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2006 J. Phys.: Condens. Matter 18 5017

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Film growth arising from the deposition of Au onto an *i*-Al–Pd–Mn quasicrystal: a medium energy ion scattering study

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Received 2 December 2005, in final form 3 March 2006

Published 16 May 2006

Online at stacks.iop.org/JPhysCM/18/5017

Abstract

The room temperature deposition of 7 ML of Au onto the fivefold symmetric surface of icosahedral Al–Pd–Mn leads to the formation of a several monolayers thick Au–Al alloy film. An AlAu film with 1:1 stoichiometry is formed, which shows no evidence of ordered structure, being either amorphous or polycrystalline. Annealing to 325 °C causes more Al to diffuse into the film, producing Al₂Au but still with no indication of structure. Experiments using 0.5 ML of pre-deposited In demonstrated a surfactant effect as the In ‘floated’ on the surface during growth and produced a reduction in film roughness. However, contrary to previous findings the film was still either amorphous or polycrystalline, with no evidence of quasi-crystalline or aperiodic structure. Experiments were also conducted using smaller doses of Au to look for the formation of an epitaxial layer and, if formed, determine the registry with the substrate. However, no change in the Pd blocking curves for the surface could be seen, suggesting that the Au does not adsorb in well defined sites. This result is not surprising when considering that even for these low doses Al is drawn into the film, changing the composition and probably the structure of the topmost layers of the substrate, so that the potential adsorption sites on the clean surface may no longer exist.

1. Introduction

The surfaces of quasi-crystalline materials have attracted a good deal of research interest in recent years. Initial studies have concentrated on determining the properties of the clean

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surfaces of these materials [1–4], but more recently attention has been given to the use of quasicrystals as templates for the growth of thin films [5, 6]. One objective of this work has been the creation of elemental epitaxial films, allowing the effects of composition and structure on the unusual properties of quasicrystals to be deconvolved. Another possibility is the formation of films with novel structural arrangements having as yet unknown electronic, chemical and physical properties. An excellent recent review of the growth of thin films on quasicrystal surfaces is provided by Fournée and Thiel [7].

Studies of the clean fivefold surface of *i*-Al–Pd–Mn [1, 2] have demonstrated that it is compatible with a truncation of a bulk structure proposed by Boudard *et al* [8]. Using scanning tunnelling microscopy (STM), dark star-shaped features have been observed on the fivefold surface [9] and theoretical studies suggest that these may be due to truncated Bergman clusters [9] or Al dimer vacancies [10]. Further STM studies of the deposition of elements including Al and Cu have indicated that these features may act as nucleation sites for the initial stages of growth [11], and in addition theoretical calculations have indicated that they are the lowest energy adsorption sites on the surface [12]. Recently, low energy electron diffraction (LEED) and helium atom scattering (HAS) have suggested that single layer highly ordered epitaxial films of Sb and Bi can be formed on the fivefold surface of *i*-Al–Pd–Mn at a coverage of about one adatom per Al atom in the surface [13]. In addition, the deposition of Pb on the clean surface has been seen to give rise to well ordered patterns as observed with STM [14].

The growth of thicker films of a few monolayers has also been studied. STM work on the deposition of Ag on the fivefold surface indicated the formation of high aspect ratio islands even at relatively low coverage [15]. Another STM study of the deposition of Pd onto the closely related ξ' -Al–Pd–Mn approximant phase demonstrated the formation of clusters that showed only slight increase in size with coverage up to 7 ML [16]. A LEED and secondary electron imaging (SEI) study of Al deposition on *i*-Al–Pd–Mn showed the formation of domains of fcc nanocrystals with their [111] axes parallel to the threefold axes of the surface [17]. In the case of the deposition of Cu onto the clean fivefold surface a film showing one-dimensional quasiperiodicity has been seen at coverages between 5 and 25 ML. STM images show that the structure is comprised of rows having spacings following a Fibonacci sequence of long and short separations [18]. However, analysis of the LEED pattern [19] and recent quantitative medium energy ion scattering (MEIS) results [20] show that the film is comprised of a series of fcc nanoscale domains or 'wires'. The one example so far proposed for the formation of a three-dimensional pseudomorphic film with icosahedral symmetry on Al–Pd–Mn is the deposition of Au in the presence of an In surfactant [21, 22]. The Au forms an alloy film with Al atoms from the substrate in a ratio consistent with the AuAl₂ cubic phase. X-ray photoelectron diffraction (XPD) patterns from the Au 4f peaks have symmetry elements consistent with an icosahedral arrangement of atoms.

A MEIS study of the deposition of Au on *i*-Al–Pd–Mn was undertaken with a view to a structural analysis of the proposed pseudomorphic structure and also as this is an ideal system to investigate using this technique. Since the Au atoms are considerably more massive than any of the substrate atoms, the overlayer signal will be clearly resolved in MEIS and the film structure can be evaluated straightforwardly by comparison of blocking dips with those of the substrate. If the overlayer has the same structure as the substrate then a similar blocking pattern should be evident. However, even in the case of an overlayer blocking pattern that is different to that of the substrate, the structure can still be deduced by comparing it with simulations for various model structures produced using the VEGAS code [23]. A good example of this type of structural analysis using MEIS is contained in the recent study of the growth of Cu films on *i*-Al–Pd–Mn [20]. In addition to the sensitivity to film structure, the energy spectra produced by this technique allow the composition of the film to be deduced with considerable accuracy.

Along with the evaluation of thicker films, analysis of films at a coverage consistent with the formation of a single epitaxial layer was also envisaged, since changes in the surface blocking features could reveal the registry of the film with the substrate and provide insight into the adsorption site during the initial stages of overlayer growth.

2. Experimental details

The experiments were carried out at the UK national MEIS facility at the CCLRC Daresbury Laboratory. A detailed description of the facility is provided elsewhere [24] but briefly it is comprised of an ion source situated in a high voltage enclosure, a transfer beamline and an endstation including ultra-high vacuum chambers for both sample preparation and ion scattering measurements. The collimated ions are scattered from a target mounted in a precision goniometer to allow exact alignment of the beam with specific crystallographic directions in the sample. Scattered ion intensity is monitored using a toroidal electrostatic analyser and position sensitive detector that simultaneously measures a range of angles and energies, with several sets being accumulated and pasted together electronically to produce a full two-dimensional intensity map. The two-dimensional data sets collected are typically processed into one-dimensional energy or angle plots giving compositional and structural information respectively.

The *i*-Al₇₀Pd₂₁Mn₉ sample was grown using the Bridgman technique at the Ames laboratory. The sample was cut by spark erosion to a fivefold surface ((1 0 0 1 0 0) plane) as determined using Laue x-ray diffraction. The surface was polished using progressively finer diamond paste to 1/4 μm before insertion into the vacuum system. The surface was further prepared by cycles of Ar⁺ ion bombardment (1.5 keV, 6 μA, 45° incidence, 1 h) and annealing (630 °C, 1–4 h) to a cumulative annealing time of over 20 h. Procedures of this type have previously been found to produce clean, well ordered, flat surfaces suitable for further experimentation [4]. In this study, the condition of the surface during preparation was monitored using LEED and AES. Deposition of Au onto the sample at room temperature was achieved using a K-cell (SciCam, Cambridge) set at 1275 °C for 30 min for the thicker films (~0.23 ML min⁻¹) and 1245 °C for 12 min for the low coverage deposition (~0.17 ML min⁻¹). For the highest source temperature, a background pressure of approximately 10⁻⁷ mbar was seen during deposition, but residual gas analysis showed this to be composed entirely of molecular N₂ that originates from PBN components in the cell. Throughout this paper coverages are quoted in terms of the average layer density of the icosahedral structure (1 ML = 5.15 × 10¹⁴ atoms cm⁻²), although it should be pointed out that many layers, including the proposed top layer [1, 2], have densities that can be more than twice this. The pre-deposition of In was also carried out using a K-cell, this time at 820 °C for 3 min but with the sample held at 400 °C. For sample annealing, radiative heating for 3 min followed by cooling back to room temperature over a period of approximately 20 min was employed, giving rise to a maximum temperature of 325 °C, which was the minimum temperature that could be realistically measured by the infra-red pyrometer used. The samples were transferred under UHV (10⁻¹⁰ mbar) into the scattering chamber for analysis. He⁺ ions at 100 keV were used and typically data were collected using an incidence angle of 31.8° with the beam orthogonal to a threefold (1 1 1 1 1) plane in the icosahedral substrate. Each data set was taken at a dose of 2.5 × 10¹⁵ ions cm⁻² and the sample moved every two data sets to minimize beam damage.

3. Results

Figure 1 shows a typical 2D data set taken from a sample with a thick Au film grown in the presence of an In surfactant. Diagonal stripes of intensity arising from the various elemental

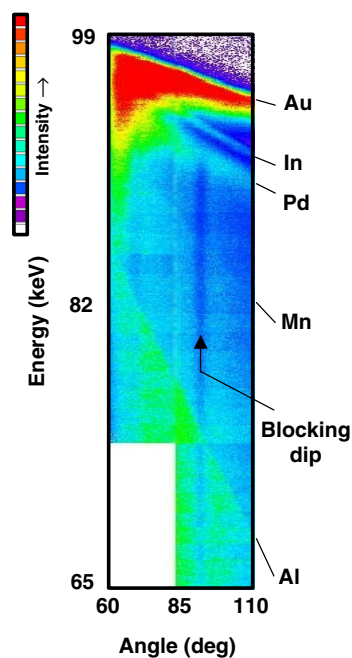


Figure 1. Two-dimensional data set taken from an *i*-Al-Pd-Mn sample with 7 ML of Au deposited in the presence of 0.5 ML of In and annealed to 325 °C. The various mass components can be easily identified along with blocking features from the quasi-crystalline structure.

(This figure is in colour only in the electronic version)

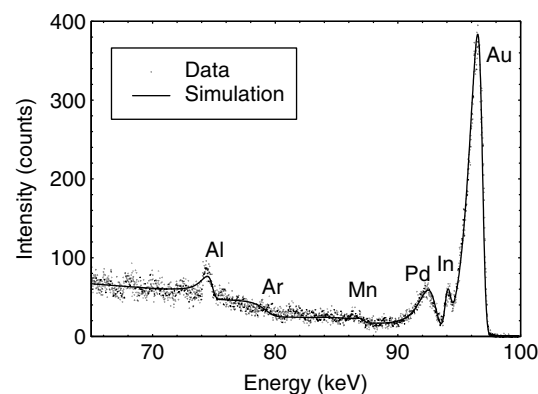


Figure 2. An energy spectrum projected from the data set shown in figure 1. The data were taken in a double alignment geometry (channelling in, blocking out) with a scattering angle of 90° and have been fitted using the SIMNRA5.0 code.

components can be seen together with features of reduced intensity running vertically which arise from the blocking of the outgoing ions by the substrate structure. It is interesting to note that no vertical blocking features run through the Au signal.

Figure 2 shows an energy spectrum taken by projecting a 2D spectrum onto the energy axis. The data have been fitted using the SIMNRA simulation program [25] utilizing a model comprising layers for the sub-surface region, an interlayer, the Au rich film and, where

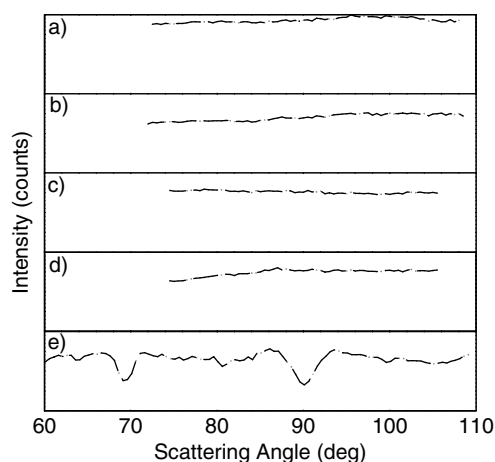


Figure 3. Angular projections for the Au signal from films prepared using (a) 7 ML of Au with no surfactant and no anneal, (b) 7 ML of Au with no surfactant annealed to 325 °C, (c) 7 ML of Au with 0.5 ML of In surfactant but no anneal, (d) 7 ML of Au with 0.5 ML of In surfactant and annealed to 325 °C and (e) the subsurface Pd signal to allow a comparison with the bulk structure. The low angle cut-off for the Au signal is determined by the ability to mass resolve the Au and Pd components. Note the lack of any blocking features in the Au signal regardless of preparation conditions.

necessary, a surfactant layer. Table 1 contains the results from the fitting of a series of samples including ~ 7 ML films grown both with and without an In surfactant, before and after annealing to 325 °C, and a sample with a lower coverage of ~ 2 ML. In general, the deposited Au forms an AlAu alloy with 1:1 stoichiometry, which transforms into Al_2Au when annealed. Partial substitution of Au within the film also appears to occur, leaving small levels of Mn throughout the films. The In signal is always seen to be at the very surface of the film even after annealing, which is typical behaviour for an element acting as a surfactant during growth. The surface roughness of the films, which gives rise to a tail on the low energy side of the Au peak, was seen to increase after annealing. The use of the In surfactant led to lower values of fitted surface roughness when compared to the non-surfactant grown sample both before and after annealing, although the difference is limited. For the thicker films, there is a thin interface region, which is depleted in Al and Mn, before the sub-surface region that is basically bulk-like. For the sample with around 2 ML of Au a 1:1 stoichiometric alloy has already formed, but since this involves less Al, the interface region does not exhibit substantial deviation from the sub-surface composition.

Figure 3 compares the angular intensity yield for the thicker Au films grown under a variety of conditions with signal from the Pd sub-surface region. Whilst the Pd signal has clear features resulting from the icosahedral structure of the substrate, there is virtually no intensity variation in the Au signal for any of the samples analysed. This indicates a complete lack of structure in any of the thicker Au rich films grown.

For the thinner 2 ML film no features would be expected in the Au signal since the Au should lie in the topmost layers where complete illumination is seen. However, if the Au forms an ordered epitaxial monolayer then the atoms should be in well defined sites, which would have an impact on the surface blocking curves of the substrate species. Since it sits higher in energy than Al and Mn and thus should exhibit no background from the sub-surface, the surface Pd signal is the best to evaluate in this respect. Figure 4 contains a comparison of the surface Pd

Table 1. Fitted values of composition thickness and roughness obtained using the SIMNRA simulation code for thin films of Au on *i*-Al-Pd-Mn deposited under various conditions.

Conditions	Thin film					Interface				Sub-surface		
	Thickness (10^{15} atoms cm^{-2})	Roughness (10^{15} atoms cm^{-2})	Au (%)	Al (%)	Mn (%)	Thickness (10^{15} atoms cm^{-2})	Al (%)	Pd (%)	Mn (%)	Al (%)	Pd (%)	Mn (%)
~7 ML Au	8.94	11.22	45	50	5	1.69	20	80	0	81	8	11
~7 ML Au 325 °C anneal	9.87	14.50	28	69	3	1.60	35	65	0	79	10	11
~0.5 ML In ~7 ML Au	7.59	10.67	49	49	2	1.76	24	76	0	81	8	11
~0.5 ML In ~7 ML Au 325 °C anneal	8.91	12.10	37	63	0	1.76	24	76	0	69	15	16
~2 ML Au	2.09	5.37	47	51	2	4.55	76	20	4	77	9	14

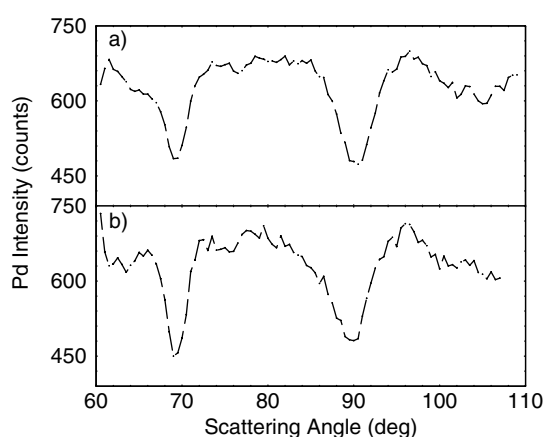


Figure 4. Blocking spectra from the surface Pd signal for (a) the clean surface and (b) one with ~ 2 ML of Au deposited. Note the similarity both in shape and overall intensity of the curves.

signal for the thin Au film and the clean surface. If the adsorbing Au atoms go into bulk-like sites this will lead to a reduction in the overall intensity and more specifically the intensity in the blocking dips, due to the larger scattering cross-section of the Au when compared to Al, Mn or even Pd. If the Au adsorbs in well defined non-bulk-like sites then this will give rise to additional features in the blocking spectrum. Comparing the data in figure 4 shows that the blocking features are essentially unchanged with very similar shape and intensity. This suggests that the Au atoms are not adsorbed in well defined sites.

4. Discussion

It is interesting to note that the deposited thick Au films initially formed an alloy with 1:1 stoichiometry on deposition and significant annealing was required to obtain the previously identified Al_2Au alloy phase. The binary alloy phase diagram [26] indicates that the AlAu alloy has primitive monoclinic structure, which has low symmetry and is perhaps unlikely to form a long-range ordered film. The transformation to Al_2Au , at least in the bulk alloy, leads to the formation of a cubic structure [26]. Well ordered cubic films can be formed on *i*-Al–Pd–Mn by sputtering [4], and hence the Al_2Au phase could possibly be expected to form an ordered cubic film. However, a previous study of this deposition system has indicated the formation of an icosahedral structure in the film. The data shown in figure 3 indicate that no short-range order is present in any of the thick-film samples analysed, even those grown in the presence of In surfactant. This excludes the possibility of either cubic or quasi-crystalline structure in the films, indicating that they are either amorphous or at best polycrystalline.

To further investigate the effect of the film structure on the MEIS blocking curves VEGAS simulations were run of icosahedral Al–Pd–Mn models where Au was substituted for the Pd, the Mn (the favoured model from previous work [22]) and both Pd and Mn sites (which would be required to achieve a composition close to the measured value). These simulations are shown in figure 5 and demonstrate that in all three cases clear blocking dips in the Au signal should be present at the same angular positions as the bulk if the Au sits in an icosahedral environment, thus further confirming the lack of icosahedral structure in the Au rich films.

The similarity between the Pd surface signal for the clean surface and Au thin film has been interpreted as Au adsorbing in sites that are not well defined relative to the substrate. To further

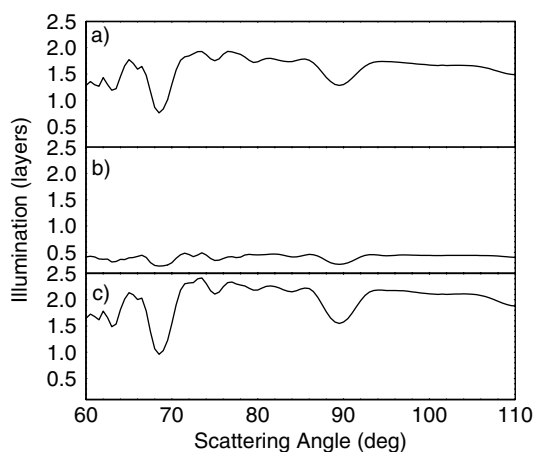


Figure 5. VEGAS simulations of blocking spectra for Au atoms sitting in various lattice sites in an icosahedral quasicrystal: (a) Au in Pd sites; (b) Au in Mn sites; (c) Au in both Pd and Mn sites. In either Mn or Pd sites, Au would give rise to bulk-like blocking features.

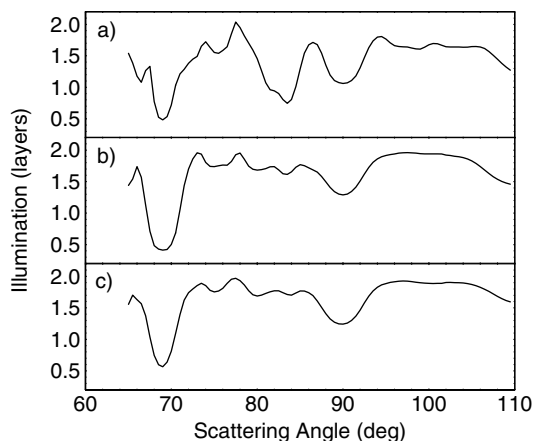


Figure 6. VEGAS simulations of the surface Pd signal for two Au terminated *i*-Al-Pd-Mn models compared with a clean surface model: (a) Au in atop sites; (b) top layer of icosahedral structure substituted for Au; (c) clean surface. For the model with Au in bulk-like sites there is less overall intensity and more specifically a deeper blocking dip at $\sim 69^\circ$. For the model with Au in atop sites a new blocking feature at $\sim 83^\circ$ is evident.

explore this issue VEGAS simulations were carried out for the clean surface and two alternative surfaces that were Au terminated. The first model involved replacing the top-most layer (which is normally Al rich) with Au atoms, thus representing the situation where Au atoms occupy sites that are essentially a continuation of the quasi-crystalline lattice. The second model involves Au atoms in atop sites directly above the surface atoms in one of many non-bulk-like sites that could be envisaged. The results shown in figure 6 illustrate the differences that can be expected in the MEIS data for these two scenarios. In the case of the Au bulk terminated surface there is a reduction in overall intensity of approximately 3%, which arises because of the larger scattering cross-section of the Au leading to more effective blocking of the subsurface atoms. The difference between the overall intensity of the two data sets in figure 4 is less than 0.5%.

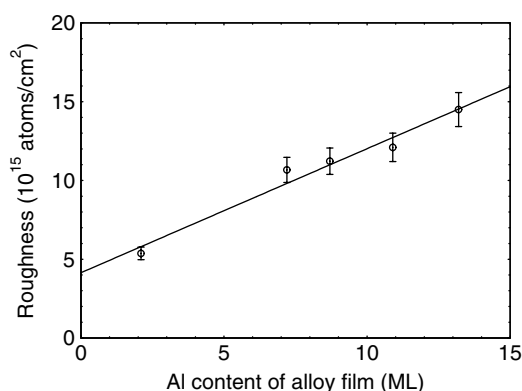


Figure 7. A plot of fitted roughness values against the amount of Al drawn into the alloy film for the five sets of conditions listed in table 1. The line is provided to guide the eye.

At the bottom of the blocking dip at 69° the effect is even more pronounced, with a difference of 38% between the clean surface simulation and that with Au in bulk-like continuation sites; this compares with a difference of approximately 7% in the data. The simulation for Au in atop sites shows a large new blocking feature appearing at 83° . Of course, this is only one of many well ordered non-bulk-like sites that could be envisaged, and they would all be expected to produce different blocking features. However, as with the example shown, the difference between the clean surface and one with Au in non-bulk-like sites could be expected to be sufficiently pronounced to be readily identifiable in the data. Figure 4 demonstrates clearly that this is not the case, since the two data sets have no distinctive differences. This lack of a well defined site for Au adsorption is perhaps not surprising when considering that even at this low coverage the deposited film appears to have mixed composition, so that Al pulled out of the substrate could potentially disrupt the surface structure.

Further evidence that the migration of Al into the alloy film has a disruptive effect on the surface comes from the increasing level of roughness seen for the higher coverages of Au. Figure 7 demonstrates a relationship between the amount of Al in the alloy film and the fitted roughness values. From this relationship it would be easy to speculate that the small positive effect of pre-deposited In on the film morphology could be due to it inhibiting in some minor way the migration of Al into the growing alloy film. If the In remained at the interface during growth it would be easy to accept this as the mechanism for the reduced roughness. However, the MEIS data demonstrate that, as would be expected for a typical surfactant, the In floats on the surface during growth, implying a more traditional mechanism such as increased lateral mobility of the atoms for the improved growth.

The question arises as to the discrepancy between this study and previous work [21, 22]. A possible explanation could be differences between the film preparation conditions used in the two experiments. In this study the Au film was deposited in a partial pressure of N_2 and annealed to a higher temperature than the previous work. However, the N_2 partial pressure would be unlikely to influence the film growth, since it should have a negligible sticking coefficient on the quasi-crystalline substrate. The presence of more reactive contaminants, such as hydrocarbons, H_2O and specifically CO, can be ruled out since the residual gas analyser showed only mass 28 with a small satellite peak at 14, and in addition AES spectra of the deposited surfaces indicated no C or O present. Moreover, the higher annealing temperature used was demonstrated by the MEIS data to give the same composition as the annealing

procedure used in the previous study, which could realistically be expected to result in the same structure. There is another potential explanation of the discrepancy. The previous studies involved the use of x-ray photoelectron diffraction images for the Au 4f peaks, which appeared to show fivefold symmetry elements consistent with icosahedral structure. One interesting feature from the MEIS work is an apparent roughening of the surface after annealing. If this were to lead to areas of the surface where the Au rich film thickness was below the inelastic mean free path of the photoelectrons then additional signal from the bulk components, Pd and Mn, could be detected, giving rise to peaks at similar energies to the Au 4f peaks (Au 4f_{5/2}, 87.6 eV, and Au 4f_{7/2}, 83.9 eV, compared with Pd 4s_{1/2}, 87.1 eV, and Mn 3s_{1/2}, 82.3 eV). Clearly any contribution from either Pd or Mn would give rise to bulk-like photoelectron diffraction features. The diffraction image presented in the previous work has been taken at the correct energy for Mn atoms, and in addition the single scattering cluster model calculations presented also indicate that the atoms responsible for the image are sitting on Mn sites [22]. The possibility of a bulk contribution to the diffraction image does not appear to have been considered in that work.

The MEIS data suggests the following possible sequence for the deposition of Au on *i*-Al-Pd-Mn. In the early stages of deposition Al is pulled from the surface of the substrate to form a thin AlAu alloy film. The surface structure is disrupted, removing the possibility of Au atoms occupying well defined adsorption sites. As the coverage increases and the film becomes thicker, further Al is drawn from the substrate, creating a depleted region in the near surface. The disruption to the surface, which gets progressively worse with increasing Au coverage, means that the growing film has no registry with the substrate, hence forming in an amorphous or at best polycrystalline fashion. Annealing this film gives rise to further migration of Al into the film to form an Al₂Au alloy whilst at the same time further roughening of the film occurs, leading to significant variation in film thickness across the surface. Pre-dosing the sample with In before Au deposition leads to essentially the same growth sequence except that the In floats above the growing film, leading to a slightly flatter surface, possibly by improving the lateral mobility of the adsorbing species. Again, annealing leads to increased roughness but this time, having started from a smoother surface, the final film is able to maintain an advantage over that grown without the In surfactant. Since it is still being disrupted by the migration of Al into the Au rich film, the interface region remains ill defined and no structure is induced in the film due to the In surfactant.

5. Conclusions

The deposition of ~7 ML of Au on *i*-Al-Pd-Mn led to the formation of an AlAu film, which transformed into Al₂Au upon annealing to 325 °C. Pre-deposited In appeared to have a slight surfactant effect, since it floated on the surface during growth and led to reduced surface roughness. However, none of the Au films grown either with or without surfactant, before or after annealing, exhibited any well ordered structure, being amorphous or at best polycrystalline. For the deposition of a thinner film below 2 ML, again an AuAl alloy formed with no well defined registry to the substrate. It is speculated that the affinity of the Au for Al, which it draws out from the substrate, disrupts the surface structure, thus inhibiting the formation of well ordered overlayers, either crystalline or quasi-crystalline.

Acknowledgments

The authors would like to thank EPSRC for funding this work under GR/S19080/01 and for direct access to the MEIS facility via GR/R88809/01. The Austrian science fund (FWF) is also

acknowledged for providing an Erwin Schrödinger fellowship for Dr Draxler (J2417-NO8). The FOM Institute, Amsterdam, is thanked for the provision of the VEGAS code and Dr Paul Quinn for the user-friendly interface to the code. Dr Gerald Kasner of the OvG University, Magdeburg, is acknowledged for providing the structural model used in the simulations.

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