ARPES of Single Crystal Uranium (001)
Angle Resolved Photoemission Spectroscopy (ARPES) of Single Crystal Uranium (001)

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Why Study Uranium?

- Actinides possess itinerant to localized “f” electron behavior
- U(001) sample quality not previously available
- First comprehensive band map of an actinide now possible
- Actinide band map calculation -- improved accuracy

Los Alamos National Laboratory
The World’s Greatest Science Protecting America
LEED pattern of U(001) at T = 273 K

First U(001) LEED pattern, long range order bulk termination

Calculation & Experiment < 2 % difference

Structural reactivity studies: O_2, D_2, H_2

I-V analysis underway
ARPES - choose azimuthal $q$ to specify $k$-vector to probe, and then vary polar $f$ to collect DOS at various $k_{||}$ and observe dispersion of bands along $k$-vector.

$$E_{\text{kinetic}} = h\nu - e\Phi - E_{\text{binding}}$$

$$k_{||} = \sqrt{\frac{2m_eE_{\text{kinetic}}}{\hbar^2}} \cdot \sin\phi$$
**a - Uranium**

![unit cell diagram](attachment:unit_cell_diagram.png)

**Brillouin Zone**

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ARPES Raw Data Stack Plot, along G to S

$\phi = 60\,\text{degrees}$

$f = 0\,\text{degrees}, \perp \text{to U(001) surface}$

Fermi Edge
Uranium Band Map Sigma to Gamma, Gamma to Y, $T = 173$ K
ARPES: $\Sigma - \Gamma - Y, \Gamma - S$

$\alpha$-Uranium (001), $T = 173$ K

Binding Energy (eV)
ARPES & WIEN2K

$\alpha$-Uranium (001), $T = 173$ K
Data Maxima, DDOS WIEN2K Calculations

Band Structure

Band Structure, Low Intensity

d-Band, Tamm surface states

f-Band, f-like, Shockley surface states

Plasmon ??

Flat band near FE due to disorder ?
Conclusions:

- Single crystal U(001) samples yield expected experimental LEED pattern (< 2% difference). Showing long range bulk termination.

- ARPES data exhibit band dispersion at 173 K and correlates favorably with DDOS WIEN2K.

- Narrow f-band near Fermi edge. Presence of d and f surface states.

- Data-Theory mismatch possibly due to: DT, e⁻ to e⁻, e⁻ to phonon contributions.

Next Steps:

- Colder Temperatures, Higher Resolution
- Fermi Surface Mapping, at ALS, Berkeley, CA
- Matrix Element Calculation, DMFT Calculation
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