

## Short Communications

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### The *k*-space components of a photoelectron from an arbitrarily oriented crystal face

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A standard rotational matrix method is described for determining the *k*-space components of photoelectrons emitted from a crystal surface, which is arbitrarily oriented with respect to the experimental frame. This simplifies the analysis of angle-resolved photoemission data from a crystal surface not aligned to the experimental chamber axes.

**Keywords:** angle-resolved UV photoelectron spectroscopy; angle-resolved photoemission; *k*-space components; ARUPS data analysis.

#### 1. Introduction

Angle-resolved UV photoelectron spectroscopy (ARUPS) is a powerful bandmapping technique. Although not requiring synchrotron radiation, a synchrotron source is commonly used to provide the exciting radiation as it produces relatively high intensity light in the VUV range. It is also highly plane polarized and may be frequency selected.

#### 2. Theory

The mean elastic scattering length of UV photoelectrons ( $\approx 10$ – $100$  Å) (Seah & Dench, 1979) makes the spectroscopies performed at these energies very sensitive to surface contamination. Various methods are used to ensure that the surface of the sample is clean (Woodruff & Delchar, 1986). When performing ARUPS from single crystals, cleaving is often used to present a clean surface to the light source. The surface orientation after cleaving may be arbitrary with respect to the experimental axes. The ARUPS analysis found in the literature (Courths & Hüfner, 1984; Plummer & Ehardt, 1982) usually assumes that the experimental and crystal-surface normals are coincident, and gives the relations

$$k_{\parallel} = k \sin(\theta), \quad (1)$$

and

$$k_{\perp} = \{(2m^*/\hbar^2)[E_{\text{kin}} \cos^2(\theta) + E_v]\}^{1/2}, \quad (2)$$

where  $E_{\text{kin}}$  is the kinetic energy of the photoelectron,  $E_v$  represents the energy at the bottom of the nearly free electron band relative to the vacuum level,  $k$  is the momentum of the photoelectron,  $k_{\parallel}$  is the momentum component parallel to the surface,  $k_{\perp}$  is the momentum component perpendicular to the surface,  $\theta$  is the angle between the perpendicular axis and the electron direction, and  $m^*$  is the effective mass of the photoelectron in the crystal. However, this condition may not generally be true.

In Fig. 1, a diagrammatic representation of an angle-resolved experiment for an arbitrary orientation of the crystal surface and normal axes with respect to the experimental axes is shown. The surface orientation may be represented by the product of three rotation matrices

$$R_i(\alpha)R_j(\beta)R_k(\gamma) = \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{pmatrix}, \quad (3)$$

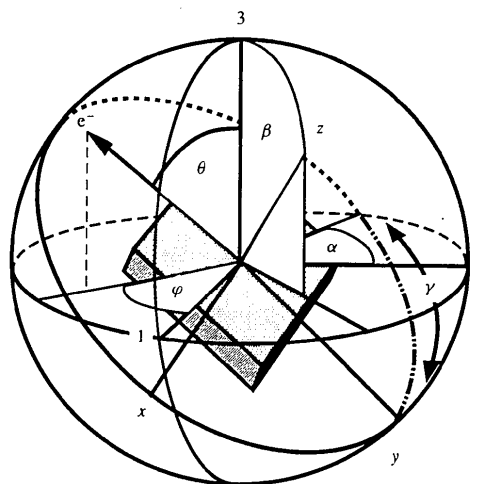
where  $i, j, k = 1, 2$ , or  $3$ , but  $i, k \neq j$ , acting on the experimental axes and  $R_{i,j,k}$  represent rotation matrices about these axes. If  $i = k$  in (3) then this is a Euler-type transformation matrix (Jeffreys & Jeffreys, 1980). The exact form of the  $R_{i,j,k}$  matrices is dependent on how the angles of rotation are defined with respect to the axes. Using the normal convention for rotations (see Fig. 2), this gives

$$R_1(\alpha) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\alpha) & -\sin(\alpha) \\ 0 & \sin(\alpha) & \cos(\alpha) \end{bmatrix}, \quad (4)$$

$$R_2(\beta) = \begin{bmatrix} \cos(\beta) & 0 & \sin(\beta) \\ 0 & 1 & 0 \\ -\sin(\beta) & 0 & \cos(\beta) \end{bmatrix}, \quad (5)$$

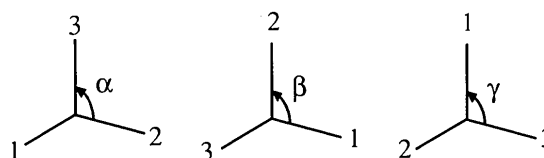
and

$$R_3(\gamma) = \begin{bmatrix} \cos(\gamma) & -\sin(\gamma) & 0 \\ \sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (6)$$



**Figure 1**

Diagrammatic representation of an ARUPS experiment. 1, 2 and 3 are the experimental axes, *x*, *y* and *z* the crystal surface and normal axes, and  $\alpha$ ,  $\beta$  and  $\gamma$  indicate the actions of  $R_3$ ,  $R_2$  and  $R_1$ , respectively.  $\theta$  and  $\varphi$  are the directions of the outgoing photoelectron,  $e^-$ , relative to the experimental axes.



**Figure 2**

The normal convention used for rotational transformations with respect to the axes.

The matrix for the transformation in Fig. 1 using (6) and (5), for example, gives (3) as

$$R_3(\alpha)R_2(\beta)R_3(\gamma) =$$

$$\begin{bmatrix} c(\alpha)c(\beta)c(\gamma) - s(\alpha)s(\gamma) & -c(\alpha)c(\beta)s(\gamma) - s(\alpha)c(\gamma) & c(\alpha)s(\beta) \\ s(\alpha)c(\beta)c(\gamma) + c(\alpha)s(\gamma) & -s(\alpha)c(\beta)s(\gamma) + c(\alpha)c(\gamma) & s(\alpha)s(\beta) \\ -s(\beta)c(\gamma) & s(\beta)s(\gamma) & c(\beta) \end{bmatrix},$$

where  $s = \text{sine}$  and  $c = \text{cosine}$ .

The momentum of the photoelectron is conserved parallel to the surface (Plummer & Ebhardt, 1982). Therefore, using (3),

$$k_x = \sum_{i=1}^3 k_i r_{i1}, \quad (7)$$

and

$$k_y = \sum_{i=1}^3 k_i r_{i2}, \quad (8)$$

where  $k_{1,2,3}$  represent the components of  $\mathbf{k}$  along the experimental axes. However,  $\mathbf{k}$  perpendicular to the surface is not conserved; therefore, using the nearly free electron model for the final state band in the material gives

$$k_z = \left\{ (2m^*/\hbar^2) \left[ \left( \sum_{i=1}^3 k_i r_{i3}/\mathbf{k} \right)^2 E_{\text{kin}} + E_v \right] \right\}^{1/2}. \quad (9)$$

Therefore, the components of  $\mathbf{k}$  are determined in the three-dimensional Brillouin zone of an arbitrarily oriented crystal. These relations are a refinement of (1) and (2) that allow a more natural determination of the experimental error, as the orientational uncertainty may now be included, and their application will allow analysis of investigations that do not pass through the  $\Gamma_{000}$  point of the band structure.

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