Real-time Integration Tools for the Comparison of ARPES Data and DFT Band Structure Predictions

Anna Capuano, Brendan Faeth, Darrell Schlom

Introduction

Angle Resolved Photoemission Spectroscopy (ARPES):

- A spectrometer measures the emission angle and kinetic energy of electrons photoemitted from a sample following excitation from an ultraviolet (UV) photon beam
- Momentum in the x and y direction can be calculated using:

$$k_x = \sqrt{(2 * (m_e))/\hbar} * \sqrt{KE} * \cos(Q) * (-\cos(\omega) * \sin(\theta) - \cos(\phi) * \cos(\theta) * \sin(\omega)) + \sin(Q) * \sin(\phi) * \sin(\omega)$$

$$k_y = \sqrt{(2 * (m_e))/\hbar} * \sqrt{KE} * \cos(Q) * (-\cos(\phi) * \cos(\theta) * \cos(\omega) + \sin(\theta) * \sin(\omega)) + \sin(Q) * \cos(\omega) * \sin(\phi)$$

Motivation:

- Out-of-plane momentum must be tuned by changing photon energy
- Lab-based plasma-discharge lamps typically available as UV photon sources provide a few discrete photon energies
  - Photon energies correspond to different plasma emission lines
- There is difficulty when determining location in momentum space without quickly comparing to theory
- Out-of-plane momentum can be calculated using:

$$k_z = \sqrt{(0.262468 * (KE + v_0)) - (k_x^2) + (k_y^2)}$$

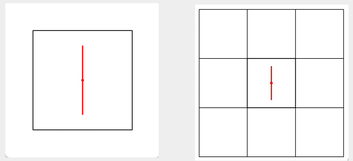
Proposed Solution:

- Integration tool that allows user to easily and quickly compare the computed band structures from theory to ARPES data collected in real time
  - Ability to reference the location of the cut through the fermi surface of ARPES data in 3D momentum space

Methods

Igor Pro and Blue Zone:

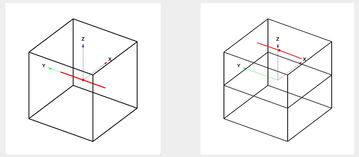
- Igor Pro Software was used to modify PARADIM ARPES collection tool Blue Zone



- BlueZone shows the current cut in reference to the Brillouin zone when provided with angles or momentums

Blue Zone 3D:

- Blue Zone was modified to Blue Zone 3D to determine location during measurements



- Shows the cut in 3D momentum space given the inner potential (V_0) or out-of-plane momentum is provided

Density Functional Theory (DFT):

- DFT data collected by theorists Betul Pamuk and Sri Gudivada
  - Quantum Espresso software used to simulate the electronic structure of $SrVO_3$

Benchmark Study Material:

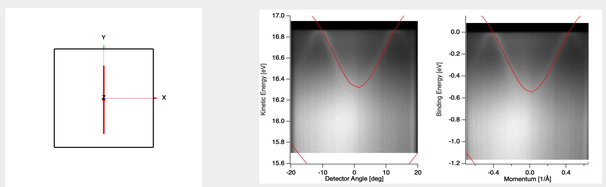
- $SrVO_3$
  - cubic symmetry
    - states share 3D behavior
  - ARPES data previously collected by Brendan Faeth

Results

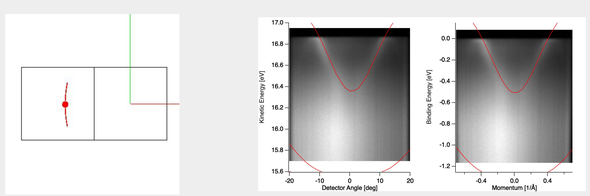
Helium Photon Energy (He-I 21.2 eV):

This photon energy is the cut in the middle of the $SrVO_3$ Fermi surface

Cut A: band should be visible since it is a cut through the middle of the surface



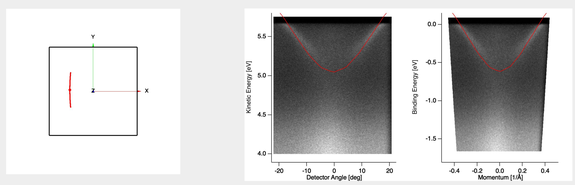
Cut B: band should also be visible, since cut A is in the middle of the Fermi surface and Strontium Vanadate has cubic symmetry.



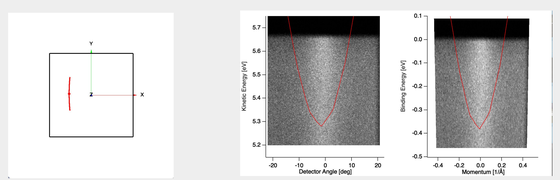
Krypton Photon Energy (Kr-1 10.03 eV):

This photon energy is the cut on the edge of the $SrVO_3$ Fermi surface

Cut A: band should be visible since it cuts through part of the Fermi surface



Cut B: band shouldn't be visible, since cut A is at the edge of the Fermi surface cut B will be off of the Fermi surface.



Conclusions and Next Steps:

Conclusions:

- Comparison between the ARPES and DFT data in real time
- Ability to determine location in 3D space while taking measurements

Next Steps:

- Continued challenge to find the necessary out-of-plane momentum that would create a fit for all of the photon energies
  - New capability must be added to the software suite to find correct fit
    - Allows for the viewing of multiple sets of data simultaneously
    - Ability to adjust parameters at the same time

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References

- "Igor Pro Version 8 ." *WaveMetrics*, 26 Feb. 2019, https://www.wavemetrics.net/doc/igorman/IgorMan.pdf.