diffraction studies of Fe-Mn, Cr-Mn, and V-Mn superlattices, Pohl et al.,[8] while still claiming, without proof, to have grown δ-Mn layers, quote the lattice parameter of δ-Mn as $a=2.985\pm0.05$ Å. It is not clear whether this number is the equilibrium value for δ-Mn at room temperature or the actual value measured on the Mn layers in the superlattices. The interlayer spacing d is listed in Table I of Ref. 8 as varying from 1.476 to 1.486 Å, although it is declared in the text to be "no real lattice spacing, but a variable used for calculation purposes only" (Ref. 8). It is therefore difficult to draw clear conclusions from the data presented in that paper.

A common problem with all the papers discussed above is that the claim about having grown δ-Mn seems to be based on the mere fact that Mn films were found to grow pseudomorphically on substrates such as Fe, Cr, or V, all of which have the bcc structure. This fact alone does not prove or justify the claim. A strain analysis is needed to establish the identity of the equilibrium phase. We summarize below the pertinent arguments (for a more detailed discussion see, e.g., Ref. 9).

Pseudomorphic epitaxy of film A on substrate B of a different material almost always strains A because the lattice parameters of A and B are almost always different. The percentage difference between the unit meshes at the film-substrate interface is the strain in the plane of the film and is called the misfit. To calculate the in-plane strain we must know both lattice parameters, i.e., that of B (which is also the *actual* in-plane lattice parameter of the pseudomorphic film) and that of the *unstrained*, so-called *equilibrium*, structure of A. If the in-plane strain is positive, i.e., A is expanded in the plane to fit the B parameter (as required by the pseudomorphism), then the elastic response will make the perpendicular strain negative, i.e., A will contract in the perpendicular direction, and *vice versa*. Again, we can calculate the perpendicular strain only if we know both the perpendicular lattice parameter of the *equilibrium* phase of A and the *actual* perpendicular lattice parameter in the film as grown. If there are more than one *possible* equilibrium phases of A (and there almost always are, stable or metastable), then the strains will be different for each phase.

It follows that when we observe pseudomorphic growth of A on B we cannot immediately tell which phase of A has been grown. To find out we must *measure* the perpendicular strain and compare it with the strain calculated for each pos-

sible equilibrium phase of A, a procedure called strain analysis. In the specific case of Mn as the film material A and a cubic {001} plane as the film-substrate B interface, there are at least *two* possible equilibrium phases of A, both metastable at room temperature, namely, γ-Mn and δ-Mn. The bulk structure of B plays no role in the process, only the size of the unit mesh at the interface does, i.e., the mere fact that the substrate has a bulk bcc structure does not allow the conclusion that the equilibrium phase of the A film is also bcc. (For example, Fe on Cu{001} is fcc, but Fe on Ag{001} is bcc, and so is Fe on Rh{001}.)

The needed relationship between the actual (measured) and the equilibrium structure of the A film must take into account the elastic properties of the equilibrium phase. For a cubic (either fcc or bcc) material growing pseudomorphically on a square net with constant a with a bulk interlayer spacing d (the *actual* structure) the relationship with the corresponding quantities of the equilibrium phase a_{eq} and d_{eq} is (see e.g., Ref. 9)

$$\frac{d}{d_{eq}} = \left(\frac{a}{a_{eq}}\right)^{-\gamma}, \tag{1}$$

where γ is a function of the elastic constants of the equilibrium phase. In the case of cubic{001}

$$\gamma = \frac{2c_{12}}{c_{11}} = \frac{2\nu}{1-\nu}, \tag{2}$$

where c_{12} and c_{11} are elastic constants and ν is the Poisson ratio.

It is obvious, therefore, that in order to carry out a strain analysis we need to know the lattice parameters *and* the elastic constants of all possible phases of A. In the case of Mn this knowledge is only approximate and uncertain, particularly for δ-Mn. We will argue below that the room-temperature lattice constant of δ-Mn can be estimated in two ways. One way is by first-principles calculations, which give $a = 2.84$ Å, the other is by extrapolation from high temperature, which gives $a = 2.98$ Å—two quite different values.

Any attempt at stabilizing δ-Mn at room temperature by pseudomorphic epitaxy requires making a choice of appropriate substrates, choice that in this case depends on which of the two values of the lattice constant is correct. If $a = 2.84$ Å is the correct value, then Fe{001}, with $a = 2.866$ Å, is a suitable substrate (misfit 0.9%): a study of the growth of Mn on Fe{001} was done and published recently[10] and will be discussed below. If $a = 2.98$ Å, then V{001}, with $a = 3.023$ Å, is a good choice (misfit 1.4%).

We present here the results of a study of the growth of ultrathin films of Mn on V{001} (Sec. II), the determination of their atomic structure by quantitative low-energy electron diffraction (QLEED) intensity analysis (Sec. III), the pertinent strain analysis (Sec. IV), and a concluding discussion (Sec. V).

II. EXPERIMENT

The preparation of a clean V{001} surface is a difficult and lengthy process. Jensen *et al.*[11] described the process in detail, which was useful to us in the initial stages, but the process needed to be somewhat modified in the present work, as described below.

The V substrate was a {001} platelet approximately $10 \times 10 \times 0.5$ mm^3. After 30 h of Ar-ion bombardment (5×10^{-5} Torr of Ar, 1 μA, 375 eV) Auger-electron spectroscopy (AES) still revealed the presence of large amounts of S, C, P, and O. The amounts were estimated from the ratios of (doubly differentiated) AES lines of each impurity to the V AES line at 473 eV: for S the line at 152 eV, for C the line at 272 eV, and for P the line at 120 eV. For O there is the problem that the O AES line at 510 eV is too close to the V line at 509 eV for accurate measurements, but the problem can be circumvented by monitoring the ratio between the V line at 473 eV and the V line at 509 eV (with O present, the peak at 509–510 eV is bigger and wider than otherwise), and by monitoring the O line at 490 eV. After the initial 30 h of Ar-ion bombardment the amounts still present were: S about 56%, C 43%, P 24%, and O 30%.

Additional Ar-ion bombardment for 12 h still left about 12% C and 6% S, but no P and no O above the noise. Annealing to 500 °C for 5 min increased the S peak enormously, but did not substantially affect the C and P peaks. Additional 14 h of bombardment did not change the situation significantly.

Argon-ion bombardments of the hot sample (850 °C) proved to be more effective in the long run. After a total of 50 h (5 cycles of 10 h each) S was reduced to 36% and P to 15%. Four additional cycles for a total of 42 h, with 10-min flashes to 1000 °C every 2 h, reduced the P peak into the noise and the S peak to 3%. At this point, the LEED pattern was a sharp 5×1. Jensen *et al.*[11] reported observing a 5×1 pattern with no S, and attributed the formation of the superstructure to the presence of 0.2 layers of oxygen. We have no explanation for this difference between Jensen *et al.*'s observations and ours. But in any case 6 more hours of bombardment, followed by 10-min anneal at 1000 °C, slow cooling (about 1 h) to room temperature, 2 more hours of bombardment followed by a 30-s flash to 1000 °C produced an AES-clean V{001} surface. The LEED pattern at this stage was a sharp 1×1 pattern with low background at all energies between 30 and 400 eV. Thus, the overall cleaning process required a grand total of 152 h of Ar-ion bombardment, 56 with the sample at room temperature and 96 with the sample hot (850 °C).

Manganese was deposited on the clean V{001} surface from a source consisting of a few Mn pellets in a W spiral that was heated resistively. The deposition rate varied between 0.5 and 0.8 Å/min. The Mn coverage was monitored by the ratio between the Mn AES line at 589 eV and the V line at 473 eV. The LEED pattern was observed, and $I(V)$ curves were collected, after approximately each incremental 3 or 4 Å; the pattern always remained 1×1. The $I(V)$ curves taken with 3 Å of Mn were already different from those of the clean substrate surface, and kept changing until the Mn film reached a thickness of about 12 Å, after which they remained stable with increasing thickness. But after reaching about 15 Å the LEED pattern deteriorated (spot broadened, background increased) and was barely visible at thicknesses of about 25 Å. The $I(V)$ curves used in the structure analysis were collected from a 12-Å thick Mn film: they are the 10, 11, 20, and 21 curves from 60 to 360 eV. We should note, for reasons to be discussed later, that the quality of the LEED pattern from the 12-Å film was notably better (sharper

spots, lower background) than that of LEED patterns from Mn films grown on Fe{001}.[10]

III. STRUCTURE ANALYSIS

The calculations of the LEED beams intensities produced by the Mn film were made with the full-dynamical program CHANGE (Ref. 12) including 81 beams and 6 phase shifts up to 360 eV. The Mn potential needed for the corresponding phase shifts was obtained from the collection of Moruzzi, Janak, and Williams.[13] The real part of the inner potential was initially chosen at 10 eV (adjustable during the analysis—the final value was 12 ± 3 eV), the imaginary part was 3 eV, and the root-mean-square amplitude of thermal vibrations $(\langle u^2 \rangle)^{1/2} = 0.121$ Å.

The calculations assumed that the Mn film was semi-infinite with an in-plane lattice constant of 3.023 Å imposed by the pseudomorphism with the V{001} substrate. The interlayer spacing d_{bulk} was varied initially from 0.9 to 1.50 Å in steps of 0.2 Å, and later from 1.42 to 1.54 Å in steps of 0.02 Å, in each case varying the change Δd_{12} of the first interlayer spacing d_{12} from -0.08 to $+0.16$ Å in steps of 0.02 Å.

The agreement between calculated and observed $I(V)$ spectra was gauged both visually and by R-factor analysis with three R factors: R_{VHT},[14] r_{ZJ},[15] and R_P.[16] Contour plots for these three R factors in the d_{bulk}-Δd_{12} plane are depicted in Fig. 1. The average values of the parameters from the three R-factor minima are $d_{bulk} = 1.46 \pm 0.03$ Å and $\Delta d_{12} = 0.11 \pm 0.03$ Å, with $R_{VHT} = 0.24$, $r_{ZJ} = 0.10$, and $R_P = 0.36$.

Figure 2 depicts the 10, 11, 20, and, 21 $I(V)$ curves, both experimental (solid) and theoretical (dotted), showing very good fit for a strained pseudomorphic film.

IV. STRAIN ANALYSIS

The experiment and the QLEED analysis show that the actual structure of the Mn film is bct with $a = 3.023$ Å (imposed by the V{001} substrate) and $d = 1.46$ Å. The question is, what is the equilibrium phase? To answer this question we must carry out a strain analysis by calculating d with Eq. (1) for all possible equilibrium phases and comparing the results with the experimental value $d_{exp} = 1.46$ Å. For the calculations we need the value of the Poisson ratio ν of Mn and the values a_{eq} and d_{eq} of the possible equilibrium phase. Two possible candidates for the equilibrium structure are: γ-Mn or δ-Mn.

In our study of ultrathin films of Mn on Fe{001} (Ref. 10) we demonstrated that the Poisson ratio of Mn is about 0.45, i.e., the material is very soft. We use this value to calculate γ from Eq. (2) for both γ-Mn and δ-Mn, obtaining $\gamma = 1.636$.

We also need the room-temperature values of a_{eq} and d_{eq} for the two possible equilibrium phases. For γ-Mn, the most reliable room-temperature parameters are those determined by Endoh and Ishikawa[2] from polycrystals of Fe-Mn alloys with small amounts of Cu added to stabilize the γ phase. The alloys have the fcc structure for all concentrations of Fe down to 15%, where they exhibit a small tetragonal distortion. Extrapolation of the data to zero Fe content yields the values $a_0 = 3.796$ Å, $c_0 = 3.592$ Å. Since the {001} plane is
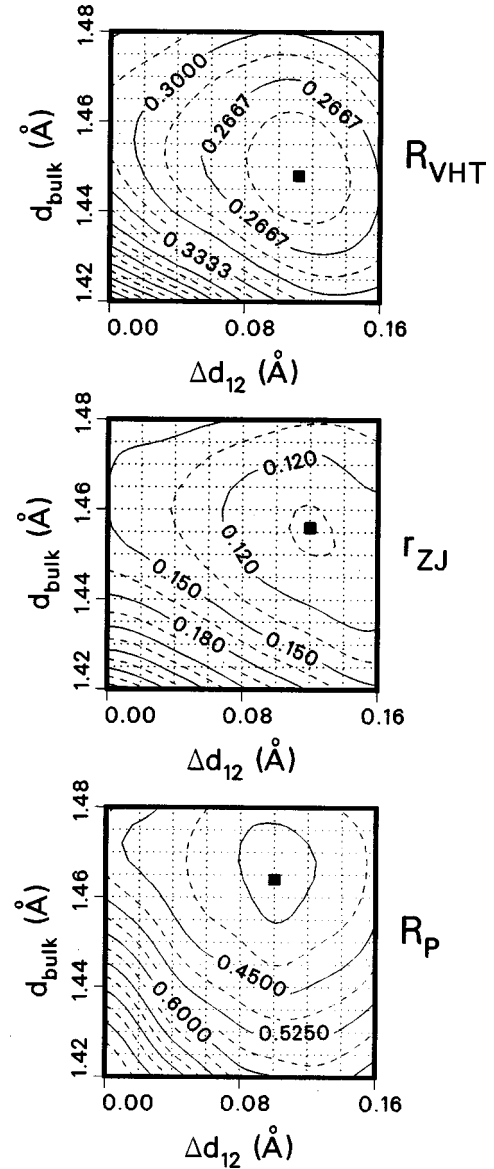

FIG. 1. Contour plot of d_{bulk} versus Δd_{12} for a 12-Å film of Mn on V{001}.

face centered, the relevant parameters are $a_{eq} = 3.796/\sqrt{2} = 2.684$ Å and $d_{eq} = 3.592/2 = 1.796$ Å.

For δ-Mn, we have a dilemma. First-principles total-energy band-structure calculations[17] show that the ground state of bcc Mn is low-spin ferromagnetic with $a = 2.78$ Å, then becomes ferrimagnetic upon expansion by 4 to 8% (from $a = 2.80$ Å to about $a = 3.0$ Å) and then antiferromagnetic upon further expansion, with a ferromagnetic phase about 20 mRy/atom higher than the antiferromagnetic phase for values of the lattice parameter larger than 3.1 Å. In order to estimate the *experimental* value a correction of these theoretical values is needed, since the theoretical values of lattice parameters calculated with augmented spherical waves (ASW) have been shown[18] to be between 1 and 2% too low with respect to experiment for all $3d$ metals (with the exception of fcc Mn, for which the theoretical value is about 3.7% too low with respect to experiment, but note that the theoretical value applies to the fcc structure, whereas the experimental ground state is tetragonal). Thus, applying a 2% correction to the 2.78 value we find that the
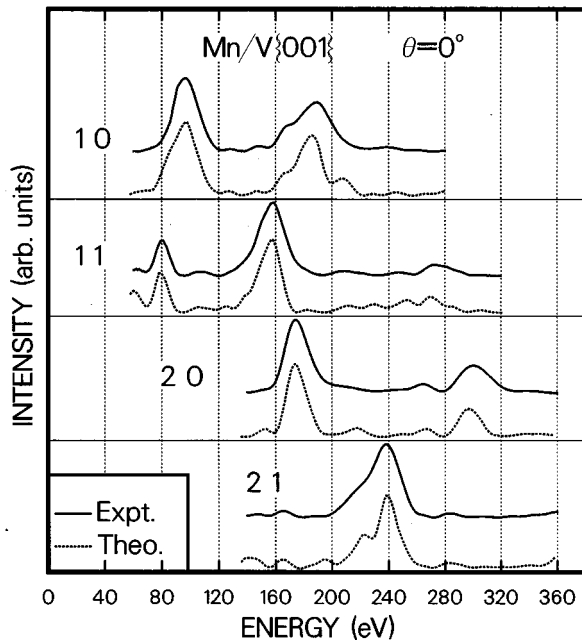
FIG. 2. Experimental (solid, from a 12-Å film) and theoretical (dotted, for a semi-infinite crystal) LEED $I(V)$ spectra for Mn on V{001} at normal incidence of the primary beam.

theoretical value for the ground state of δ-Mn at room temperature is $a_{eq} = 2.84$ Å, i.e., $d_{eq} = 1.42$ Å.

A different value of the room-temperature lattice constant of δ-Mn is obtained if we extrapolate the high-temperature value to room temperature. For this extrapolation we need to make estimates of thermal expansion coefficients, and correct them for their decrease at lower temperatures (the linear extrapolation of the lattice parameter of the α phase of Mn from 1000 °K to room temperature is too low by about 1.5% with respect to the measured value[19]). Using the high-temperature data reported by Pearson[1] and applying a 1.5% correction we obtain $a = 2.98$ Å.

The conclusions that can be drawn from the present experiments are quite different depending on which lattice-constant value is assumed for δ-Mn, i.e., either the theoretical value $a_{eq}^t = 2.84$ Å, hence, $d_{eq}^t = 1.42$ Å, or the extrapolated value $a_{eq}^e = 2.98$ Å, hence, $d_{eq}^e = 1.49$ Å, as we now show.

For γ-Mn from Eq. (1) we find $d = 1.478$ Å. If we assume the extrapolated value of the lattice constant (2.98 Å) for δ-Mn from Eq. (1) we get $d = 1.455$ Å. In this case, although the calculated value for δ-Mn agrees better with experiment, considering the error bars on the d_{exp} value (1.46 ± 0.03 Å), we cannot choose confidently between the two possible equilibrium phases.

If we assume the (corrected) theoretical value of the in-plane lattice constant (2.84 Å) we can immediately disqualify δ-Mn from being the equilibrium phase with the following argument. In order to adapt to the lattice constant of the V{001} substrate (3.023 Å), δ-Mn would be expanded in the plane, hence, would be expected to contract in the perpendicular direction, i.e., to have a d value smaller than $d_{eq} = 1.42$ Å. But the experimental value $d_{exp} = 1.46$ Å is larger than 1.42, hence, δ-Mn cannot be the equilibrium phase. In fact, from Eq. (1) we obtain $d = 1.28$ Å, much lower than d_{exp}.

V. DISCUSSION

Obviously, an important quantity in a discussion about the possibility of stabilizing δ-Mn at room temperature by pseudomorphic epitaxy is the value of the lattice constant at room temperature. Unfortunately, as we noted in the preceding section, such value is not known with confidence.

The theoretical value $a^t = 2.84$ Å for δ-Mn was found above by an empirical correction to theory, but it is possible that there is another metastable phase of Mn that fits V{001} well, especially if the volume is expanded by magnetic effects. The extrapolated value $a^e = 2.98$ Å fits the lattice constant of V{001} better, but it disregards possible effects of phase transitions from disorder to order, which generally reduce the lattice constant, and cannot be measured. The volume per atom is quite different for the phases under scrutiny: for $a^t = 2.84$ Å, $V^t = 11.45$ Å^3, for $a^e = 2.98$ Å, $V^e = 13.23$ Å^3, while the experiment gives $V_{exp} = (3.023)^2 \times 1.46 = 13.34$ Å^3.

Some consequences of accepting $a^t = 2.84$ Å as the correct lattice constant of δ-Mn at room temperature are worth noting. As pointed out above, the present experiments exclude δ-Mn from being the equilibrium phase (because despite the in-plane expansion of 2.84 to 3.023 Å, the *actual* interlayer spacing, 1.46 Å, is larger than the equilibrium value 1.42 Å). The same argument would exclude δ-Mn from being the equilibrium phase of the Mn films grown on Fe{001} (because despite the in-plane expansion of 2.84 to 2.866 Å, the *actual* interlayer spacing, 1.614 Å,[10] is larger than the equilibrium value 1.42 Å). The latter exclusion is particularly significant, because the small misfit between δ-Mn and Fe{001} (+0.9%) would suggest good growth of Mn films. One might conclude that if δ-Mn does not grow pseudomorphically on Fe{001} then it probably cannot be stabilized by pseudomorphic epitaxy on *any* substrate.

Table I summarizes the data pertinent to ultrathin films of Mn on Pd{001},[20] Fe{001},[10] and V{001} (this work), as determined by QLEED and calculated with Eq. (1) and $\nu = 0.45$ for γ-Mn and for δ-Mn with either lattice constant. It is clear from the table that with $a = a_{eq}^t = 2.84$ Å δ-Mn (labeled δ-Mn^t in the table) does not grow on any of the three substrates listed in the table (compare d_{calc} with d_{exp}). By contrast, if $a = a_{eq}^e = 2.98$ Å, δ-Mn could possibly grow on Pd{001} (but the misfit, at −7.7%, is quite large), and would probably grow on Fe{001} and on V{001}. These conclusions would not change even if the Poisson ratio of δ-Mn were $\nu = 0.3$, a value common to most metals.[21] In fact, with $\nu = 0.3$, putting $a = a_{eq}^t = 2.84$ Å we calculate $d_{calc} = 1.346$ Å (outside the error bars of $d_{exp} = 1.46 ± 0.03$ Å), whereas putting $a = a_{eq}^e = 2.98$ Å we get $d_{calc} = 1.472$ Å, acceptably close to the experimental value.

The alternative to δ-Mn is of course γ-Mn, which, according to the data in Table I, probably grows on Pd{001} and perhaps also on Fe{001}, despite a misfit of almost 7%. On V{001} γ-Mn would be the preferred phase only if the lattice constant of δ-Mn were indeed 2.84 Å. But the misfit of γ-Mn to V{001} is unusually large (almost 13%) and would not normally allow the growth of well-crystallized 10- or 12-layer films, although we should note that the value of the Poisson ratio near 0.5 means that the material is soft, and large epitaxial strains produce small strain energies. But,

TABLE I. Data for ultrathin films of Mn on Pd{001} (Ref. 20), Fe{001} (Ref. 10), and V{001} (this work). The table headings are: Substrate, as indicated; a_{sub} = lattice constant of the corresponding substrate; d_{exp} = bulk interlayer spacing as determined by QLEED for Mn/Pd, Mn/Fe, and Mn/V; Phase = γ-Mn or δ-Mn; Misfit, to the corresponding Mn phase, as indicated; d_{calc} = interlayer spacing d as calculated with Eq. (1). The data used in the calculations are for γ-Mn, a_{eq} = 2.684 Å, d_{eq} = 1.796 Å (bct tetragonal); for δ-Mn^e, a_{eq} = 2.980 Å, d_{eq} = 1.490 Å (bcc); for δ-Mn^t, a_{eq} = 2.840 Å, d_{eq} = 1.420 Å (bcc); Poisson ratio ν = 0.45. (For the calculations, four significant figures have been kept even though the experimental error is estimated to be ±0.03 Å.)

Substrate	a_{sub} (Å)	d_{exp} (Å)	Phase	Misfit	d_{calc} (Å)
Pd{001}	2.751	1.715	γ-Mn	+2.5%	1.726
			δ-Mn^e	−7.7%	1.700
			δ-Mn^t	−3.1%	1.496
Fe{001}	2.866	1.614	γ-Mn	+6.8%	1.613
			δ-Mn^e	−3.8%	1.588
			δ-Mn^t	+0.9%	1.399
V{001}	3.023	1.460	γ-Mn	+12.6%	1.478
			δ-Mn^e	+1.4%	1.455
			δ-Mn^t	+6.4%	1.283

considering the experimental fact that the Mn films are better crystallized on V{001} (the LEED pattern is sharper and the background lower) than on Fe{001}, one would have to reach the strange conclusion that γ-Mn grows better on V{001} with 12.6% misfit than on Fe{001} with 6.8% misfit.

In the end, we cannot determine with confidence which of the two phases of Mn, γ-Mn, or δ-Mn, grows pseudomorphically on either Pd{001}, Fe{001}, or V{001}, and we may even doubt whether δ-Mn can be stabilized by epitaxy at room temperature at all. The possibility mentioned above, that the equilibrium phase of the grown film is a metastable phase other than γ or δ, still exists. A solution of this problem would probably be found if we had available the so-called epitaxial paths[22] of all possible tetragonal phases, magnetic and nonmagnetic, of Mn.

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