Electronic structure of $Sm(Ni_{1-x}Co_x)_3$ alloys – XPS and *ab initio* study

A. Majtyka,[1] M. Sikora,[2] D. Blachliński,[2] G. Chełkowska,[2] and J. Deniszczyk[1]

[1] *Institute of Materials Science, University of Silesia in Katowice, 75 Pułku Piechoty 1A, 41-500 Chorzów, Poland*

[2] *A. Chełkowski Institute of Physics, University of Silesia in Katowice, Uniwersytecka 4, 40-007 Katowice, Poland*

The complex band structure investigations for $Sm(Ni_{1-x}Co_x)_3$ alloys were performed using the X-ray photoelectron spectroscopy (XPS) and an *ab initio* calculations. The aim of the study was to determine how the electronic structure changes with concentration in these compounds. Experimental XPS spectra indicated that the Ni/Co substitution results in a reconstruction of the valence band (VB), especially the intensity near the Fermi level decreases with Co content. The *ab initio* based simulated XPS valence band spectra agree qualitatively with experimental ones apart from the structure of Sm-4f sub-spectra where the multiplet decomposition is observed. Analysis of the calculated electronic structure of $Sm(Ni_{1-x}Co_x)_3$ alloys confirmed the VB reconstruction and showed that the valence of Sm ions and the location of Sm-4f band with respect to Fermi level depend on the local atomic environment of Sm ions.