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The surface core-level shift in Y(0001)

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Abstract. We have calculated the 4p core-level shift at the (0001) surface of yttrium using the SCF–LMTO–ASA method in a supercell geometry. We find a value of 0.6 eV to increased binding energy, in good agreement with the experimental value.

Angle-resolved photoemission measurements on Y(0001) indicate that the binding energy of the (spin–orbit split) 4p core level for atoms at the surface is greater than that for atoms in the bulk [1]. From comparisons with photocurrent calculations made using the NEWPOOL code [2] we estimate that the shift is in the range 0.7–0.9 eV.

We have calculated the electronic structure at the Y(0001) surface using the SCF–LMTO–ASA method. We model the surface by defining a supercell comprising five layers of Y atoms and a similar number of empty layers. We show in figure 1 the calculated local densities of states (LDOS) for the 4p levels at the 'surface' (S) and in the 'bulk' (B), i.e. the layer in contact with the vacuum and the middle Y layer, respectively. (For the latter, the DOS in the valence band region is very similar to that obtained in previous

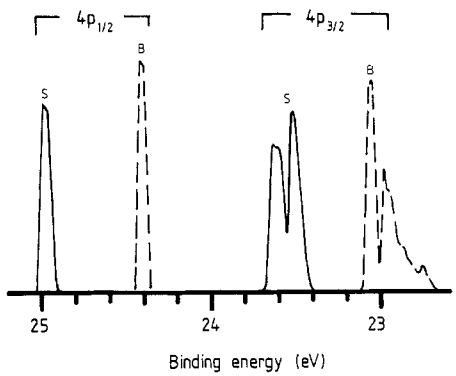

Figure 1. The calculated LDOS for the 4p levels.

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calculations for the infinite crystal [1], indicating that it closely resembles the bulk.) The calculations show a shift of 0.6 eV to increased binding energy, in good agreement with the photoemission measurements.

References

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[2] Larsson G C 1986 *Surf. Sci.* **152/153** 213