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To cite this version:

HAL Id: jpa-00218838
https://hal.archives-ouvertes.fr/jpa-00218838
Submitted on 1 Jan 1979

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Electronic band structure and properties of $\alpha$-U (*)

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Résumé. — Utilisant une version relativiste de la méthode LAPW, nous présentons des résultats d'une étude détaillée de la structure de bande électronique ainsi que de quelques propriétés physiques de l'uranium dans la phase orthorhombique. Les densités d'états totales et partielles sont utilisées pour discuter les résultats de photo-émission de Veal et Lam. Les surfaces de Fermi des bandes prédominantes 6 et 7 présentent une symétrie élevée ainsi que quelques particularités topologiques (nesting) qui peuvent être comparées aux mesures actuelles d'effet dHvA d'Arko et Schirber. Le calcul du facteur de forme neutronique en présence d'un champ magnétique est en bon accord avec les mesures de Maglic et al.

Abstract. — We present some results of a detailed study of the electronic band structure and some physical properties of orthorhombic uranium using a relativistic version of the LAPW method. Total and projected (by orbital angular momentum) densities of states are used to discuss the photo-emission data of Veal and Lam. The Fermi surfaces of the dominant 6th and 7th bands are found to have high symmetry (and some nesting features) of interest to dHvA measurements being pursued by Arko and Schirber. The theoretical magnetic field induced neutron form factor is found to be in good agreement with the measurements of Maglic et al.

The anomalous physical properties of $\alpha$-U have made it a subject of great interest for experimental and theoretical study. Unfortunately, its complex structure (orthorhombic with 4 atoms/unit cell) and the resulting lack of symmetry have made its theoretical study by conventional energy band methods exceptionally difficult and costly. Thus, while we were able to study the light and heavy actinide metals [1] in their cubic (high temperature) structures, the study of $\alpha$-U awaited development of a computational scheme which was not only rapid and efficient but which avoided the so-called asymptote problem which plagued our earlier efforts.

In this paper we report some results of our relativistic energy band studies on $\alpha$-U using a relativistic version of the linearized augmented plane wave method [2-3] (LAPW). This scheme has been successfully applied to the study of some actinide compounds, notably UGe$_2$ [4], UIr$_3$ [2], and URh$_3$ [5]. We have determined the energy band structure, density of states (DOS), orbital angular momentum projected DOS (for use in analysing the XPS experiments of Veal and Lam [6], detailed Fermi surface cross-sections in close collaboration with the work of Arko and Schirber [7] reported elsewhere at this conference), wavefunctions and magnetic field induced spin densities, neutron magnetic form factors (in close collaboration with and to understand the measurements of Maglic et al. [8]), and generalized susceptibilities, $\chi(q)$ (for investigating possible electronically driven phonon anomalies and charge density waves). Because of space limitations we are able only to give a brief indication of this extensive work here. A full report is being prepared for publication elsewhere.

The three lattice parameters and the atomic positional parameter, $a$, were obtained by extrapolating the temperature dependent X-ray measurements of Barrett et al. [9] to the temperatures assuming that the system was cooled under pressure in order to avoid the anomalies associated with transitions at $T < 43$ K. Using these parameters ($a = 5.360$ Å, $b = 11.086$ Å, $c = 9.328$ Å, and $\mu = 0.102$) our model warped muffin tin potential was constructed in the standard overlapping charge density model using the Kohn-Sham-Gaspar ($\alpha = 2/3$) exchange. In our calculation we use the $t^6$ $d^8$ $s^1$ configuration. Different estimates including a pseudo-self-consistent model (as was used earlier for UGe$_2$) to determine an improved choice of configuration, indicate that a configuration in which roughly 0.25 to 0.5 electron are transferred from the f to the d levels is more appropriate. The calculated band structure was fitted with a Fourier series and used in our determinations of the Fermi surface, DOS and $\chi(q)$.

Figure 1 shows the $l = 3$ angular momentum projected DOS. We see a good deal of structure in the total DOS (not shown) arising from the lower symmetry and the hybridized set of s, p, d, and f bands. There is a rapidly increasing total DOS just above $E_F$. (*) Supported by the U.S. NSF, the AFOSR, and the DOE.

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Our calculated Fermi surface cross-sections are presented and discussed elsewhere in these proceedings. In the remaining space we present the magnetic field induced spin densities decomposed by $l$-value. The Fourier transform of these spin densities make the dominant contribution to the neutron magnetic form factor. Figure 2 compares the free ion $f$ state charge density (broken curves) with the $l = 3$ decomposed radial density at (or close to) the Fermi energy, 1.135 Ry. All densities are normalized to unity over the $r$ space shown (solid curves) so that they must be multiplied by their occupation. (The $f$ contribution is roughly 80% with the majority of the remainder comprised of $d$-character.) We find that the two $l = 0$ densities agree very closely, the $l = 1$ densities are slightly shifted for large $r$, and the $l = 2$ densities deviate only near the sphere radius. The major difference is in the $l = 3$ densities with the band result showing the large radial expansion expected for itinerant electrons in the lower half of the band. It is this expansion which is responsible for the contracted values of the magnetic neutron form factor seen by Maglic et al. [8].

Our results indicate that the $f$-electrons in $\alpha$-U are not only quite itinerant in nature (and hence treatable by a band model), but are dominantly present in the experimental data.

References


