Introduction to research background

Chengyu Fang

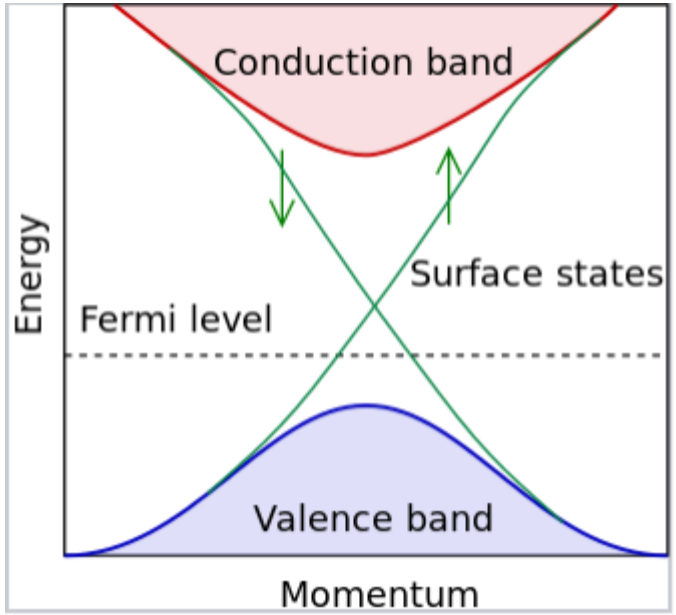
ShanghaiTech University

ARPES Group Research Experience

- Used ARPES experiments data to demonstrate the band structure of materials
- Used ARPES beam line in National Synchrotron Radiation Laboratory(NSRL) to study Topological Insulator(TI) with group members.
- Simulated Synchrotron light after the focus of zone plate to design the pattern of zone plate in Shanghai Synchrotron Radiation Facility(SSRF).

What is ARPES and Topological Insulator(TI)

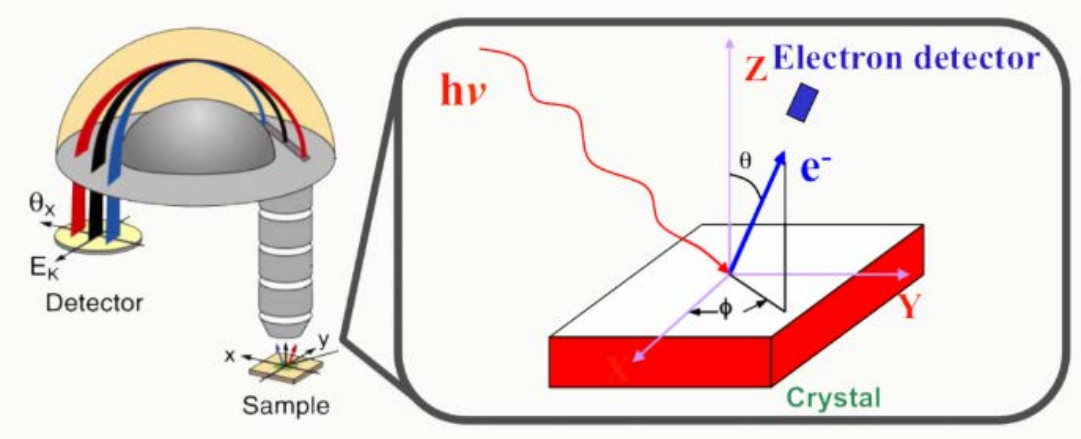
- ARPES: It's a direct experimental way to detect the electronic structure of the solids in reciprocal space.
- Topological Insulator: It's a kind of material which is intrinsically insulating in the bulk but conducting on the surface. The reason why it's conductive on the surface is the existence of surface state.



From Wikipedia: https://en.wikipedia.org/wiki/Topological_insulator

What Is ARPES

ARPES Instrument Sketch Map



From Stanford Shen's Laboratory Webpage

Theory

- Conservation of Energy

$$E = \hbar\omega - E_B - \phi$$

$\hbar\omega$is the incoming photon energy

$E_B$is the binding energy

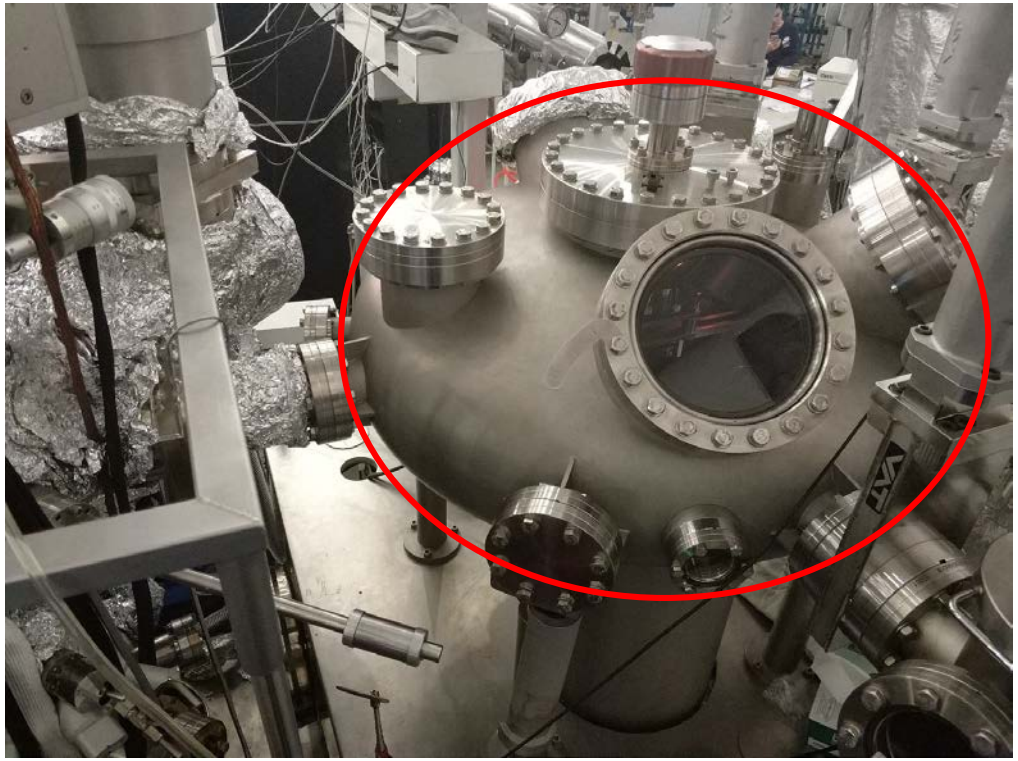
$\phi$is the electron work function

- Conservation of Momentum along the surface of material

$$\hbar k_{crystal} = \hbar k_{vacuum} = \sqrt{2mE}\sin\theta$$

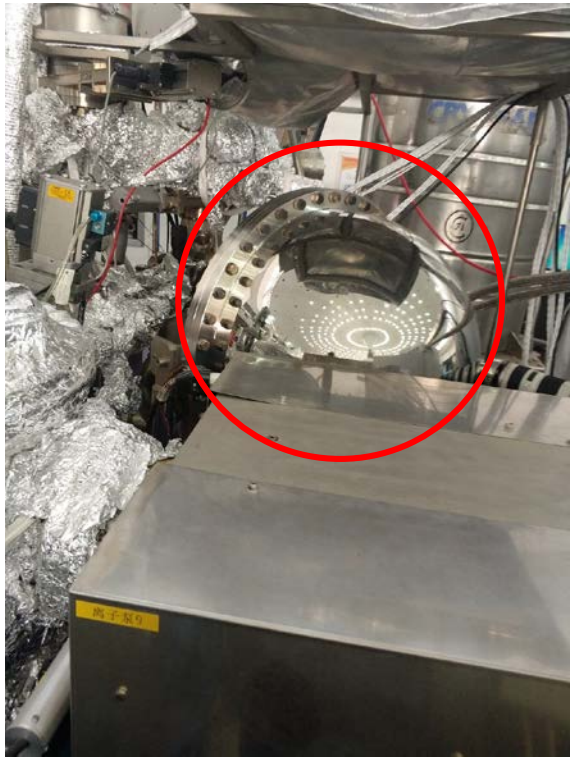
What is ARPES

- Practical AREPS Instrument in Hefei NSRL beam line station



Magazine

Main Chamber



Semi-Sphere Analyzer

What I Did In NSRL Experiment

- **I analyzed the ARPES data independently.**
- Take Bi2Te3(Topological Insulator) as an example to show what I did

The original data contains: 2 Angles, Energy, Intensity of the electrons

Step1: Transfer the degree information into the momentum(k) info.

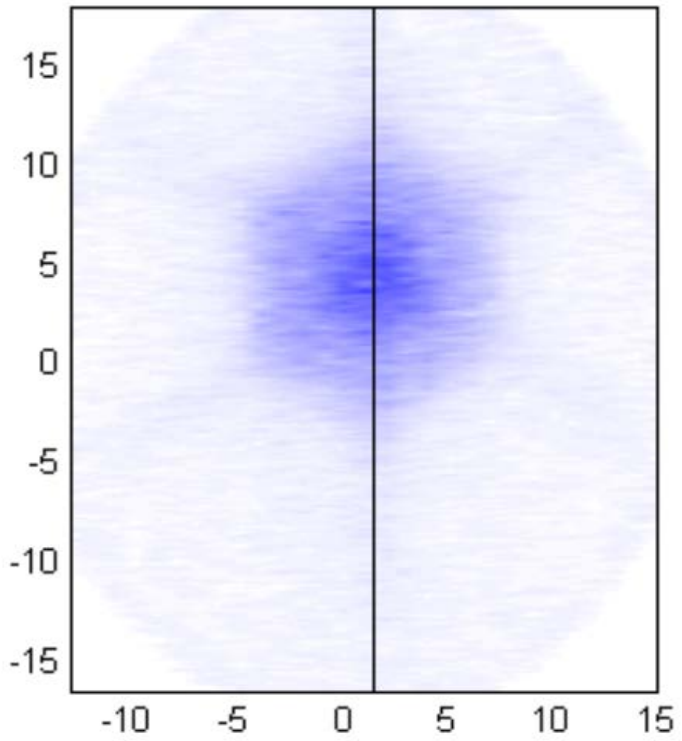
k_x and k_y: The energy and degree can tell us the momentum of electrons along the surface of the material.

k_z: We can change the energy of the photon to detect the momentum in z direction.

Step2: Plot every single point on the $k_x - k_y$ coordinate

What I Did In NSRL Experiment

Result of Step1 and Step2

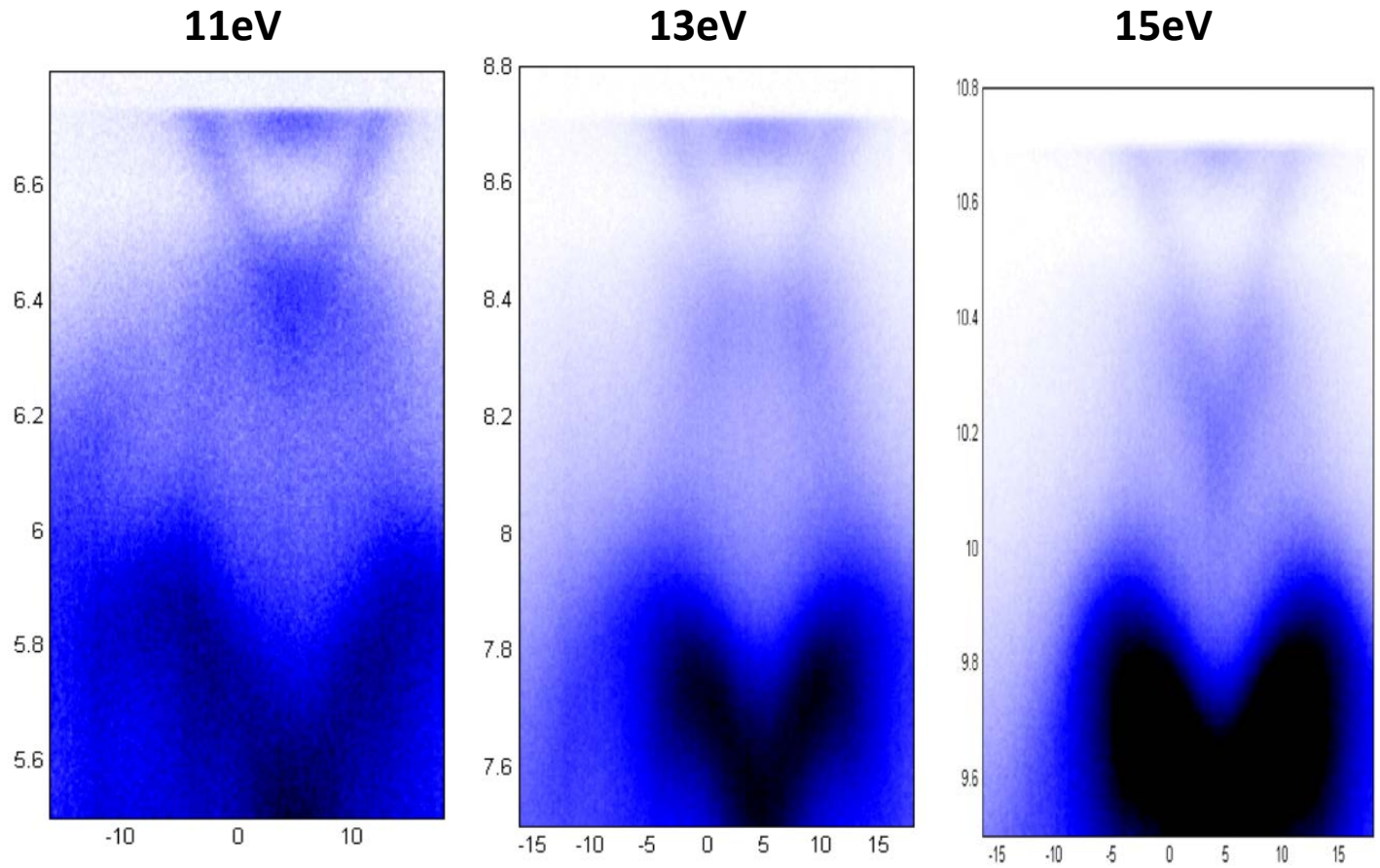


DA30map 19eV
G-M

- **Step3:** Decide the position of the gamma point by looking at the symmetry properties of the figure. The Gamma point locates at the symmetric center.

What I Did In NSRL Experiment

- **Step 4:** Use the energy data directly from the original data and then get the E – k relationship.
- **Step 5:** Repeat Step1 to Step4 with a different photon energy.



What is Zone Plate(ZP)

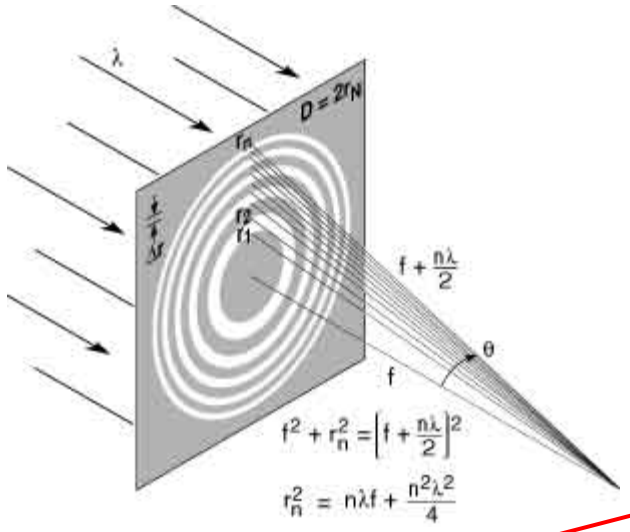
- Zone plate is an optical device used to focus light. Unlike general lenses or curved mirrors however, zone plates use diffraction instead of refraction or reflection.

- Why do we use ZP but not general lenses in Synchrotron ARPES?

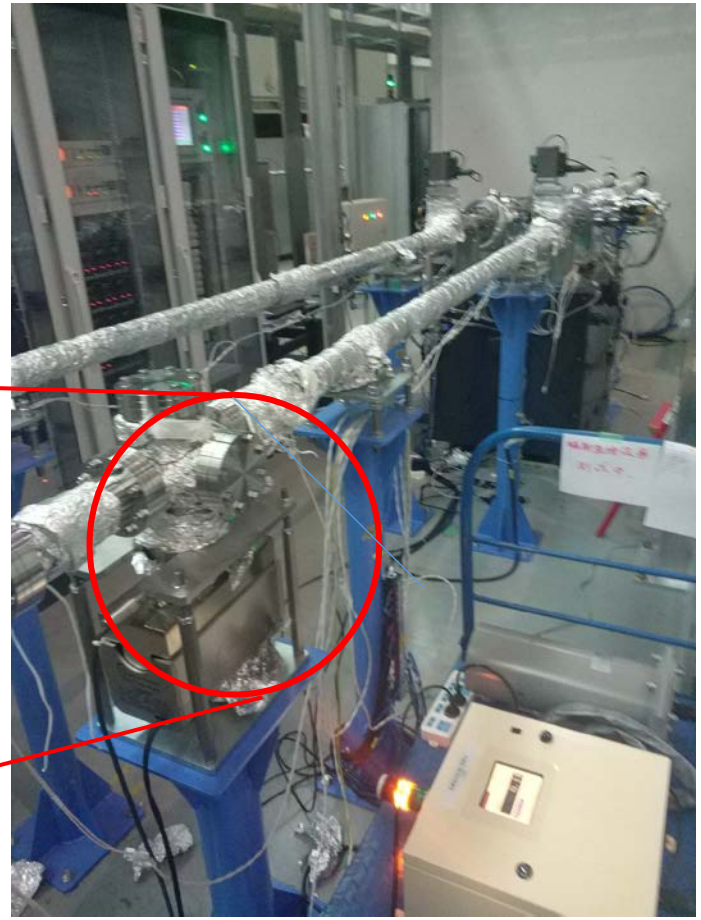
The energy of the outgoing photon of the Synchrotron is extremely high. We know the higher the energy is, the higher the frequency is. According to the dispersion relationship, the refractive index is extremely high. So it’s hard to produce this kind of lens.

What I Did In SSRF ARPES Construction

- Simulated the behavior of the light after inserting the zone plate in light path.



From http://xdb.lbl.gov/Section4/Sec_4-4.html

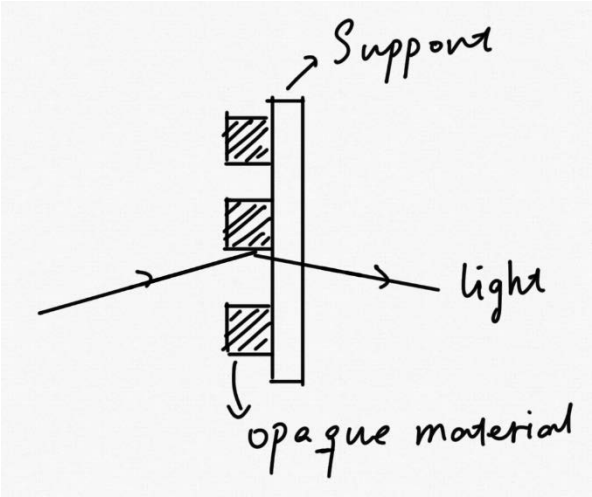


Beam line in SSRF

What I Did In SSRF ARPES Construction

Simulation details

- Consider the thickness of the zone plate which induces the reflection and absorption on the wall
- Consider the existence of the support of the zone plate so that the empty part of the zone plate is not totally transparent



Sketch for the practical zone plate

Photoelectron Lab Research Experience

- Used the Density Functional Theory(DFT) to calculate band structure of semiconductors Si and GaAs with Local Density Approximation(LDA) and HSE hybrid functional
- Calculated the band structure of AlInAsSb digital alloy to predict the property of Avalanche Photodiode (APD)
- Ongoing: Calculation of the electron-electron scattering rate of AlInAsSb digital alloy

What is Density Functional Theory(DFT) and Tight Binding Model(TBM)?

- Both of DFT and TBM are calculation methods to get the electronic structures of the solid-state material.
- DFT: If we know the distribution of the electrons, then we can use the functional we assumed to calculate the energy of the system. By minimizing the system's energy, we can get the distribution of the electrons and then get the electronic structure. As for the functional, we have different assumptions like LDA and HSE hybrid functional.
- TBM: Using an approximate set of wave functions based upon superposition of wave functions for isolated atoms located at each atomic site.(It's bad for metal. It can be used in quasiparticle calculation)

Why Do We Study the AlInAsSb Digital Alloy's electronic structure?

- Experiment shows that AlInAsSb digital alloy has low noise factor.
- Excess noise factor of APD is a function of carrier ionization ratio k.

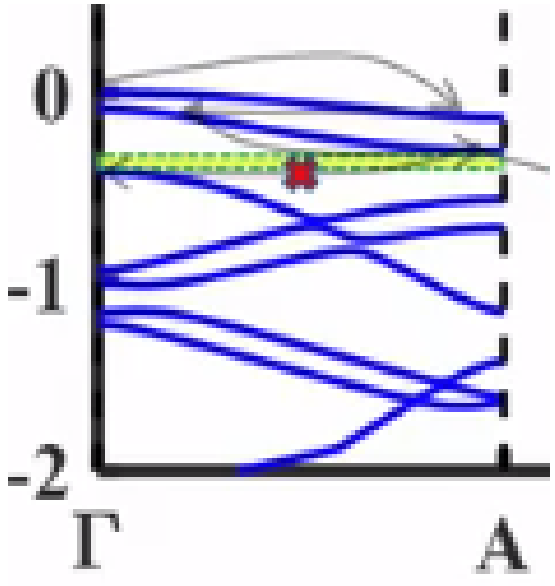
$$k = \frac{probability(hole\ ionization)}{probability(electron\ ionization)}$$

- The band structure of the material can reveal the properties of impact ionization of the material.
- I used the DFT theory to calculate the band structure of the digital alloy. Also the band structure is useful for my ongoing scattering simulation project.

AlInAsSb digital alloy Band structure Calculation

- I used HSE hybrid functional to calculate the AlInAsSb then get a more obvious mini gap in the valence band.(The result in the RHS is calculated by Tight Binding Model.)

The low-noise characteristic of the APD is a consequence of the existence of a mini gap in the valance band



From Joe C. Campbell, Seth R. Bank,
"Low-noise, digital-alloy avalanche photodiodes,"