Electronic structure studies of DyNi₄Cu

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Electronic structure of the DyNi₄Cu compound, crystallizing in the hexagonal CaCu₅-type of structure has been studied using the XPS method with monochromatized Al K_{α} radiation as well as the self-consistent spin-polarized TB-LMTO (tigh-binding linear muffin-tin orbital) method. The self-consistent band calculations were performed for the experimental lattice parameters (a=4.918 Å, c=3.991 Å), which were determined by X-ray diffraction. Our calculations show that DyNi₄Cu is ferromagnetically ordered at 0 K. The analysis of the valence band shape in vicinity of the Fermi level shows that this part of the spectrum comes mainly from 3d electrons of Ni and Cu atoms (peaks at -1 eV and -4 eV). The features of the experimental XPS valence band spectra near the Fermi level are reproduced in our calculations. Peaks below -7.5 eV are connected with the contribution of the f-electrons of Dy. The obtained peaks positions in the valence band are in good agreement with the binding energies of metallic dysprosium, copper and nickel.

Core levels of Dy, Cu nd Ni are also investigated.

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 $9.7~\mathrm{cm}$