XPS study of $RNiSb_2$ (R = Pr, Nd) compounds

A. Szytuła[1], B. Penc[1], and A. Jezierski[2]

[1]*M. Smoluchowski Institute of Physics, Jagiellonian University*
Reymonta 4, 30-059 Kraków, Poland
[2]*Institute of Molecular Physics, Polish Academy of Sciences*
M. Smoluchowskiego 17, 60-179 Poznań, Poland

The electronic structure of the ternary $RNiSb_2$ (R = Pr, Nd) compounds which crystallize in the tetragonal primitive $ZrCuSi_2$-type structure was studied by X-ray photoemission spectroscopy. R *3d* core-levels and valence bands were investigated. The X-ray photoemission spectroscopy results of $PrNiSb_2$ valence band are compared with the previously calculated density of states. The obtained results indicate that the valence bands are mainly determined by the Ni *3d* band. The analysis of the XPS spectra of R $3d_{5/2}$ and R $3d_{3/2}$ on the basis of the Gunnarsson - Schönhammer model gives a hybridization of *4f* orbitals with the conduction band.

The experimental data concerning the valence band of these compounds are compared with the calculated data based on the KKR – CPA method. The calculated data for the room temperature (paramagnetic region) give the peaks corresponding to the R *4f* states at the Fermi level $E_F = 0$. A different distribution of the peaks corresponding to the Ni *3d* states is observed. For $PrNiSb_2$ three peaks at 2.0, 2.3 and 3.5 eV is observed while for $NdNiSb_2$ a broad maximum between 5.0 and 8.0 is visible. The experimental data for $PrNiSb_2$ are in good agreement with the calculated ones while those for $NdNiSb_2$ do not agree.

Name of the presenting author (poster session II): Andrzej Szytuła
e-mail address:szytula@if.uj.edu.pl
http://www.if.uj.edu.pl