LETTER TO THE EDITOR

Observation of a (7 × 1) surface reconstruction on Y(11$\bar{2}$0)

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Abstract. A study of the surface reconstruction of Y(11$\bar{2}$0) has shown a sixfold-symmetric low-energy electron diffraction pattern in contrast to the twelvefold-symmetric pattern reported earlier. This indicates that only one orientation of close-packed atoms exists on the surface; the collapse of the surface unit cell is uniaxial along the [0001] direction. This produces the same commensurate surface structure as found previously for the (11$\bar{2}$0) (7 × 1) reconstructions of Ho and Er. Why the earlier study of Y showed a two-domain reconstruction has not been determined, but we suggest that this structure was influenced by the presence of surface defects, inducing the collapse of the unit cell along the [10$\bar{1}$0] direction to form an incommensurate domain with approximately equal probability to that of the commensurate (7 × 1) domain.

In an earlier letter [1] we reported the observation of a reconstruction of the (11$\bar{2}$0) surface of Y. The reconstruction involved the collapse of the relatively open ideal surface unit cell into a close-packed structure very similar to that of a (0001) surface. The low-energy electron diffraction (LEED) pattern displayed twelvefold symmetry and was interpreted as the superposition of two congruent sixfold-symmetric patterns rotated by $\pi/2$ with respect to each other. The surface comprised domains of close-packed atoms, with one domain structure being commensurate with that of the bulk and the other incommensurate. The uniform intensity of each of the 12 principal spots indicated that the total areas covered by each domain were approximately equal. No spots that could be attributed to the (ideal) substrate structure were visible, indicating that the reconstruction extended for many atomic layers. As this was the first surface reconstruction to be observed on a metal with a hexagonal close-packed (HCP) structure it was not known whether such a domain structure was typical for this surface, but it was suggested [1] that the reconstruction observed for Y might be common to other HCP elements in the rare earth series. A recent study of the (11$\bar{2}$0) surfaces of Ho and Er [2] has shown that these also collapse to a close-packed structure, but display sixfold-symmetric LEED patterns with no sign of any spots produced by an alternative orientation of close-packed atoms. Due to the commensurate relationship between the close-packed surface unit

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Figure 1. LEED pattern from Y($11\bar{2}0$) (7 × 1); beam energy: 50 eV.

cell and the underlying bulk cell, the reconstructions of Ho and Er have been assigned the Wood notation ($11\bar{2}0$) (7 × 1) [2]. No such notation could be applied to the reconstruction of Y($11\bar{2}0$) as the unit cell of one of the domain structures was incommensurate with that of the bulk.

In the light of the differences between the surface reconstruction of Y and those of the other rare earth elements studied, we have repeated our study of Y($11\bar{2}0$). In order to determine whether the two-domain structure is a characteristic of the Y($11\bar{2}0$) reconstruction or is dependent on the sample preparation, a new sample was cut from the same high-quality single-crystal boule as the original sample. The experimental equipment and *in situ* cleaning procedure used were as described in the previous studies of Y [1, 3]. Any difference in behaviour between the two Y samples can be ascribed to the different extent of ubiquitous surface defects—slight misalignment of either surface with respect to the crystallographic axes (producing terraces of steps), surface roughness, or levels of surface contamination.

We find that the LEED pattern from Y($11\bar{2}0$) is sixfold symmetric (figure 1), in contrast to the twelvefold-symmetric pattern observed previously. The orientation of the LEED pattern indicates that the ($11\bar{2}0$) surface unit cell has collapsed uniaxially along the [0001] direction to form a close-packed structure which has a unit cell commensurate with that of the bulk. The numerical relationship between the vectors of the surface unit cell and those of the bulk unit cell leads to the reconstruction notation (7 × 1).

In the previous studies [1, 2] the state of the surface structure was monitored using the intensity of a surface-order-dependent state (SODS) observed in the UV photoemission spectrum at a binding energy of ≈9.5 eV. This has been found to be very sensitive to the degree of surface sixfold symmetry [1, 3] and thus reduces in intensity of the reconstructed surface reverts to its ideal (twofold-symetric) structure or if the surface crystallography becomes disordered. Plotting the intensity of this feature as a function of temperature clearly shows a transition from a surface structure of sixfold symmetry to one of a lower symmetry. Figure 2 shows such a curve for the present study of Y($11\bar{2}0$); some of the corresponding data for the previous studies of Y [1] and Er [2] are shown
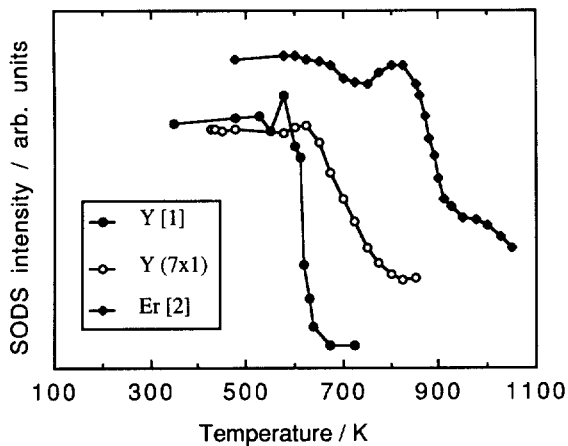
Figure 2. SODS intensity as a function of temperature for erbium and yttrium.

for comparison. The transition occurs in the region of $\simeq$600–800 K, with the mid-point at 700 $\pm$ 25 K (compare with 610 $\pm$ 10 K in the previous study). The higher transition temperature implies a higher stability for the (7 $\times$ 1) reconstruction compared with the two-domain structure. When the latter was destroyed by heating there was no sign of the (7 $\times$ 1) phase remaining at 700 K. This implies that the destruction of the incommensurate phase at $\simeq$610 K induced the premature destruction of the (7 $\times$ 1) phase at a temperature $\simeq$ 100 K below its nominal transition temperature. Due to the large change of surface atom density accompanying the rearrangement from the reconstructed to the ideal surface structures, it is perhaps not surprising that the two domains could not revert to the ideal structure independently.

The shape of the curve of SODS intensity versus temperature for Y is qualitatively closer to that displayed by Er(11$\bar{2}$0) [2] than in the previous study of Y [1]. This may indicate that at high temperatures the surface does not have the ideal bulk termination structure (in contrast to the earlier results [1]). A relatively high photoemission intensity at the Fermi energy at high temperatures also indicates that the surface is not fully ordered; the density of states for Y is heavily weighted at the Fermi energy [4] and so the photoemission from a disordered surface would be expected to display a similar distribution. Another observation that strengths the similarity between the Y(11$\bar{2}$0) (7 $\times$ 1) reconstruction and those of Ho and Er [2] is the dependence of the surface structure on the rate at which the temperature is varied. In the previous study of Y(11$\bar{2}$0) [1] it was observed that if the sample was cooled from an anneal temperature of 875 K to room temperature over a time period of $\simeq$30 min then the ideal surface structure was quenched in and the reconstruction was inhibited. In order to promote the reconstruction it was necessary to cool the samples slowly over a period of many hours. This is in contrast to the reconstructions of Ho and Er [2] which occurred spontaneously; in the case of Ho the reconstructed surface could not be destroyed by temperatures up to 1000 K. In this study of Y(11$\bar{2}$0) the ideal surface could not be obtained at room temperature, although the degree of crystalline order on the reconstructed surface (as determined by the intensity of the SODS) was found to improve if the samples were cooled at a controlled rate over many hours.

In conclusion, we have shown that the surface reconstruction of Y(11$\bar{2}$0) conforms to the behaviour found for the (11$\bar{2}$0) surfaces of other rare earth metals. We suggest that the earlier study of the Y reconstruction was influenced by the presence of surface

defects, the most likely of which were terraces of steps formed due to the surface not being exactly perpendicular to the [11$\bar{2}$0] direction; Laue x-ray diffraction indicated that the surfaces of both Y samples were within 1° of (11$\bar{2}$0). If the terraces are oriented in a particular direction, they may act as nucleation regions for the incommensurate reconstruction; as the reconstruction to a close-packed structure requires a $\simeq 60\%$ increase in atom density at the surface, it seems likely that steps must influence the formation of the reconstructed domains. Conversely, it is possible to interpret the results of these studies of (11$\bar{2}$0) surface reconstructions as indicating that surface defects (on the Y sample of this study, Ho and Er [2]) *inhibit* the formation of an incommensurate domain. This is thought to be less likely as this interpretation would require that all of these samples have defects with the required surface structure. An alternative explanation to steps assumes that the level of contamination influences the formation of domains. As the surfaces of bulk single-crystal samples of rare earth metals always have a residual contamination level of a few atomic per cent (usually C and O), this is a possibility that cannot be ruled out.

References

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