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Band effects in the 5p levels of Ho(0001)

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Abstract. Recent bandstructure calculations have indicated that the 5p core levels of the lanthanide metals may influence the bonding significantly. We have investigated this possibility with angle-resolved UV photoemission from the 5p levels of Ho(0001), using synchrotron radiation. Spectra taken at normal and off-normal emission show a changeover in the relative intensities of the $5p_{1/2}$ and $5p_{3/2}$ peaks, and the spectra taken at equal emission angles either side of the surface normal (for a constant photon incidence angle) are found to differ significantly. As these phenomena would not occur if the 5p levels were 'true' core levels, i.e. showing negligible dispersion, we conclude that they must have a significant bandwidth.

The electronic structure of the lanthanide metals has been an area of some controversy for many years [1]. This has centred on the treatment of the highly localized 4f levels within the local density approximation but recent bandstructure calculations for Gd [2] have indicated that some attention must also be paid to the treatment of the 5p core levels. Temmerman and Sterne [2] found that a 7% difference in the theoretical c/a ratio was obtained between treating the Gd 5p levels as 'true' core levels and treating them as relaxed band states. Such a large difference implies that band effects should be detectable in angle-resolved UV photoemission (ARUPS) spectra from the 5p levels. In Gd the 5p ARUPS spectra show multiplet splitting [3] due to magnetic interactions, making this element unsuitable for evaluation of 5p band effects. Therefore we have investigated band effects in the 5p levels of Ho, which is unaffected by such magnetic effects, by means of ARUPS from the (0001) surface.

The Ho(0001) sample was cut from the same high-quality single-crystal boule as the (11 $\bar{2}$ 0) sample used in our study of the surface reconstruction [4]. The boule, grown by Dr D Fort (School of Metallurgy and Materials, University of Birmingham, UK), had an impurity concentration of approximately 0.1 at%, with C and O the dominant impurities. The sample was spark-machined from the boule and polished *ex-situ* using standard metallographic techniques.

The photoemission experiments were performed using the toroidal grating monochromator on beamline 6.2 of the Synchrotron Radiation Source, SERC Daresbury Laboratory, UK. The spectrometer used was a Vacuum Generators ADES 400 system with three-grid low-energy electron diffraction (LEED) optics used as a retarding field analyser for Auger electron spectroscopy (AES). The overall energy resolution for ARUPS was 0.25 eV. The base pressure of the system was approximately

2×10^{-10} mbar.

In-situ sample cleaning was performed by repeated cycles of Ar^+ bombardment (beam energy 3–4 kV, current density $\sim 20 \mu\text{A cm}^{-2}$) and annealing at 875 K. Surface cleanliness and order were monitored principally by ARUPS—contamination shows an additional weight in the spectra at approximately 6 eV binding energy and the intensity of the surface-order-dependent state (SODS) at 9.6 eV binding energy is known to be extremely sensitive to the quality of the surface [4, 5]. Spectra from $\text{Ho}(0001)$ in the binding energy range 0–12 eV, including the SODS, are shown and discussed elsewhere [4–6]. After approximately 20 cleaning cycles a high SODS intensity and low contamination level were reproducibly obtainable, the cleanliness and crystallinity being confirmed by AES (C and O levels of a few at%) and LEED (sharp 1×1 spots on a relatively low background).

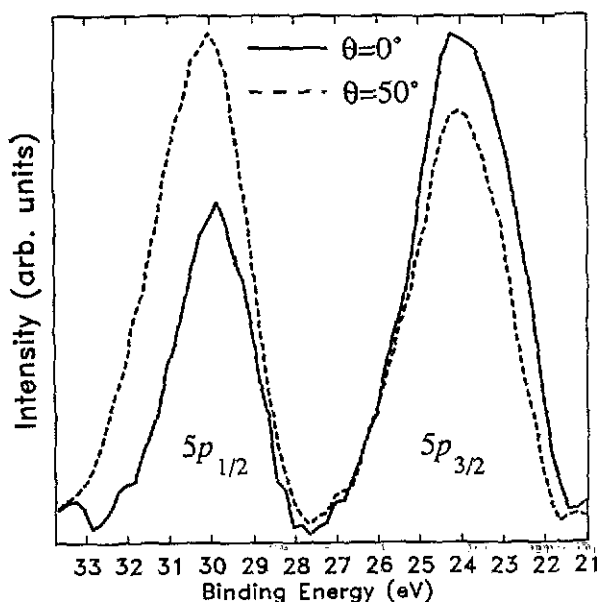


Figure 1. Angle-resolved spectra of the 5p levels of $\text{Ho}(0001)$. The inelastic background has been subtracted using a polynomial fit: photon energy 60 eV, p-polarized radiation, incidence angle 30° .

Figure 1 shows ARUPS spectra taken at normal ($\theta = 0^\circ$) and off-normal ($\theta = 50^\circ$) emission. At normal emission the intensity ratio of the $5p_{1/2}$ and $5p_{3/2}$ peaks is, to a good approximation, that expected from the relative occupancies of these levels, i.e. 1:2. At off-normal emission this no longer holds—the $5p_{1/2}$ peak is more intense than the $5p_{3/2}$ peak. Although at $\theta = 50^\circ$ the surface sensitivity is greatly enhanced this intensity changeover cannot be attributed to either a surface core level shift (~ 0.6 eV for Ho [7, 8]) or a chemical shift due to residual surface contamination since these would affect both peaks equally. However, if the 5p levels possess significant bandwidth it is entirely feasible that the intensities of the spin-orbit split components might vary with emission angle. Further evidence is provided by an additional experiment employing two different experimental geometries (figure 2). The photon incidence angle is kept constant while the emission angle is set to the same value either side of the surface normal. The difference between these geometries is the polarization of the light relative

to the momentum of the emitted electron. If the 5p levels were 'true' core levels, i.e. with no momentum dependence, then spectra recorded in these two geometries should be identical, since in both cases the surface sensitivity is the same. Figure 3, which shows the results of this experiment, demonstrates that the two different geometries produce different spectra.

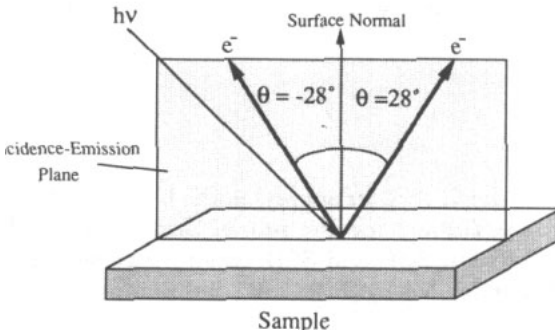


Figure 2. The two geometries used to test for momentum dependence. The emission angles were chosen arbitrarily, with the incidence angle (55°) dictated by the spectrometer layout.

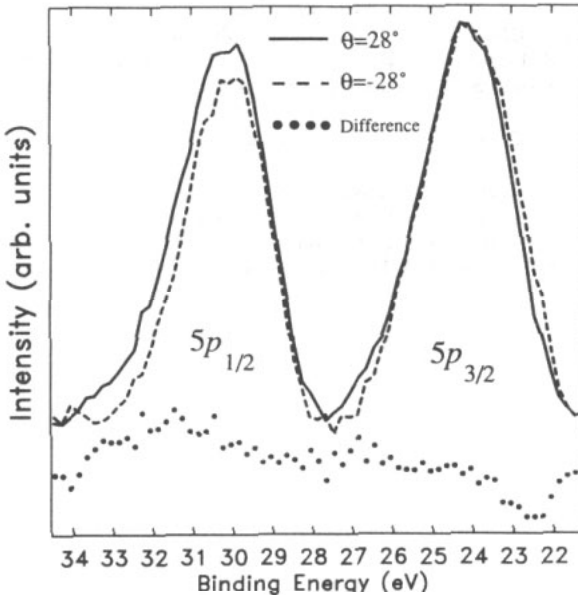


Figure 3. Angle-resolved spectra of the 5p levels of Ho(0001). Geometry as in figure 2, photon energy 60 eV, p-polarized radiation. The inelastic background has been subtracted using a polynomial fit.

There are several conclusions to be drawn from these results. As this phenomenon seems unlikely to be limited to the heavy rare earths it follows that caution should be applied when attempting to use the combination of shallow p levels and ARUPS to measure surface core level shifts (SCLS). To date the only such measurements, of the

Y(0001) 4p levels [9, 10], have employed *ab initio* photocurrent calculations, which implicitly include band effects, rather than curve fitting. It also appears that the results of Temmerman and Sterne [2] have been vindicated. The 5p levels of Ho and, by analogy, those of other heavy lanthanides (including Gd) probably do possess a significant bandwidth, and should therefore be treated on an equal footing with the valence electrons in bandstructure calculations. This puts the heavy rare earths in the unusual position of having core-like valence electrons (4f) and band-like core levels (the 5p)!

Acknowledgments

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