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Electronic and Magnetic Properties of UCu_2Si_2 Compound

J.A. Morkowski [1], G. Chełkowska [2], R. Troć [3], A. Szajek [1], M. Richter [4], C. Neise [4]

[1] *Institute of Molecular Physics. Polish Academy of Sciences. ul. M. Smoluchowskiego 17. 60-179 Poznań. Poland*
[2] *A. Chełkowski Institute of Physics, Silesian University, ul. Uniwersytecka 4, 40–007 Katowice, Poland*
[3] *W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, P.O. Box 1410, 50–950 Wrocław, Poland*
[4] *Leibniz-Institut für Festkörper- und Werkstoffforschung, IFW Dresden, PF 270116, D-01171 Dresden, Germany*

Ternary intermetallic compounds UT_2Si_2, where T denotes a transition metal, show a rich variety of electronic and magnetic ground state properties such as Pauli paramagnetism, ferro- and antiferromagnetism. In almost all cases only uranium atoms are observed to be magnetic. The X-ray and neutron diffraction measurements showed that UCu_2Si_2 crystallizes in the body-centered-tetragonal $ThCr_2Si_2$-type structure with space group *I4/mmm*. The neutron diffraction studies on polycrystalline samples of UCu_2Si_2 reveal ferromagnetic ordering of the uranium magnetic moments aligned below about $T_C = 103$ K. The uranium ordered moment at 4.2 K was reported to be either $1.61 \pm 0.05\ \mu_B$ [1] and $2 \pm 0.1\ \mu_B$ [2]. Comprehensive approach to UT_2Si_2 series, including T = Cu, based on *ab-initio* calculations was presented by Sandratskii and Kübler [3]. They obtained magnetic moment on uranium atom equal to only $0.88\ \mu_B$. Recently performed measurements on single crystal UCu_2Si_2 [4] gave $T_C = 100$ K and observation of an antiferromagnetic phase in the range of 100–106 K. The saturation moment was found to be $1.75\ \mu_B$ at 2 K and the electronic specific heat coefficient as 20 mJ/(K^2 mol).

In this paper we present measurements based on a single crystalline sample with crystallographic parameters collected in Table 1.

Table 1. Crystallographic characteristics for UCu_2Si_2: space group *I4/mmm*, lattice parameters $a = 3.985$ Å, $c = 9.945$ Å, positions of atoms (x,y,z) in the unit cell.

Atom	Site	x	y	z
U	2b	0	0	½
Cu	4d	0	½	¼
Si	4e	½	½	0.6177

The band structure calculations were performed by the Full Potential Linear Muffin-Tin Orbitals method (FP LMTO) using the LMTART code (version 6.5) [5] and Full-Potential Local-Orbital Minimum-Basis Scheme (FPLO, version 5.10-20) [6]. The results of magnetic moments obtained using local spin density approximation (LSDA) were much too small (~$0.5\ \mu_B$) because of cancelation of spin and orbital moment. The calculations where the so-called orbital polarization was assumed based on Brooks scheme [7] in FPLO method gave much larger magnetic moment on uranium atoms, as well as much closer to the experimental results: $2.09\ \mu_B$. This result was obtained using the reciprocal space mesh contained 1992 $\boldsymbol{k}$ points within the irreducible wedge of the Brillouin zone. The exchange and correlation potential in the local spin density approximation (LSDA) was taken in the form proposed by Perdew & Wang [8]. The density of states (DOS) at Fermi level is equal 4.84 states/(eV f.u.), which corresponds to the electronic specific heat coefficient equal to 11.39 mJ/(K^2 mol).

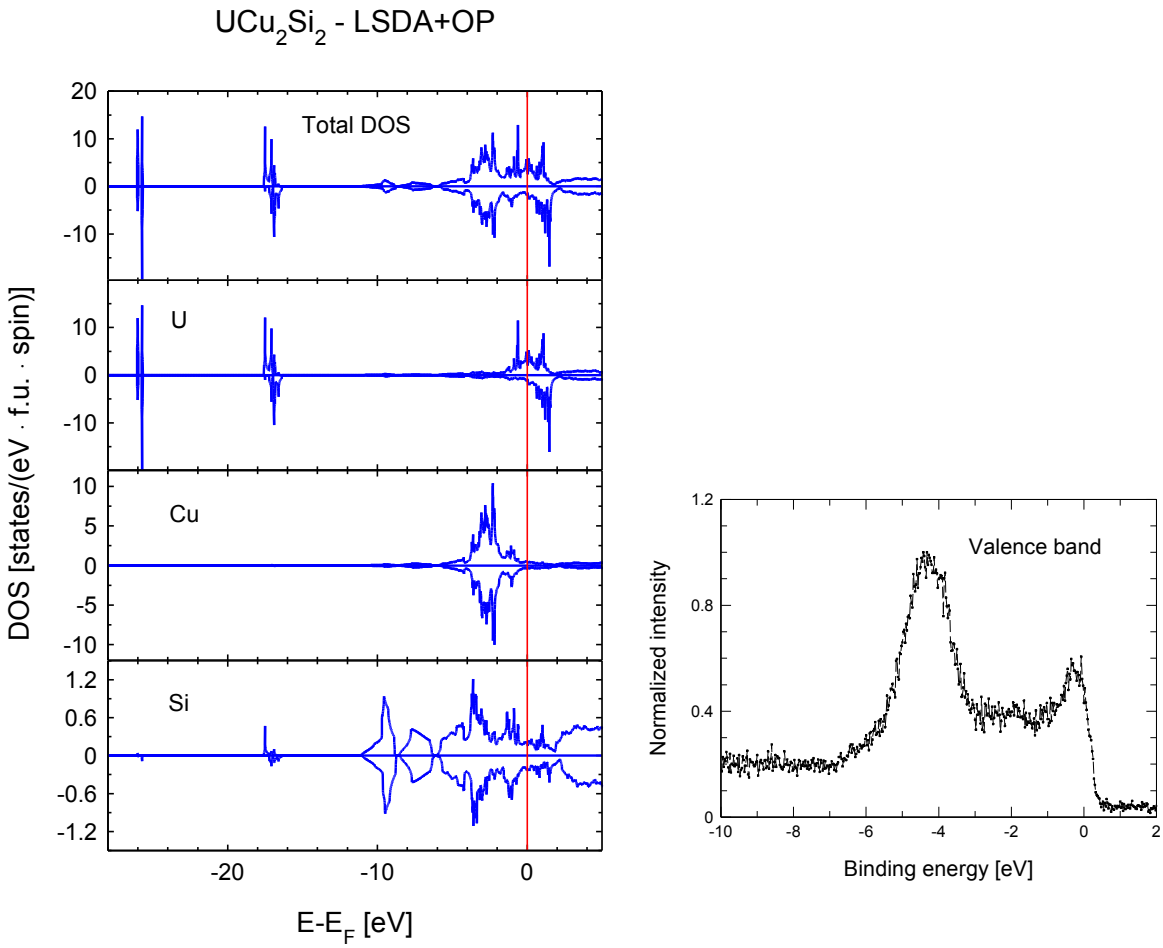

Fig. 1. *Left panel*: Densities of electronic states for UCu_2Si_2: total and local contributions from the particular atoms, calculated by the method of ref. [6].
Right panel: The experimental XPS spectrum of valence band.

The calculations without spin polarization were used to reproduce the experimental XPS spectra. Such procedure was used because the experiment was performed at room temperature, well above T_C. In Fig. 1 (right panel) experimental spectrum of valence band is presented. The peak for zero binding energy is formed mainly by U(5f) electrons and for about –4 eV by Cu(3d) ones.

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