Gd/W(110) Interface Formation Studied by W 4f Surface Core-Level Spectroscopy

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W 4f core-level spectra of Gd films on W(110) show components which can be identified as being due to bulk and interface W. The results suggest that the W/Gd interface is abrupt, *i.e.* no interface alloying occurs. At submonolayer coverages a further component is seen which is attributable to intermediate ($n \times 2$) phases.

Keywords: surface core-level spectroscopy; Gd on W(110).

1. Introduction

One route to the preparation of clean rare-earth surfaces is growth on the (110) faces of refractory metals such as W, Nb and Mo. It has been found that on these substrates rare-earth metals grow as single crystals. It is known that W and Gd do not form bulk alloys and compounds, making W(110) an ideal substrate for growth of Gd. Rare-earth crystals grown on the refractory metals show hexagonal low-energy electron diffraction (LEED) patterns, consistent with the (0001) surface of an h.c.p. single crystal. However, the identification of the structure as h.c.p. cannot be determined by qualitative LEED alone since other structures have the same two-dimensional symmetry. Therefore, the designation (0001) can only be regarded as provisional. The interface is not epitaxial since there is a change of symmetry, and there is typically a 15% lattice mismatch between the substrate (110) and rare-earth (0001) lattices which will cause strain in the rare-earth layers. In the case of Gd/W(110), Weller, Alvarado, Gudat & Campagna (1985) suggest that this strain is only relieved with film thicknesses > 100 Å. At submonolayer coverages, Gd on W is known to go through a series of ($n \times 2$) structures in the following sequence: (10×2), (7×2), (6×2), (5×2), and then a $c(5 \times 3)$ before hexagonal structures are observed for coverages > 0.6 monolayers (Kolaczkiewicz & Bauer, 1986) Although there have been many previous core-level studies of rare earths on W(110) (Federov *et al.*, 1994, and references therein), these have all been of rare-earth 4f thick-film surface shifts.

2. Experimental

The measurements were performed on the Liverpool/Manchester photoemission beamline (4.1) (Dhanak, Robinson, van der Laan & Thornton, 1992). A Vacuum Science Workshop HA54 analyser was used. The combined analyser and photon bandwidths resulted in a total energy resolution of 120 meV at $h\nu = 70$ eV. The chamber, with a base pressure $< 10^{-10}$ mbar, was fitted with Omicron 4 grid LEED optics, also used as a retarding field analyser for Auger electron spectroscopy. The W(110) sample was cut and polished to within $1°$ from a commercially obtained boule with a purity rated at $> 99.99\%$. *In situ* preparation was carried out by roasting in 1×10^{-6} mbar of oxygen at 1473 K, followed by flashing to 2073 K. LEED showed a sharp (1×1) pattern on a low background. The surface cleanliness was monitored by Auger electron spectroscopy and core-level photoemission since the W 4f surface shift is known to be highly sensitive to contamination and, in particular, hydrogen adsorption (Riffe, Wertheim & Citrin, 1989). The sample was periodically flashed to maintain cleanliness.

The Gd was evaporated from a water-cooled tungsten basket evaporator (Dowben, LaGraffe & Onellion, 1989) which was extensively outgassed prior to deposition. The substrate was held at room temperature to ensure layer-by-layer growth (Kolaczkiewicz & Bauer, 1986). A photon energy of 70 eV was used to ensure high surface sensitivity. The spectra were taken during deposition and thus there is no absolute calibration of coverage. For a 1 h evaporation the estimated total film thickness is $\simeq 5$ monolayers. This estimate is made by considering the attenuation of the W 4f signal as a function of deposition (see Fig. 1), and using a Gd mean free path of ~ 2 monolayers for electrons with a kinetic energy of 34 eV (Gerken, Barth, Kammerer, Johansson & Flödström, 1982).
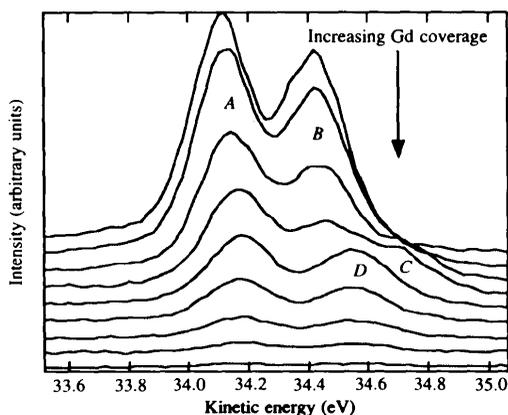
3. Results and discussion

Fig. 1 shows the W $4f_{7/2}$ core level as a function of evaporation time. The data show two peaks from the clean surface, *i.e.* bulk (*A*) and surface (*B*) components. As Gd is deposited, an intermediate feature (*C*) appears on the high kinetic energy side of the surface peak. After 40 min

Table 1

Peak positions determined from the fits of Fig. 2.

Peak	Assignment	Shift (meV)
Bulk	A	0
Clean surface	B	316
Intermediate	C	570
Interface	D	384

evaporation only two components are obvious: A and D. At higher coverages no further features can be observed, and so it seems reasonable to attribute peak D to the buried Gd/W interface.

To determine the quantitative behaviour of the various components we employed a least-squares curve-fitting procedure. The peaks were modelled using standard photoemission line shapes (Joyce, del Guidice & Weaver, 1989). Our assumptions were that the spectra could be fitted using only those components that could be visually identified, and that the binding energies and line shapes of components B, C and D did not vary as a function of coverage. The binding energy of peak A clearly changes by a small amount with increasing Gd coverage and so in all fits its energy was not fixed. This apparent small shift could be attributable to an extra component of the bulk peak A to a higher kinetic energy which could not be resolved in this experiment. Two peaks were used to fit the clean W(110) spectrum, giving the parameters for peaks A and B. The 15 min spectrum was fitted with three peaks, using the parameters for peaks A and B (allowing their intensities and the energy of peak A to vary), giving the parameters for peak C. The 40 min spectrum was fitted with two peaks, using the line-shape parameters for peak A (allowing its intensity and energy to vary), giving the parameters for peak D. The fitting results are summarized in Table 1 and the fits are shown in Fig. 2. Some confidence in our assumptions is given by the fit
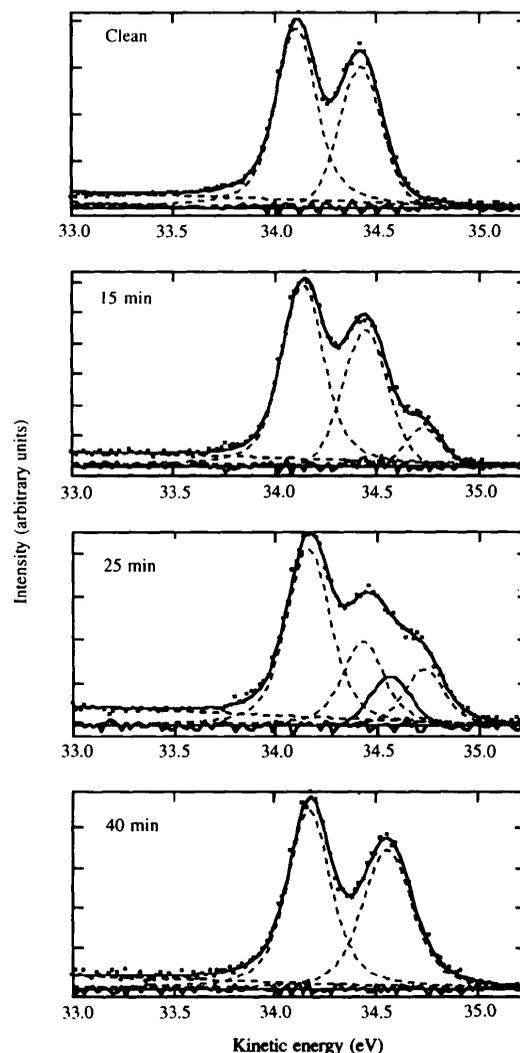
to the 25 min spectrum, also shown in Fig. 2. This shows that an excellent fit can be obtained using the parameters for B, C and D from the previous fits, allowing only their intensities to vary.

4. Conclusions

Since at saturation coverages only one interface component (D) is seen, it would appear that the interface is very abrupt, i.e. no interface alloying occurs. This is supported by the similarity of the surface and interface shifts, which shows that there is not a strong chemical interaction between the W and Gd. This result is not surprising as for W and Gd no alloying occurs. The appearance of an intermediate peak (C) is not unreasonable and can be associated with the sub-monolayer ($n \times 2$) structures. The individual components of peak (C), which correspond to the various $n \times 2$ structures were not clearly resolved in this study.

Figure 1

Flux-normalized photoemission spectra of the W $4f_{7/2}$ level with increasing Gd coverage: $h\nu = 70$ eV, incidence angle = $5°$, emission angle = $35°$ (relative to the surface normal).

Figure 2

Curve fitting results for selected spectra from Fig. 1, showing components and residuals.

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