Instructions for the advanced lab course

Angle-resolved photoelectron spectroscopy

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1 Introduction

Modern physics aim at a fundamental understanding of macroscopic phenomena in terms of microscopic processes. The phenomena to be explained by condensed matter physics include electric conductivities of different materials varying by orders of magnitude, or their vastly different optical properties. The underlying electronic properties are described within the formalism of quantum mechanics. In case of crystalline solids, the result is an electronic band structure. Electronic states are characterized by two quantum numbers, their band index and their crystal momentum. The band structure is directly experimentally accessible through angle-resolved photoemission spectroscopy (ARPES). ARPES uses UV light to photoemit electrons from the surface of a solid. These electrons are detected with energy and angular resolution. Energy and momentum conservation then allow to reconstruct the electronic band structure of the surface. In the lab course, you will apply ARPES to graphene, a two-dimensional material, in which the electronic structure can be fully reconstructed.

2 References

The Zulassungsarbeit provides both the background on the theoretical and experimental concepts required to conduct the experiment. Additional literature on photoelectron spectroscopy, surface science, and solid state physics can be found in the following references:

1. Max Ünzelmann: *Aufbau und Charakterisierung eines Versuchs für das physikalische Praktikum für Fortgeschrittene - Angle-Resolved Photoemission Spectroscopy*. Zulassungsarbeit, Universität Erlangen-Nürnberg, 2015 (German). All theoretical and experimental information of this experiment.


3. Harald Ibach and Hans Lüth: *Solid-State Physics: An introduction to
3 Preparation

Please prepare a written manuscript that covers the points listed in Sec. 3.1 to 3.3.

3.1 Basics of Condensed Matter Physics

- **Crystal structure**: real space and reciprocal space, first brillouin zone
- **Band structure**: Bloch theorem, $k$-vector
- **Graphene**: atomic and electronic structure, unit cell, Brillouin zone, band structure
3.2 Photoelectron Spectroscopy

- **General description**: photoelectric effect, kinetic energy, binding energy, work function

- **Angle-resolved photoelectron spectroscopy**: determination of $\vec{k}_\parallel$, conservation of $\vec{k}$

- **Experimental implementation**: generation of ultrahigh vacuum, hemispherical electron analyzer, preparation of samples in ultrahigh vacuum

- **Determination of the band structure from experimental spectra**

3.3 Band Structure of Graphene

As you can see from Fig. 1, the photoemission intensity has maxima around the K and M points. Only this part of the band structure will be measured within the lab course. Estimate the angular range required to cover $1.2 \, \text{Å}^{-1} \leq |\vec{k}_\parallel| \leq 1.8 \, \text{Å}^{-1}$. Assume a sample work function of 4.1 eV.

![Figure 1: Band structure of graphene as measured from ARPES. From Ref. 5.](image)

**Figure 1**: Band structure of graphene as measured from ARPES. From Ref. 5.
4 Experimental Instructions

1. **Orientate the sample.** LEED will be used to laterally orientate the sample. A rotational feedthrough allows to rotate the sample around its surface normal. Place the sample in front of the LEED optics. Switch on the supply of the LEED system. Slowly increase the filament current to 4.2 A (emission current \( \approx 70 \, \mu A \)), set the screen voltage to 6 kV, and the energy to 75 eV.

Describe the diffraction pattern. To prepare the sample for ARPES measurements along the \( \Gamma M \)-direction, rotate until this direction is aligned horizontally. Sketch the resulting LEED pattern. Describe the procedure in your lab book. To switch off the LEED system, slowly decrease the filament current. Turn off the screen voltage, then the main power of the supply.

2. **Optimize the sample positioning.** Place the sample in front of the light source. Light the He gas discharge lamp (tutor!). You should see a light spot on the sample. If you do not, move the sample until the light spot is centered on it. Move the analyzer around the sample to \( \phi = 130^\circ \) (figure 2). In this position, both the angle of incidence and emergence amount to 40°. Look through the window, at which the reflected beam is expected, and turn the sample until you see the reflected light spot through the slit in the analyzer. Note the angle of the sample.

Turn on the analyzer control. Enter the parameters that are set on the control (\( E_{\text{Pass}} \), Sweep, Offset) into the software. Take a first spectrum with a short integration time using the following settings: Startenergie = \(-1\) eV, Endenergie = 18 eV, Schrittweite = 0.1 eV. Pick an energy at which the count rate is high. Use the software to set the detector to this energy. Note the count rate on the rate meter in the rack. Set the rate meter to a reasonable sensitivity. Position the sample to maximize the count rate.
3. **Start the UPS-Measurement.** Record ARPES spectra of the π-band of graphene in the proximity of the M-point. (What is it that complicates observing other parts of the band structure of graphene?) In your preparation you calculated the corresponding range of photo-emission angles. Take a spectrum every 5°. Note that the reading gives the angle between the measured direction of emission and the axis of the transfer rod. The analyzer detects electrons emitted along the surface normal when the scale reads 90°, as illustrated in Fig. 2. **Never move the analyzer to more than 190°!**

The measurement parameter should be **Integrationszeit = 2000 ms** and **Schrittweite = 0.02 eV**. Save each spectrum (the software will open the window for that). Create a new folder with your group number. The software will write the data into textfiles. Choose the file name $M_{deg50}$ for the 50° spectrum recorded at a polar angle of 50° along the $\Gamma M$ direction. Use this nomenclature consistently for the other emission angles, and the $\Gamma K$ direction, respectively.

4. **Measure the $\Gamma K$-direction.** Switch off the analyzer supply. Make sure that the channeltron high voltage is off. Position the sample in front of the LEED optics again. Switch on the LEED supply and rotate the sample until the $\Gamma K$ direction is aligned with the measurement plane. Repeat the optimization of the counting rate.

Then start the UPS measurement. In analogy to the $\Gamma M$ direction (paragraph 3), take spectra in the range you calculated before. Use the same angular spacing, integration time, and step width as you did along the $\Gamma M$ direction.
5. **Measurement of the work function.** To calculate the sample work function, you need to measure the width of the spectrum (Why?). You already measured the Fermi edge (the high-energy cutoff) of the spectrum. Now, in addition, measure the low-energy cutoff of the spectrum in normal emission.

5 **Analysis**

- Plot the spectra (count rate as a function of kinetic energy). To determine peak positions $E_Z$, use a Gaussian fit with a linear background:

$$I(E_{kin}) = A \cdot e^{-(E_{kin}-E_Z)^2} + B \cdot E_{kin} + C$$

Select reasonable start parameters manually.

- Now determine the binding energy $E_{Bin}$ and the wave vector $\vec{k}_\parallel$ of each peak in the spectra. Plot the resulting band structure $E(k_\parallel)$ along both high symmetry directions.

- Calculate the position of the M and K-points. Indicate them in the plots.

- Fit a linear function to the band structure in the vicinity of the K-point. Calculate the Fermi-velocity $v_F$ from the fit and determine the distance between the Dirac-point and the Fermi level. What is the origin of this difference?