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Direct observation of the f-c hybridization in the ordered uranium films on W(110)

Qiuyun Chen(陈秋云), Shiyong Tan(谭世勇), Wei Feng(冯卫), Lizhu Luo(罗丽珠), Xiegang Zhu(朱燮刚), Xinchun Lai(赖新春)

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Direct observation of the f–c hybridization in the ordered uranium films on W(110)*

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A key issue in metallic uranium and its related actinide compounds is the character of the f electrons, whether it is localized or itinerant. Here we grew well ordered uranium films on a W(110) substrate. The surface topography was investigated by scanning tunneling microscopy. The Fermi surface and band structure of the grown films were studied by angle-resolved photoemission spectroscopy. Large spectral weight can be observed around the Fermi level, which mainly comes from the f states. Additionally, we provided direct evidence that the f bands hybridize with the conduction bands in the uranium ordered films, which is different from previously reported mechanism of the direct f–f interaction. We propose that the above two mechanisms both exist in this system by manifesting themselves in different momentum spaces. Our results give a comprehensive study of the ordered uranium films and may throw new light on the study of the 5f-electron character and physical properties of metallic uranium and other related actinide materials.

Keywords: uranium films, 5f-electron character, angle-resolved photoemission spectroscopy

PACS: 74.25.Jb, 68.55.–a, 07.79.–v **DOI:** 10.1088/1674-1056/28/7/077404

1. Introduction

Uranium (U), being the heaviest natural element, exhibits rich physical properties:[1,2] three allotropes, anisotropic thermal expansion, a series of three low-temperature charge density wave (CDW) structural phase changes in the normal state, and a superconducting transition below 2 K.[3] It is also the only element in the periodic table with the CDW transition at ambient pressure.[4] In the normal state, the first CDW transition occurs at 43 K (α_1), the second at 38 K (α_2), and the last at 22 K (α_3).[5–7] Upon heating, α-U transforms into a tetragonal structure (935 K) and finally crystallizes to a body-centered cubic phase (1045 K) prior to melting at 1406 K at ambient pressure.[8] Many of these unusual properties found in U are thought to be closely related to the delocalization of the partially filled U 5f states.[2] It is proposed that the 5f states of the actinides are different from the 4f states in lanthanides and are more extended due to a node in the radial wave function, which gives much stronger hybridization.[9]

Metallic U provides a unique platform to understand the role of f electrons in the complex behavior of the actinides. Moreover, the production of epitaxial films has led to the discovery of a variety of new electronic, magnetic, and structural phenomena. The interaction of the deposited material with the substrate can lead to properties which may differ dramatically from those of the bulk. For U, it is reported that a hexagonal hcp-U phase can be obtained by deposition of thin U metal films onto the W(110) substrate,[10,11] and theoretical calculations predicted that the unusual hcp-U phase has an electronic instability, leading to a possible CDW or magnetic ordering.[12] It is also reported that different orientations of the α-orthorhombic phase can be obtained by depositing U onto a variety of buffer/seed layers on sapphire.[13,14]

A key point to understand the above exotic properties is to understand the electronic structure and f-electron character of U, whether it is localized or itinerant, which depends on the external conditions.[15] The electronic structure of α-U has been studied both experimentally and theoretically in the previous studies.[12,16,17] The Fermi surface of the α-U single crystals at ambient pressure from 0.02 K to 10 K with magnetic fields up to 35 T has been studied by torque magnetometry, and a rich set of orbits for α-U at low temperature have been observed.[16] Theoretical study of α-U/W(110) thin films has been performed by density functional theory (DFT) calculations, and it is proposed that the total density of states is dominated by the 5f states in the vicinity of the Fermi level.[12] Many-body electronic structure of metallic α-U has also been studied using a quasiparticle self-consistent GW method.[17]

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool to study the electronic states in solid materials.[18–23] Earlier pioneer ARPES measurements have been carried out on the high quality U single crystals,[24] and they found a well-ordered orthorhombic crystallographic structure representative of the bulk material.[25] The valence band structure of the α-U single crystal has been studied by ultraviolet photoemission spectroscopy and x-ray photoe-

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mission spectroscopy.[24] Later on, the band structure has been obtained by further ARPES measurements performed at 173 K.[25] For the ordered overlayers of U metal on a W(110) substrate, bandlike properties of the U 5f states were observed, which was proposed to arise from direct f–f interaction,[10] and scanning tunneling microscopy/spectroscopy (STM/STS) results further showed that the density of states close to the Fermi level is dominated by the 5f states.[11] Previous ARPES and STM studies have shed light on the electronic structure of U. However, the Fermi surface topology of either α-U single crystals or ordered U films has never been revealed by ARPES. Moreover, previous ARPES experiments carried out on the ordered films on W(110) were measured with 50–98 eV photons, with the energy resolution of about 100 meV. Since the energy scale of the heavy quasiparticles is relatively small in f-electron compounds, ARPES measurements with higher energy resolution are necessary to resolve the fine structures of the f states.

In the present study, well-ordered U epitaxial films were grown on a W(110) surface, and the surface topographies of the films were studied by STM. The Fermi surface topology and band structure of the grown films were investigated by ARPES. Comparing with previous ARPES results, we observed some fine structures of the ordered films with better energy resolution. More importantly, our results reveal direct evidence for the hybridization of the f states and conduction electrons, which is different from the previously proposed mechanism of the f–f interaction. We proposed that both the f–f interaction and f–c hybridizaiton exist in this system and manifest themselves in different momentum spaces.

2. Experimental details

Sample preparations and film growth were performed in several ultra high vacuum (UHV) chambers. These chambers are connected using a radical distribution chamber with a base pressure of 5×10^{-10} mbar. Ordered U films were prepared by *in situ* deposition onto the prepared W(110) substrate. After a long time outgassing of the U metal source, U metal was evaporated from a tungsten crucible, which was heated to about 2000 K during evaporation. The evaporation rate (3 Å/min) and the thickness of the deposited films were calibrated by the quartz oscillator. The base pressure was better than 5×10^{-10} mbar during evaporation. The directly deposited U film was a nonordered overlayer. After annealing at 800 K for 5 min, the ordered U films could be obtained. The samples were transferred immediately to STM and ARPES chambers under UHV conditions.

STM experiments were performed in an ultrahigh vacuum, low temperature STM apparatus with a base pressure of 5×10^{-11} mbar. All the measurements were performed at 78 K with an electro-chemically etched tungsten tip. All topographic images were recorded in the constant current mode. ARPES measurements were performed with a UVLS discharge lamp (21.2 eV, He-Iα light). All data were collected with a Scienta R4000 electron analyzer. The overall energy resolution was 15 meV or better, and the typical angular resolution was 0.2°. A freshly evaporated gold sample was used to determine the Fermi level.

3. Results and discussion

Structurally ordered U films were grown at room temperature onto a W(110) substrate. About 70 Å U was deposited by evaporation from a tungsten crucible. A sharp hexagonal low energy electron diffraction (LEED) pattern was observed, which is consistent with the previously reported results of U films on W(110),[10] and is not compatible with any of the known bulk phases of U metal at ambient pressure (orthorhombic α, tetragonal β, and bcc γ phases). The LEED pattern suggests that this growing and annealing procedure leads to the formation of a close-packed hcp structure with an interactomic U–U distance of 3.15±0.1 Å, which is in line with the results of Molodtsov *et al.*[10] and Bautista *et al.*[11] This suggests that the substrates, thickness of the films, growing and annealing conditions are especially important to obtain different phases. This is not surprising, since the two-dimensional morphology of thin films and interactions with the substrate can lead to properties which differ dramatically from those of the bulk. For thinner U films deposited on W(110), it has come to the agreement that they are in a hexagonal phase. However, if a buffer layer was added between tungsten and the U films, the orthorhombic structure of α-U can be obtained. Especially, by changing the buffer layer, the orientational relationship can also be changed.[13]

Figures 1(a)–1(c) show the constant current STM images of the ordered U films on the W(110) surface, where flat terraces can be found. We did not observe obvious islands on top of the terraces, and smooth areas can be found. Figure 1(d) shows the profile along the line aa' in Fig. 1(c), from which a typical step height of 2.55 Å for the ordered U films can be found.

Figure 2(a) shows the valence band structure of the ordered U films obtained by ARPES, and its corresponding angle-integrated energy distribution curves (EDCs) are displayed in Fig. 2(b). Two main spectral features can be observed, located at the binding energies (BEs) of 0.07 eV and 0.3 eV, marked by A and B, respectively. In the previous ARPES study of ordered U films on W(110), only one peak with no clear dispersion located at about 0.2 eV BE was observed within the energy range of 0–0.5 eV. This is not contradicting, since those data were taken with 50–98 eV photons with the energy resolution of around 100 meV. The band at

0.2 eV is probably consisted of two subbands, as observed in Fig. 2 with higher energy resolution. Combined with theoretical calculations, it is suggested that 90% of these features originate from the f character.[10]

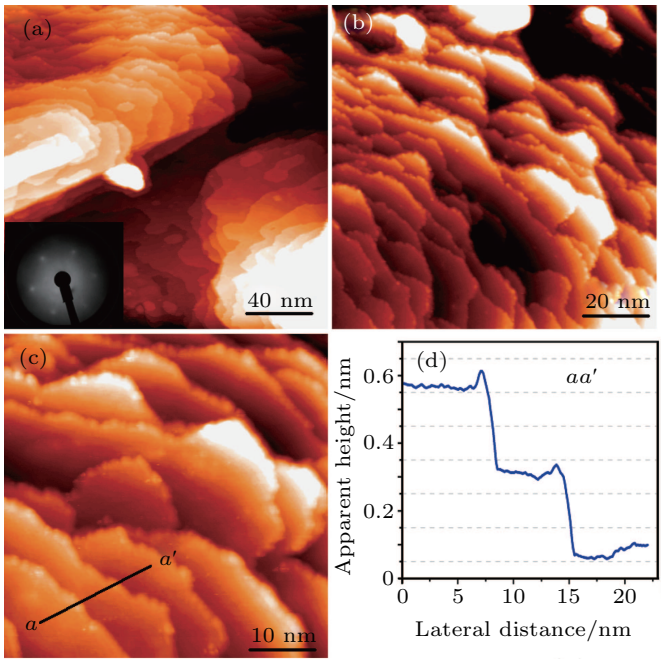


Fig. 1. (a)–(c) STM images of the freshly deposited U films on the W(110) substrate after annealing at 800 K for 5 min with the sizes of (a) 200 nm ×200 nm, (b) 100 nm×100 nm, and (c) 50 nm×50 nm. The inset in panel (a) is LEED pattern of the ordered U films. (d) Line profile of aa' in panel (c). All the images are obtained with $V_g = 1$ V and $I_t = 80$ pA.

Besides the two sharp features, three humps can also be observed, located at the BEs of 1.3 eV, 1.5 eV, and 2.3 eV, respectively. From the band structure in Fig. 2(a), we can observe two weak bands with no obvious dispersion located at 1.3 eV and 1.5 eV, which contribute to the two observed humps. The origins of these two bands are still not clear, but this behavior is similar to that of the crystal-field splittings observed in Ce-based compounds.[26] It probably arises from the splittings by the crystal electric field effects according to the point group symmetry of the system. However, more evidence needs to be given to clarify this point. The left 2-eV feature has been discussed more frequently in the previous studies, and several proposals have been given. Some attributed it to a 5f shake-up satellite,[27] and later on this shake-up sattellite was proposed to be emission from part of the 5f band.[10] Some groups found evidence of a d-band emission due to its different resonant behavior in respect to the main 5f signal.[28] Others might think that it is likely a surface state with d character.[24] From our results, this feature may originate from the d states, since it shows obvious dispersive character. However, we can not identify whether it is from the bulk or the surface state.

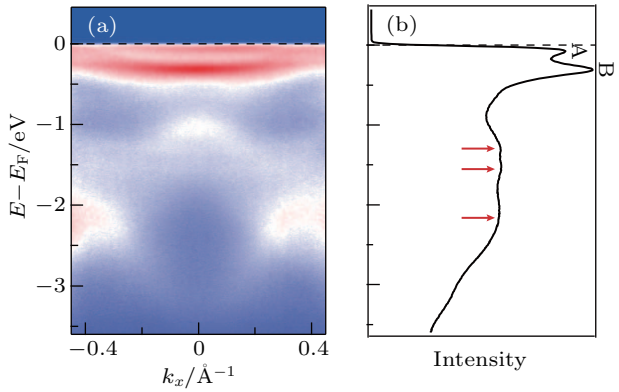


Fig. 2. (a) Valence band structure of the ordered U films on W(110) taken at 20 K. (b) Angle-intergrated EDCs of panel (a).

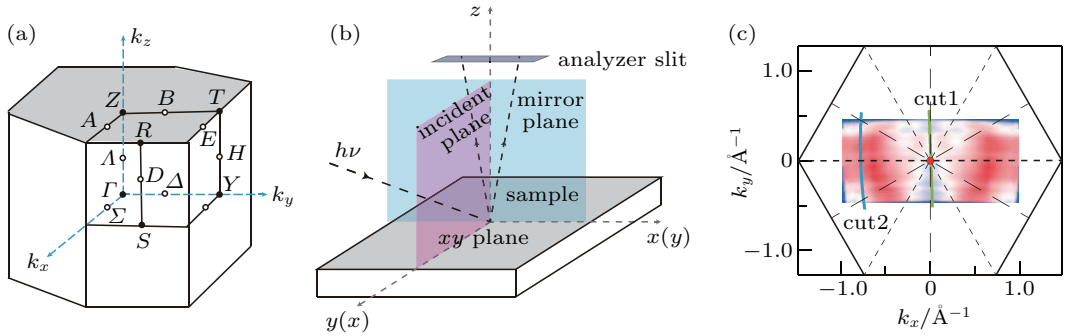


Fig. 3. (a) Bulk Brillouin zone of α-U. The projected surface Brillouin zone of the (001) surface has been marked gray. (b) Experimental setup for ARPES. (c) Photoemission intensity map of the ordered U films at the Fermi level (E_F) integrated over a window of ($E_F - 10$ meV, $E_F + 10$ meV).

Figure 3(a) shows the Brillouin zone of the bulk α-U and the projected (001) surface Brillouin zone has been marked gray. Experimental setup for our ARPES measurements is displayed in Fig. 3(b). Photoemission intensity map of the ordered films is displayed in Fig. 3(c). One main feature is that there are large spectral weights near the Fermi level, which makes it difficult to observe the fine structure of the Fermi surface. However, we can still observe a rounded Fermi pocket near the Brillouin zone center, which has a close neighbor of a square-like Fermi pocket with large spectral weight. The Fermi surface of U is rather complicated from theoretical calculations, as reported by Fast *et al.*[6] Here we can only observe part of the Fermi surface experimentally.

To concentrate on the fine structure near the Fermi level,

figure 4 shows the photoemission intensity plot along cut1 in Fig. 3(c). Two main features can be observed: a nearly flat band located at 0.07 eV BE, which contributes to the large spectral weight near the Fermi energy, as also can be clearly observed from the EDCs plotted in Fig. 4(b). This is consistent with the observed band-like feature in previous ARPES results.[10] Also an electron-like band was observed crossing the Fermi level, which contributes to the large electron Fermi pocket around the zone center in Fig. 3(c). Interestingly, we found that this electron-like band intersects with the f band locating at 0.3 eV, which results in the redistribution of the f spectral weight and indicates that this electron-like conduction band may also hybridize with the f band.

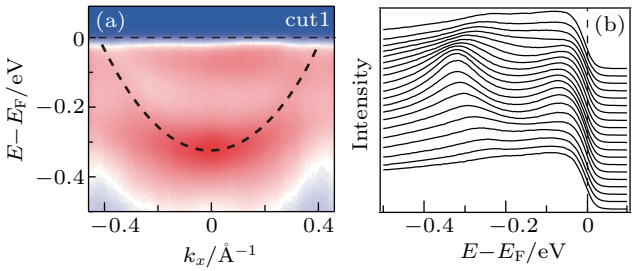


Fig. 4. (a) Photoemission intensity plot along cut1 in Fig. 3(c). (b) Energy distribution curves of the plot in (a).

Figure 5(a) presents the photoemission intensity plot along cut2 in Fig. 3(c), from which two hole-like bands can be observed. Difference can be found in the f spectral weight near the Fermi level at different k, which shows the enhancement of the spectral weight inside the two conduction bands. For f-electron systems, due to the hybridization between the conduction band and the f states, a dispersive band-like feature could be observed around the Fermi level at the locations where the f band intersects with the conduction band, which is schematically displayed in Fig. 5(b). The hybridization of the f band and the conduction band can be well described by a simple mean-field hybridization band picture, and more details can be found in Ref. [29]. When the f band hybridizes with the conduction band, the conduction band will start to bend when it comes towards the f energy level. This hybridization process forms a weakly dispersive hybridized band, which can be clearly observed in Fig. 5(b) and has been verified in the Ce-based heavy-fermion compounds.[21,26,30] The hybridized quasiparticle band has two main features: redistribution of the spectral weight and a shift in binding energy at different k. From Fig. 5(a), we can observe the difference of the intensity at different k. Figure 5(d) enlarges the EDCs of the f states at different k values, and we found slight dispersion of the f band near the Fermi level. The observation of both the energy dispersion and the redistribution of the intensity indicates the formation of a quasiparticle band due to the ongoing hybridization between the conduction electrons and f states. The hybridization emerges at the locations where the conduction bands approach or cross the Fermi level, while at other regions where no conduction bands cross the Fermi level, the f band does not show observable energy dispersions. By comparing the peak positions of the quasiparticle band at different momentum locations, we found that the energy dispersion of the hybridized band is about 5 meV in the ordered U films.

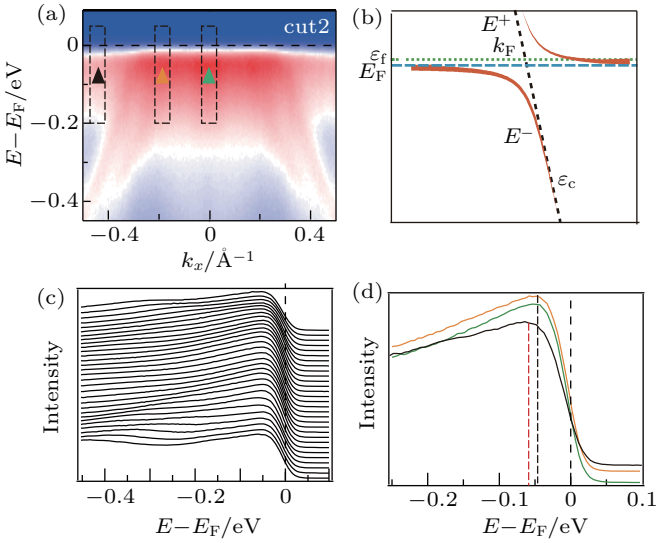


Fig. 5. (a) Photoemission intensity plot along cut2 in Fig. 3(c). (b) A schematic diagram showing the hybridization process of the f bands (ε_f) and a conduction band (ε_c) in panel (c) under a periodic Anderson model in the Kondo lattice. The red curve is the hybridized band. (c) Energy distribution curves of the plot in (a). (d) Comparison of EDCs measured at different momentum locations. The black, yellow, and green curves represent the integration windows marked by the dashed blocks with the corresponding colors.

In the previous ARPES studies of the ordered U films, the dispersion of the U 5f states was also observed, and it was proposed to be caused by direct f–f interaction, rather than by hybridization between f bands and conduction bands, which is different from the 4f-derived bands in Ce systems.[10] In our results, we have observed two kinds of dispersive bands at different momentum spaces. For the hybridization behavior in Fig. 4(a), it is consistent with the results of Molodtsov *et al.*, which may arise from direct f–f interaction. While for the hybridization behavior plotted in Fig. 5(d), direct evidence can be found for the hybridization between the f states and conduction electrons. These results suggest that the two mechanisms of the f–f interaction and f–c hybridization can both be observed in the ordered U films in different momentum spaces.

4. Conclusion

To summarize, we have grown well-ordered U metallic films on a W(110) surface, and the topography of the grown films has been studied by STM. Further APRES results present both the Fermi surface topology and electronic structure of the ordered films. The 5f spectral weight can be observed near the

Fermi level, indicating the bandlike feature of the f electrons in the ordered U films. More importantly, We have observed two kinds of hybridization behaviors in different momentum spaces, which indicates that both the f–f interaction and f–c hybridization exist and contribute in the hybridization process. Our results may shed light on the understanding of the 5f-electron character and physical properties in this and other actinide compounds.

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