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ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF UFe_2 SYSTEM

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The electronic structure of the UFe_2 compound was studied by X-ray photoemission spectroscopy and *ab initio* self-consistent tight binding muffin tin orbital method. This compound crystallizes in a cubic Laves phase. The calculated valence band spectrum is characterized by two peaks due to $\text{U}(5f)$ and $\text{Fe}(3d)$ states. We have found a good agreement between the experimental valence band spectrum and theoretical *ab initio* calculations. The carrier concentration estimated from the Hall effect amounts to $\approx 10^{22} \text{ cm}^{-3}$.

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1. Introduction

Uranium compounds exhibit a rich variety of electrical and magnetic properties, due to peculiar behaviour of the $\text{U}(5f)$ states. Numbers of experimental and theoretical studies have been made on these compounds. However, it is still unclear which of the two approaches, the localized $5f$ electrons or the itinerant $5f$ ones, supplies a better basis for the description of the properties of these compounds. An essential question is whether the band-structure calculation can be a good starting point for the description of their $\text{U}(5f)$ states. To understand this problem, the photoemission experiments have been performed for many uranium compounds [1]. Among intermetallic compounds of actinides with $3d$ metals the most frequently studied one is UFe_2 . This compound crystallizes in a Laves phase with the cubic structure of $C15$ type.

Aldred [2] summarized the earlier work and showed that the material is a ferromagnet with a total magnetic moment of $1.09 \mu_B/\text{f.u.}$ and rather small anisotropy. Andreev et al. [3] focused particularly on the small anisotropy, and concluded that the $5f$ electrons of uranium must be largely itinerant. Popov et al. [4] showed that the UFe_2 has a sizable rhombohedral distortion at T_C . Neutron elastic scattering measurements [5] have established that the Fe moment is

0.6 μ_B and that the moment on the U atom is almost zero because of the cancellation of the spin and orbital moments, which are both about 0.23 μ_B , but oppositely directed. Theoretical and experimental investigations of uranium intermetallic compounds provide important information on the development of their electronic structure with emphasis on the 5*f*-states, in particular.

In this paper we present the electronic and transport properties of the UFe₂ compound.

2. Experimental details

The UFe₂ compound was prepared by induction melting of stoichiometric amounts of the constituent elements in a water-cooled boat, under an argon atmosphere. The crystal structure was established by a powder X-ray diffraction technique using Cu K_α radiation [6].

The X-ray photoemission spectroscopy (XPS) spectra were measured with Al K_α radiation of 1486.6 eV at room temperature using a SPECS EA 10 PLUS energy spectrometer. The energy spectra of the electrons were analysed by a hemispherical analyser (FWHM_{MgK α} = 0.8 eV for Ag 3*d*_{5/2}). Calibration of the spectra was performed according to Baer et al. [7]. All emission spectra were measured immediately after the sample cleaning in vacuum of 8×10^{-11} mbar. The cleaning procedure of the sample surface is described in more details elsewhere [8]. The 4*f*_{7/2} peak of gold was located at 84.0 eV and the Fermi level was located at $E = 0$ eV. The Hall effect was measured on plate-shaped sample with the dimensions of $11 \times 3 \times 0.35$ mm³ using a DC technique at 145 and 230 K. The field dependence of the Hall resistivity was measured in a magnetic field up to 4 T.

3. Band calculations

Electronic structure was calculated by the tight binding linear muffin tin orbital (TB LMTO) method [9] for experimental lattice parameter $a = 7.062$ Å [6]. The calculations were performed without spin polarisation because the XPS spectra were measured at room temperature, it means above the Curie temperature $T_C = 165$ K. The XPS spectra were calculated from the partial electronic densities of states (DOS) weighted with atomic photoemission cross-sections [10]. The finite experimental resolution was taken into account in the calculations by convoluting the weighted DOS with an energy dependent Lorentzian function with a half-width 0.6 eV.

4. Results and discussion

In Fig. 1 we plot the experimental (upper solid line) and calculated (middle solid line) XPS spectra for the UFe₂ compound from the Fermi energy (E_F) located at $E = 0$ to a binding energy of about 4 eV. The calculated valence band spectrum is characterized by two major peaks located 0.6 (solid bottom line) and 2 eV (broken line) below the Fermi level due to U(5*f*) and Fe(3*d*) states, respectively. The Fe(3*d*) band contains 6.6945 electrons and its centre of gravity is located about 0.1 eV below the Fermi level. The peak of U(5*f*) electrons located below E_F is only a minor part of the entire band. The occupied part of the band contains 3.07 electrons. The U(5*f*) centre of gravity is located about 0.06 eV above E_F . It means

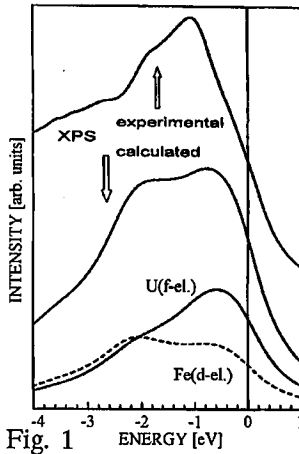


Fig. 1

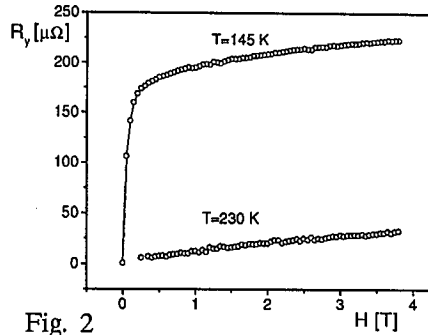


Fig. 2

Fig. 1. The experimental and calculated XPS spectra for the UFe_2 compound.

Fig. 2. The Hall resistivity as a function of magnetic field, measured at two different temperatures (above and below $T_C = 165$ K) for the UFe_2 compound.

that the uranium gives a contribution to the XPS spectra near the Fermi level. The experimental spectrum has a humped feature around 2 eV below E_F , which is well reproduced by our calculations. The agreement between the experimental XPS and calculated valence band photoemission spectra is good. The theoretical results are also in good agreement with our previous calculations [11, 12] performed for USi_3 .

Figure 2 shows the Hall resistivity as a function of the external field, measured at $T = 145$ K (ferromagnetic state) and $T = 230$ K (paramagnetic state) for the UFe_2 compound. For such a material the field dependence $R_y(H)$ should be given by $R_y = R_0 H + R_S J$, where R_0 is the ordinary (normal) Hall coefficient, R_S is the anomalous Hall coefficient, H — the applied magnetic field, and J is the magnetic polarization. In the fields below saturation the initial slope of $R_y(H)$ curve is essentially R_S . At high fields the slope will be R_0 . The carrier concentration determined from this slope amounts to $\approx 10^{22} \text{ cm}^{-3}$ at $T = 145$ K. Similar result was reported very recently in Ref. [13] for $\text{Nd}_2\text{Fe}_{14}\text{B}$.

5. Conclusions

The calculated valence band spectrum for the UFe_2 compound is characterized by two major peaks located near -0.6 and -2 eV due to $\text{U}(5f)$ and $\text{Fe}(3d)$ states, respectively. We have found a good agreement between the experimental XPS and calculated valence band photoemission spectra.

The carrier concentration estimated from the Hall effect amounts to $\approx 10^{22} \text{ cm}^{-3}$, which is value typical of intermetallic compounds containing f - and d -electron elements.

Acknowledgments

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