

Course Synchrotron radiation
Topic of project: Angle resolved photoelectron spectroscopy (ARPES).
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Introduction

This report is a partial requirement to pass the synchrotron radiation course, and describing about the Angle resolved photoelectron spectroscopy (ARPES) in short. This is a spectroscopic technique used to find bulk and surface electronic structure of materials. In the following the technique is briefly described with some experimental examples.

Angle resolved photoemission spectroscopy

(ARPES), also known as ARUPS (angle resolved ultraviolet photoemission spectroscopy), is a direct experimental technique to observe the distribution of the electrons (more precisely, the density of single particle electronic excitations) in the reciprocal space of solids. ARPES is one of the most direct methods of studying the electronic structure of the surface of solids¹. The schematic of experimental setup is shown in Fig. 1.

Theory:

In ARPES incident photons with a well-defined energy, $h\nu$ and polarization are directed towards the sample with an angle of incidence, θ_i measured from z-axis (not shown in fig.1). The azimuthal angle, ϕ , is usually selected such that a high symmetry direction of the crystal lies with in the plane of detection. The kinetic energy, E_k , of the emitted electrons is measured by the electron analyzer at various emission angles, θ .

Using the energy conservation law,

$$E_f - E_i = h\nu \quad (1)$$

Where $E_f = E_k + \phi$, then

$$E_k + \phi - E_i = h\nu \quad (2)$$

Using the equation $E_k = h\nu - E_B - \phi$ we have

$$E_k + \Phi - h\nu = E_i = -E_B \quad (3)$$

E_k = kinetic energy of the outgoing electron — can be measured.

$h\nu$ = Incoming photon energy — known from experiment.

Φ = electron work function (energy required to remove electron from sample to vacuum)
— can also be measured.

$E_i = -E_B$ binding energy of electron.

Therefore it is possible to find out information about E_k (energy of K).

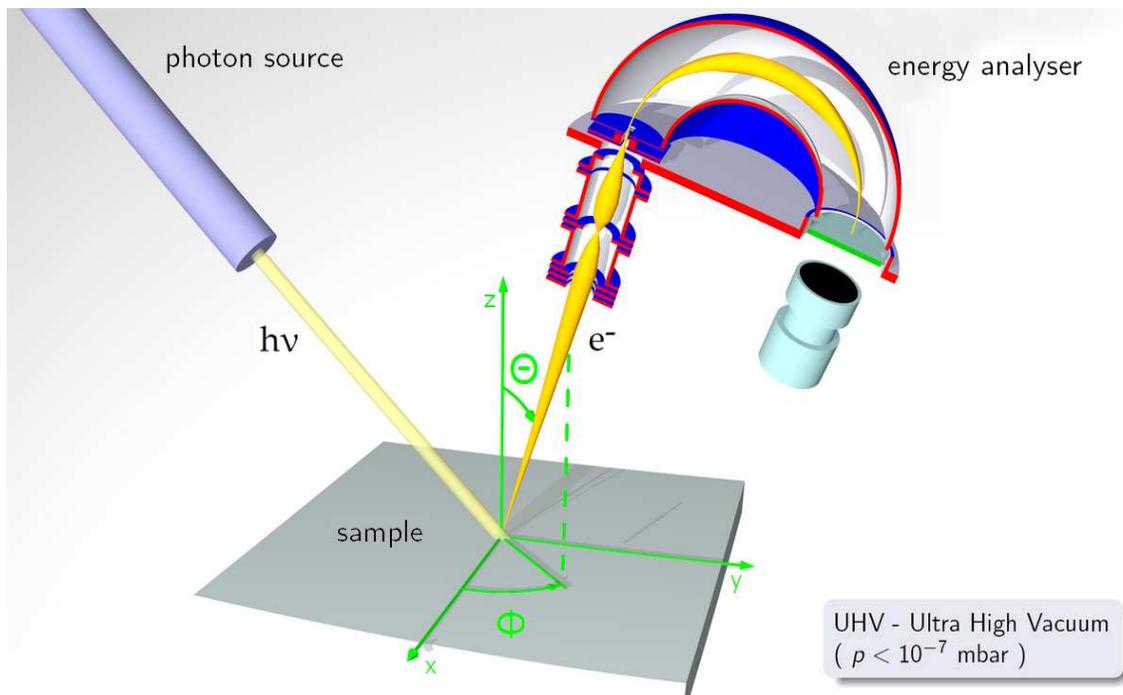


Figure 1 Schematic description of angle resolved photoelectron spectroscopy setup.¹

Experimental examples

A series of angle resolved photoemission spectra of a **Mo**(001) single crystal surface is shown in Fig.2. The **Mo**(001) surface is known to show surface reconstruction from a (1x1) to an incommensurate c(2.2x2.2) phase upon cooling below $T_c=230\text{K}$. By analyzing the photoelectron spectra, changes in the electronic structure, which are related to the surface reconstruction, could be measured. The photoelectron spectra in the figure were collected at $T=52\text{K}$ and with K_{\parallel} along the surface S axis. The spectra consist of

surface states(S_1), surface resonance states(SR_1 , SR_2) and bulk valence band states(B_1). Two-dimensional Fermi-surface contours can be obtained by determining the Fermi wave vector $k_{II}(E_F)$ at which S_1 crosses the Fermi level.²

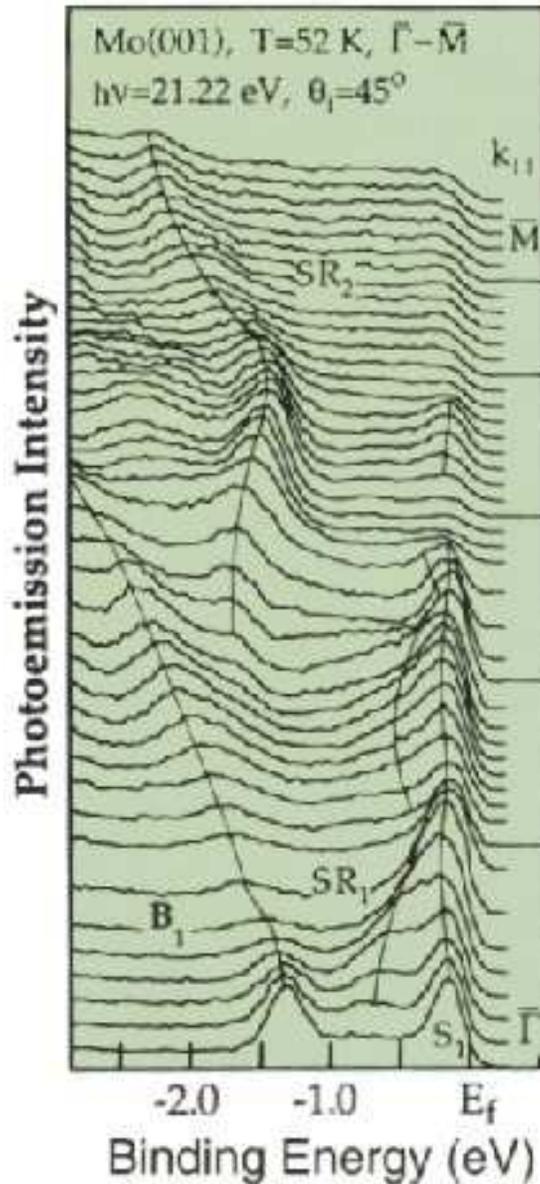


Figure 2 series of angle resolved photoemission spectra of a **Mo(001)** single crystal surface.²

In the following Fig. 3 another example of ARPES of $\text{Si}(001)2 \times 1\text{-K}$ surface is shown. In which ARUPS spectra were measured for both the clean and K deposited samples. Fig. 3a and 3b show representative ARUPS spectra of the saturation $\text{Si}(001)2 \times 1\text{-K}$ surface measured at the polar angles θ along (110) and (010) directions, respectively: Incident

light is at 45° along the opposite azimuth. For each spectrum, the cleaning and K deposition was carried out each time since the surface appeared rather unstable.³

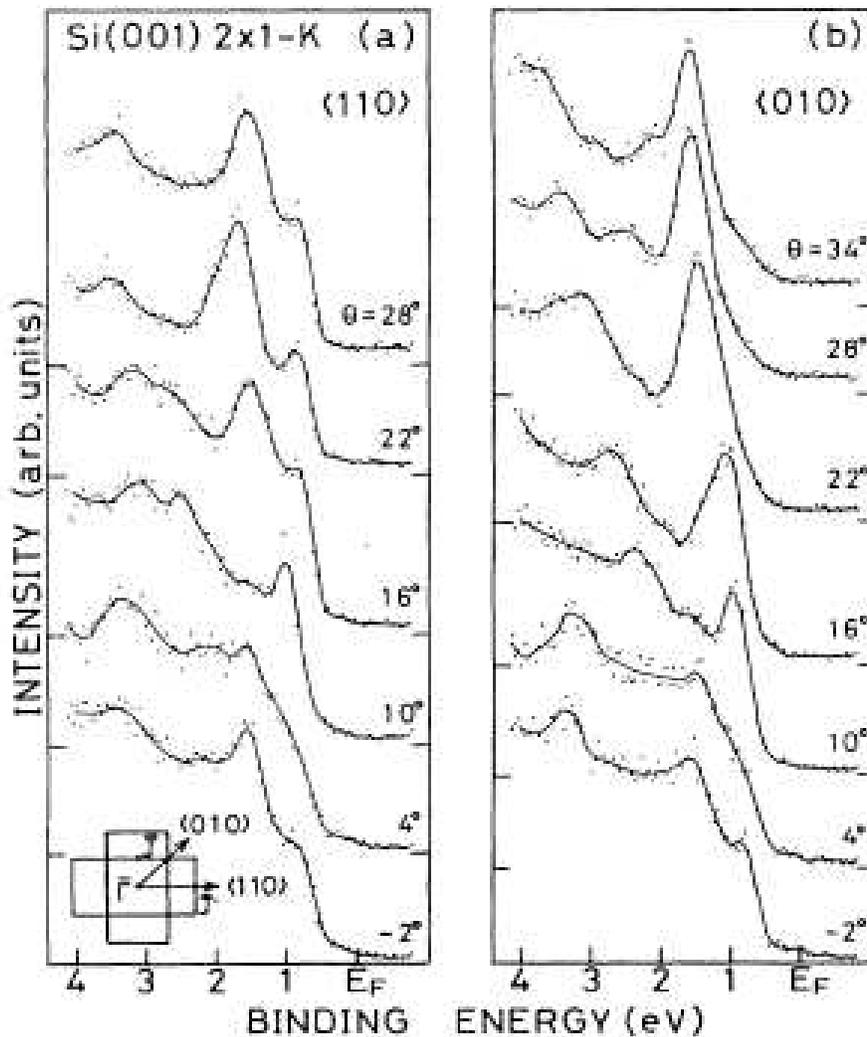


Figure 3 ARUPS spectra of the saturation Si(001)2x1-K surface as a function of polar angle θ . Azimuths are along (a) (110) and (b) (010) directions. Inset shows relation to two-domain 2x1 surface Brillouin zone.³

Reference:

- 1) www.wikipedia.com
- 2) <http://pfwww.kek.jp/index.html>
- 3) Y. Enta, T. Kinoshita, S. Suzuki, and S. Kono, Physical review B, Vol. 36, Number 18 (1987).