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X-RAY PHOTOEMISSION SPECTRA OF $Dy(Co_{1-x}Al_x)_2$ SYSTEMS

A. SZAJEK, A. JEZIERSKI, A. KOWALCZYK, J. BASZYŃSKI

Institute of Molecular Physics, Polish Academy of Sciences
Smoluchowskiego 17, 60-179 Poznań, Poland

ST. BARTKOWSKI, M. NEUMANN AND G. BORSTEL

Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

The electronic structure of $Dy(Co_{1-x}Al_x)_2$ compounds (Laves phase — $MgCu_2$, C15) for Al concentrations $x = 0.0$, 0.1, 0.2 was investigated by X-ray photoelectron spectroscopy. The results were compared with the *ab initio* band structure calculations.

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1. Introduction

The study of magnetic behaviour of cobalt in rare-earth (R) or yttrium compounds is an interesting matter. As a function of the rare-earth parameter, composition and local environment, the saturation cobalt moments vary from nil to a value close to that characteristic of a pure metal [1]. One of the most interesting phenomena in $R(Co_{1-x}Al_x)_2$ alloys is the increase in the Curie temperature with concentration of nonmagnetic Al atoms. In the most spectacular case for $Tm(Co_{0.9}Al_{0.1})_2$ T_c is about 15 times higher than for $TmCo_2$ [2]. The aim of the present paper is to evaluate the band structure results $Dy(Co_{1-x}Al_x)_2$ by comparing them with experimental data, mainly from photoemission spectra.

2. Experiment and electronic structure calculations

The $Dy(Co_{1-x}Al_x)_2$ ($x = 0.0$, 0.1 and 0.2) compounds were prepared by induction melting of the constituents in a water-cooled boat under an argon atmosphere. The ingots were inverted and melted several times to insure homogeneity. Then the samples were wrapped in Ta-foil, sealed in a quartz tube filled with argon and annealed for two weeks at 900°C, and then rapidly cooled to room temperature.

The X-ray photoelectron spectroscopy (XPS) data were obtained with monochromatized Al K_α radiation of 1486.6 eV. The energy spectrum of the electrons was analyzed by hemispherical mirror analyzer with an energy resolution of 0.4 eV.

All emission spectra were measured immediately after breaking a sample in vacuum of 10^{-9} Tr.

The band structure was calculated by the tight binding linear muffin tin orbital method in the atomic sphere approximation (TB LMTO–ASA) [3] with the spin–orbit interactions taken into account. The calculations for the disordered alloys with Al concentrations $0 < x < 1$ can be simulated by hypothetical ordered ternary compounds with the same stoichiometry. In our case the calculations were performed for the ordered compounds Dy_2Co_4 and Dy_2Co_3Al with the experimental lattice constants ($a = 7.196$ Å and 7.329 Å) [4].

The calculated XPS spectra were obtained from the partial densities of electronic states (DOS) weighted with atomic photoemission cross-sections [5]. The finite experimental resolution is taken into account in calculations by convoluting the weighted DOS(E) with an energy dependent Lorentzian function parametrized by the HWHM = 0.2 eV.

3. Results and discussion

In Fig. 1 the DOS(E) for Dy_2Co_4 and Dy_2Co_3Al are presented. The main contribution to the peak near the Fermi level, located at $E = 0$ eV, is from Co atom and f electrons of the Dy one, and to the peak about −5 eV from f electrons of Dy atoms only. The DOS at the Fermi level is equal to 27.8 and 30.1 states/(eV·unit cell) for Dy_2Co_4 and Dy_2Co_3Al, respectively. The role of Al

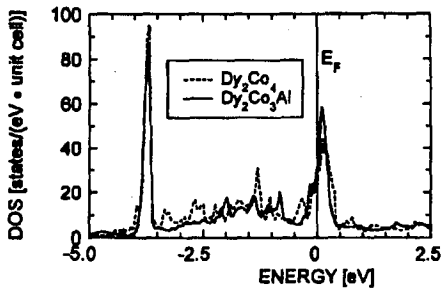

Fig. 1. The density of states for Dy_2Co_4 and Dy_2Co_3Al, the vertical line describes the Fermi level.

atoms is especially important because they introduce internal negative pressure which expand the systems. In the case of the so-called exchange enhanced paramagnets like YCo_2 or $LuCo_2$ the phase transition to the ferromagnetic order is observed [6]. In the case of magnetically ordered compounds the increase in the Curie temperature T_c is observed. For $Dy(Co_{1-x}Al_x)_2$ the increase is from 145 K to 208 and 166 K for $x = 0.1$ and 0.2, respectively. Within the RKKY model T_c is proportional to DOS(E_F) [7, 8]. The relative increase in DOS(E_F) in our calculations is in good agreement with experimental data for T_c, especially that the Dy_2Co_3Al corresponds to $x = 0.25$ which lies in the decreasing slope of the curve T_c vs. x [2].

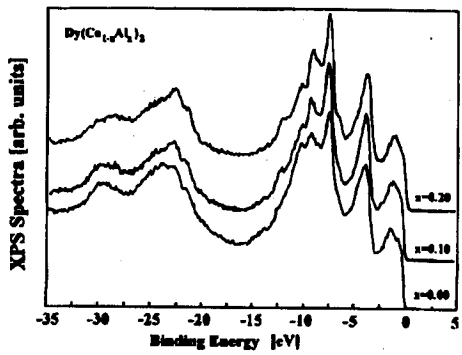

Fig. 2. The experimental XPS spectra for Dy_2Co_4 and Dy_2Co_3Al.

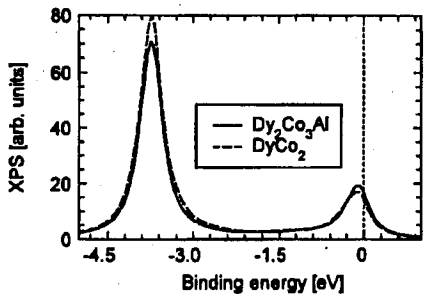

Fig. 3. The calculated XPS spectra for Dy_2Co_4 and Dy_2Co_3Al.

In Fig. 2 the experimental XPS spectra are presented. Small shifts towards the Fermi energy are observed with concentration x of Al atoms. The calculated XPS spectra (Fig. 3) cannot detect deep states (below 5 eV from the Fermi level) like it is shown in Fig. 2 but the shape of curves and positions of peaks are in good agreement.

Acknowledgments

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References

[1] E. Burzo, H.R. Kirchmayr, A.C. Chełkowski, in: *Landolt-Börnstein Handbook, III/19d2*, Ed. H.P.J. Wijn, Springer, Berlin 1990.

[2] V.V. Aleksandryan, K.P. Belov, P.Z. Levitin, A.S. Markosyan, W.W. Snegirev, *Pis'ma Zh. Eksp. Teor. Fiz.* **40**, 77 (1984).

[3] H.L. Skriver, *The LMTO Method*, Springer, New York 1984; O.K. Andersen, O. Jepsen, M. Sob, in: *Electronic Structure and Its Applications*, Ed. M. Yussouff, Springer, Berlin 1987, p. 2; J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, *Phys. Rev. B* **46**, 6671 (1992); G. Krier, O. Jepsen, A. Burkhardt, O.K. Andersen, *The TB-LMTO-ASA Program*, source code version 4.7, available upon request from the program authors.

[4] A. Szajek, A. Kowalczyk, J. Baszyński, A. Jezierski, T. Mydlarz, *J. Magn. Magn. Mater.* **157-158**, 723 (1996).

[5] J.J. Yeh, I. Lindau, *At. Data Nucl. Data Tables* **32**, 1 (1985).

[6] H. Yamada, I.S. Dubenko, R.Z. Levitin, A.S. Markosyan, *J. Phys., Condens. Matter* **5**, 3965 (1993).

[7] P.-A. Lindgård, *Phys. Rev. B* **16**, 2168 (1977).

[8] B. Szpunar, P.-A. Lindgård, *Phys. Status Solidi B* **82**, 449 (1977).