9.7 cm

Electronic structure of Ce_2TSi_3 (T=Rh,Pd) compounds

A. Szytuła[a], A. Jezierski[b] and B. Penc[a]

[a]Instutute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków

[b]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań

Electronic structure of the ternary Ce_2TSi_3 (T=Rh, Pd) compounds wich crystalize in the hexagonal AlB_2 structure was studied by X-ray photoelectron spectroscopy (XPS). Core-levels and valence bands were investigated. The XPS valence bands are compared with the ones calculated using TB LMTO method. The photoemission measurements were performed using a commercial LHS 10 SPECS spectrometer with the following radiation sources: non-monochromatized MgK_α (hν=1253.6 eV), monochromatized and non-monochromatized AlK_α (hν=1486.6 eV). The measurements were made at room temperature in high vacuum ($2 \cdot 10^{-9}$ mbar). The VB XPS spectra of Ce_2RhSi_3 and Ce_2PdSi_3 are established mainly by 4d states of Rh and Pd- atoms. The XPS spectra of 3d Ce consists of three peaks that correspond to the f^0, f^1 and f^2 configurations. The gap between energies of the f^1 states corresponding to the energy levels of $3d_{5/2}$ and $3d_{3/2}$ states give a spin-orbit splitting Δ_{SO}, which is equal to 18.7 eV for Ce_2PdSi_3 and 18.5 eV for Ce_2RhSi_3. Based on the Gunnarsson-Schönhammer theoretical model, the intensity ratio $f^0/(f^0+f^1+f^2)$ gives the f-occupation probability in the final state. The obtained results suggest that about 0.25 ions have the f^0 configuration. The shift of the shake down satellites in relation to the main peak is about 3.3 eV in Ce_2PdSi_3 and 3.6 eV in Ce_2RhSi_3. The intensity ratios $r = f^2/(f^1+f^2)$ for Ce_2PdSi_3 and Ce_2RhSi_3 are near 0.5. Such r values correspond to a very large value of Δ(about 300 meV). Similar, large Δ's (about 220 eV) are observed in Ce stannides and antimonides of the 1:2:2 type.

13.4 cm

Subject category :

4. Rare Earths and Actinides, Alloys and Compounds

Presentation mode :
poster

Corresponding author :
A. Szytuła

Address for correspondence :
Instutute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków

Email address :
szytula@if.uj.edu.pl