Photoelectron spectroscopy

Rare earth materials

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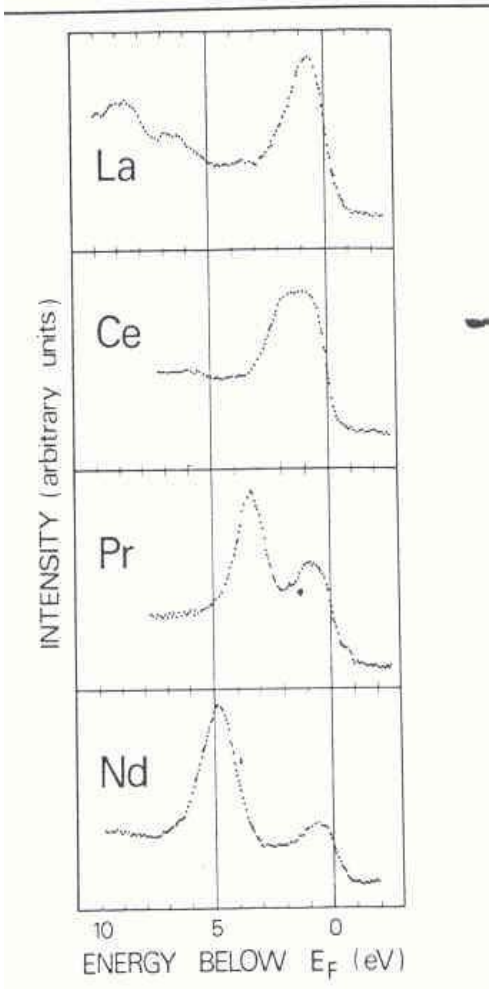
Contents

Introduction
rare earth elements

Element	Atomic Number	Electronic Ground State
La	57	$5d^1\ 6s^2$
Ce	58	$4f^1\ 5d^1\ 6s^2$
Pr	59	$4f^3\ 6s^2$
Nd	60	$4f^4\ 6s^2$
Pm	61	$4f^5\ 6s^2$
Sm	62	$4f^6\ 6s^2$
Eu	63	$4f^7\ 6s^2$
Gd	64	$4f^7\ 5d^1\ 6s^2$
Tb	65	$4f^9\ 6s^2$
Dy	66	$4f^{10}\ 6s^2$
Ho	67	$4f^{11}\ 6s^2$
Er	68	$4f^{12}\ 6s^2$
Tm	69	$4f^{13}\ 6s^2$
Yb	70	$4f^{14}\ 6s^2$
(Lu)	71	$4f^{14}\ 5d^1\ 6s^2$

Electronic structure of rare earth elements



La ,Ce, Pr,and Nd metals with a low number of f electrons have been selected because of their particularly simple spectra.

All other earths ,except for Eu and Gd, shows multiple final states which require a rather eleborate interpretation.

The structure arising at binding energies higher than 5eV in the La spectrum correspond to 5p electron excited by the X-ray satellite $K\alpha_{3,4}$The first peak just below the Fermi level in the spectra of La ,Pr and Nd is attributed to the d states of the valence bond

The spectrum of Ce does not show clearly the separation between d and f states.the flat shape of the broad peak indicates however that two unresolved structures are present.

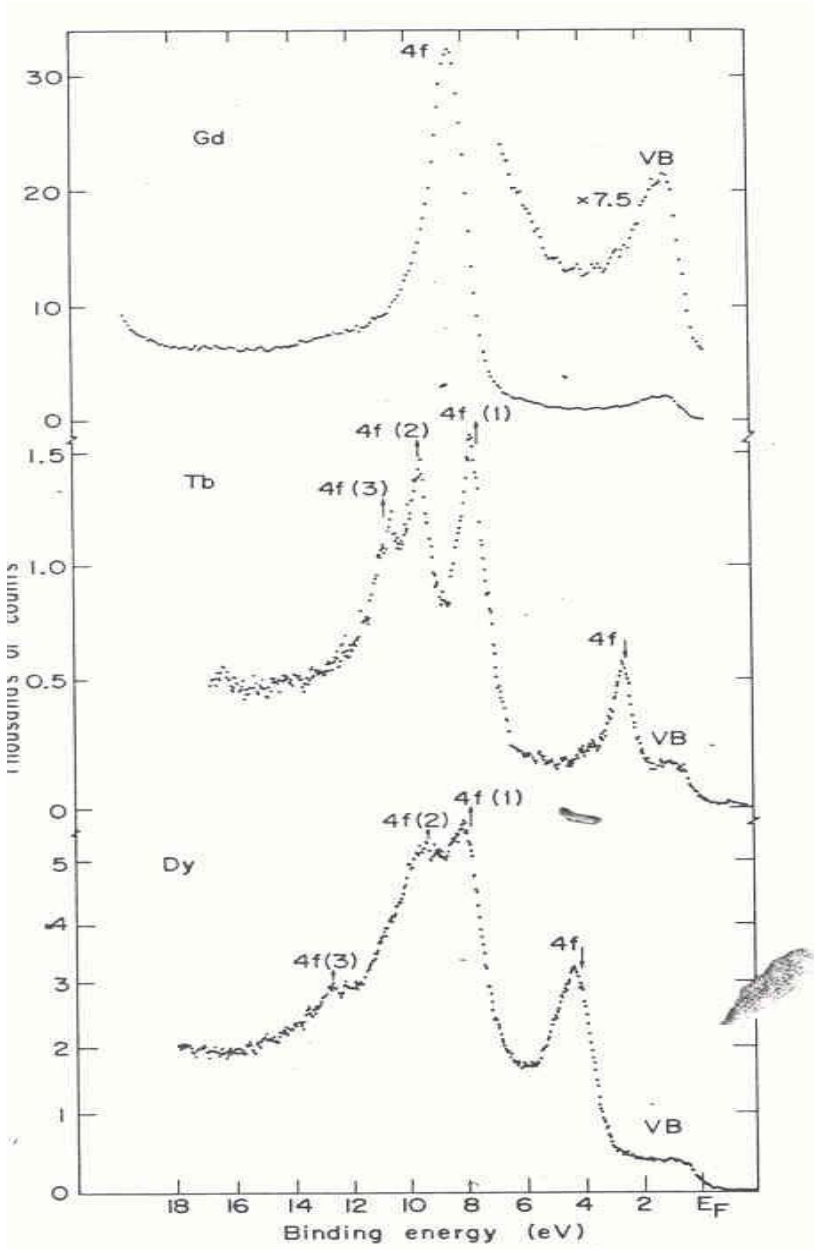
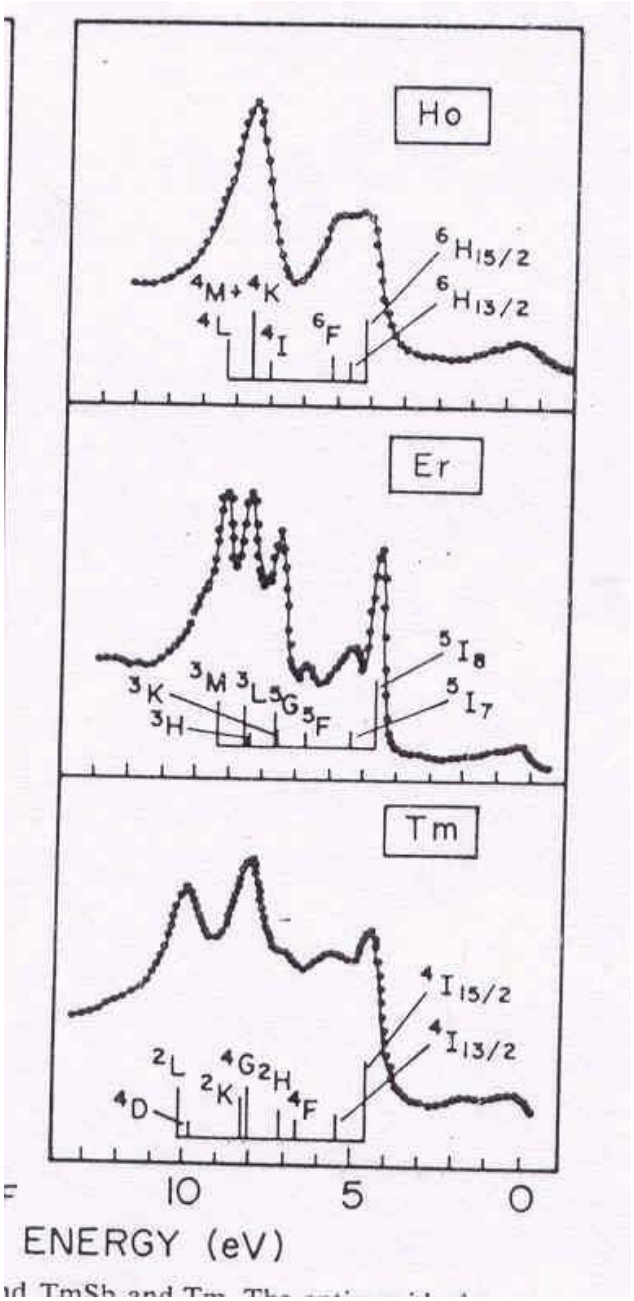


Fig. 1. X-ray photoemission spectra of the 4f and valence band region of Gd, Tb and Dy.

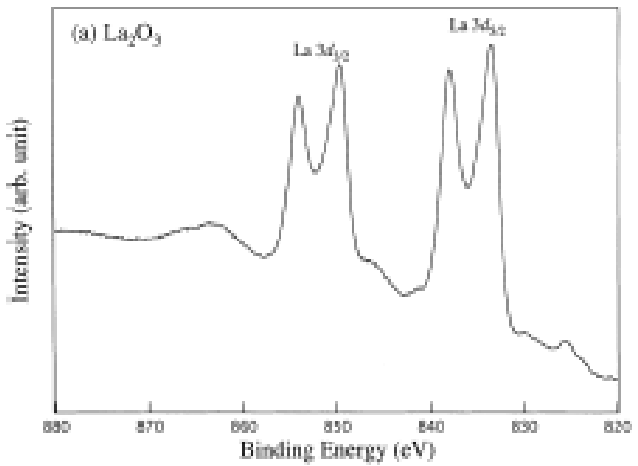


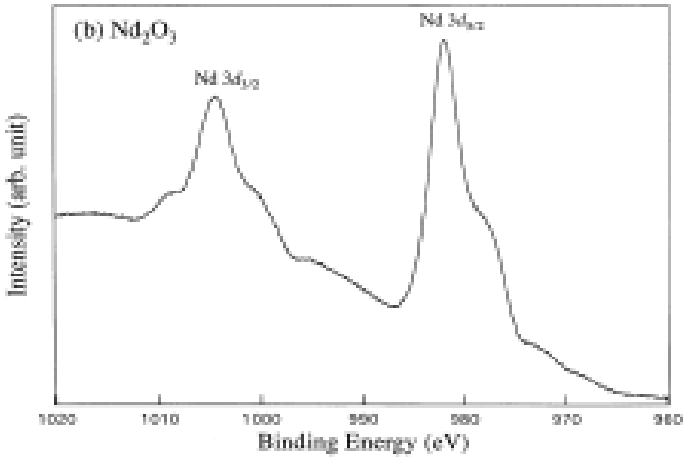
X -ray photoemission spectra of the 4f and valence band region of Ho, Er and Tm

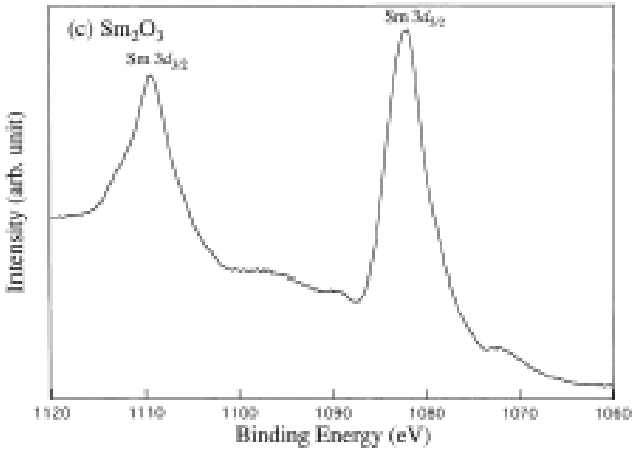
Electronic structure of rare earth materials [rare earth oxides]

- Clear double-peak structures were observed for La_2O_3, Ce_2O_3
- Broad foot of the low-binding-energy side for 3d XPS were observed for Pr_2O_3, Nd_2O_3 and Sm_2O_3
- Sinlge-peak structures were observed for Eu_2O_3, Gd_2O_3 and Dy_2O_3

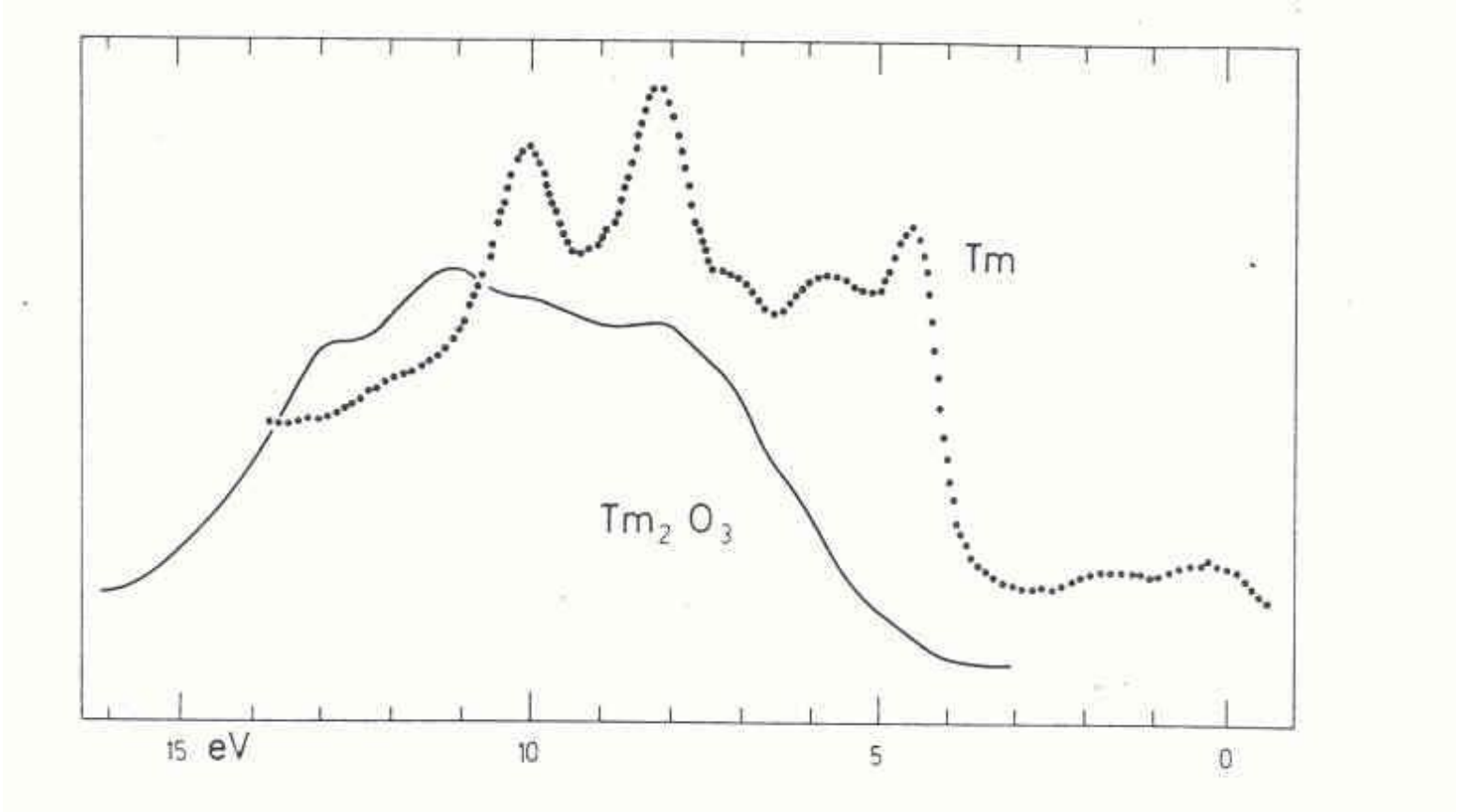
X-ray photoemission spectra of rare earth oxides







The photoemission spectrum in the 4f region of metallic thulium and thulium oxide



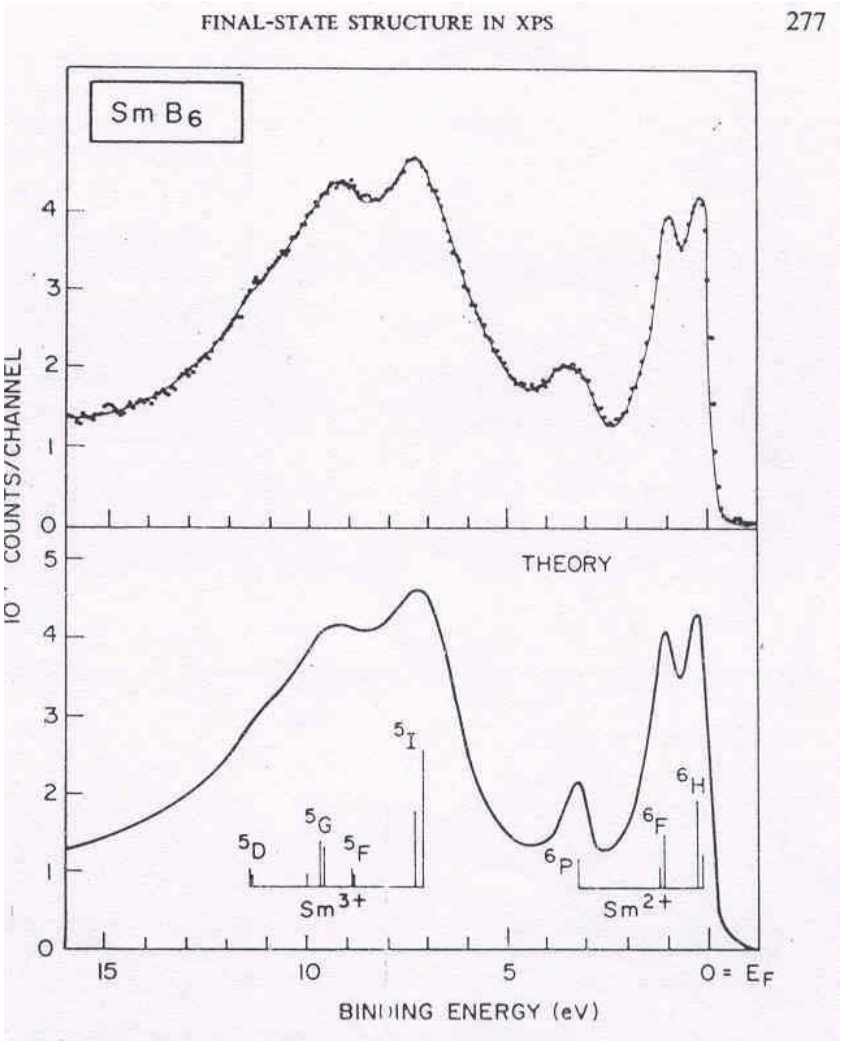
Binding energy [eV]

X-ray photoemission spectra SmB_6

It crystallizes in the CsCl structure,with metal ions on the one site and regular octahedra on the other.

The material in metallic above 50k ,and semiconducting below ,but the conductivity in the low temperature phase does not follow an activation energy.

It is proto type ICF material



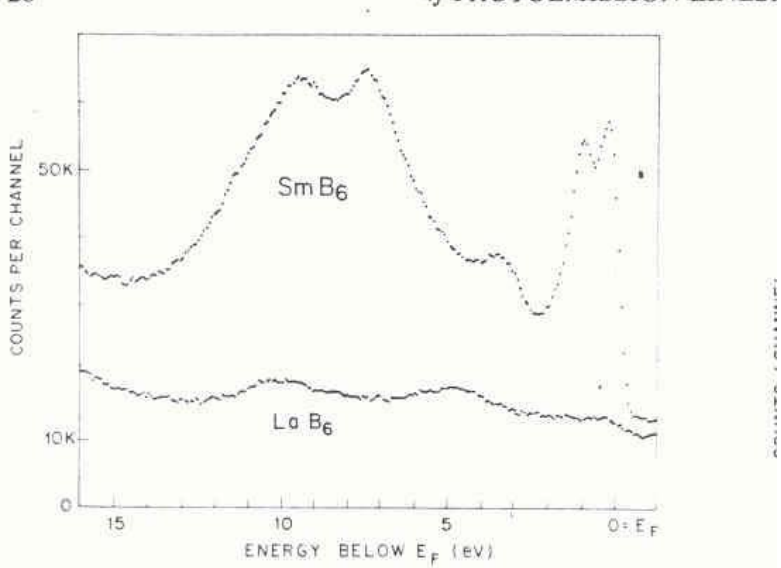


Fig. 1. High resolution X-ray photoemission spectra of the valence band and 4*f* region of SmB_6 and of metallic LaB_6.

The Sm contribution to the Valence band SmB_6

Conclusion

- X - ray photoemission spectra of 4f electrons and complexities in the multiplet of rare earth elements are discussed.
- We measured the rare earth 3d XPS for rare earth oxides
- The shapes of the rare earth $3d_{5/2}$ show dramatic changes for La to Sm and that no satellite is observed for Eu to Dy.
- X-ray photoemission spectra of SmB_6 is compared with data for LaB_6 allows a detailed analysis of the Sm 4f spectrum.

- References

Y. Baer et al,Phys.Rev.Lett. **31**, 1973, 35-37.

F.R.Mcfelly et al, Phys.Lett. **45A,** 1973, 227-228.

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