# CALCULATION OF ELECTRON ENERGY DISTRIBUTION IN PHOTOEMISSION

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The energy distribution function of electrons, normalized for photon absorption, in photoelectron emission can, in the direct transitions model, be represented in the form

$$N(E,\omega)=\frac{\sum_{n,s}\int d^3\kappa P_n(\kappa)\cdot|M_{ns}(\kappa)|^2\delta(E-E_n(\kappa))\,\delta(E-E_s(\kappa)-\hbar\omega)}{\sum_{n,s}\int d^3\kappa\,|M_{ns}(\kappa)|^2\delta(E_n(\kappa)-E_s(\kappa)-\hbar\omega)}, \tag{1}$$

where n, s are band indices; E is the electron energy; $\hbar\omega$ is the photon energy; $M_{ns}$ are matrix elements of optical transitions; $P_n(\kappa)$ is the transition probability; the integration is carried over the Brillouin zone.

To calculate integrals of the type $K(E)=\int d^3\kappa F(\kappa)\delta(E-E(\kappa))$, Gilat and Raubenheimer [1] proposed a simple and effective method. The idea is to divide the irreducible part of the Brillouin zone into elementary cells in each of which a linear interpolation is used for the functions $F(\kappa)$, $E(\kappa)$, which makes it possible to carry out the integration over each cell analytically. In earlier papers, cubes, or, more generally parallelepipeds, were selected as the cells. With such a choice, the integral over the cell is expressed in terms of the values of the functions $F(\kappa)$, $E(\kappa)$ at its corners and of $\nabla_\kappa E(\kappa)$ in the center of the cell. The Gilat–Raubenheimer method was also applied to the calculation of integrals of the type

$$I(E,\omega)=\int d^3\kappa F(\kappa)\,\delta(E-E(\kappa))\,\delta(\omega-\omega(\kappa)). \tag{2}$$

Thus, in [2], expressions are derived for the contribution to the integral $I(E,\omega)$ of a cell in the shape of a rectangular parallelepiped. At the same time, in the cell four regions are distinguished in which the integral is represented in the form of different analytical expressions.

Later, Jepson and Anderson [3], and independently Lehmann and Taut [4], proposed the selection of cells in the shape of tetrahedra. Such a partition of the Brillouin zone has a number of merits of which we shall only mention the fact that the necessity of calculating $\nabla_\kappa E(\kappa)$ drops out. In [4, 5] simple analytical expressions are derived for the contributions of a tetrahedron to the integral $K(E)$. However, no similar expressions for the integrals $I(E,\omega)$ are cited in the literature. The present communication is concerned with the derivation of the contribution of a tetrahedron to the integral $I(E,\omega)$.

The integral (2) can be represented in the form

$$\int_L\frac{F(\kappa)}{|\nabla_\kappa E(\kappa)\times\nabla_\kappa\omega(\kappa)|}\,dl=\sum_t\int_{L_t}\frac{F(\kappa)}{|\nabla_\kappa E(\kappa)\times\nabla_\kappa\omega(\kappa)|}\,dl. \tag{3}$$

Here L is the intersection line of the surfaces $E(\kappa)=E$ and $\omega(\kappa)=\omega$ in the reciprocal space; $L_t$ is the part of the line L enclosed in the tetrahedron numbered t; the summation is carried out over all the tetrahedra in the irreducible part of the Brillouin zone.

Let the vectors $\kappa_i$ ($i=0,1,2,3$) denote the positions of the vertices of a tetrahedron. We assume that the angular magnitudes $E(\kappa_i)\equiv E_i$, $\omega(\kappa_i)\equiv\omega_i$, $F(\kappa_i)\equiv F_i$ are known. Inside the tetrahedron we approximate the surfaces $E(\kappa)=E$, $\omega(\kappa)=\omega$ by the planes

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$$E_0 + a(\kappa - \kappa_0) = E; \quad \omega_0 + b(\kappa - \kappa_0) = \omega, \tag{4}$$

where

$$a = \sum_{i=1}^{3} (E_i - E_0) r_i; \quad b = \sum_{i=1}^{3} (\omega_i - \omega_0) r_i;$$

$$r_1 = \frac{\kappa_{20} \times \kappa_{30}}{v}; \quad r_2 = \frac{\kappa_{30} \times \kappa_{10}}{v}; \quad r_3 = \frac{\kappa_{10} \times \kappa_{20}}{v}; \quad \kappa_{ij} = \kappa_i - \kappa_j;$$

$v = \{\kappa_{10}, \kappa_{20}, \kappa_{30}\}$ is the sixfold volume of the tetrahedron. In the majority of cases the function $F(\kappa)$ can also be interpolated linearly inside the tetrahedron

$$F(\kappa) = F_0 + \nabla_\kappa F(\kappa_0) \cdot (\kappa - \kappa_0). \tag{5}$$

Taking expansions (4) and (5) into account, we obtain for the integral over a single tetrahedron

$$I_t = [F_0 + \nabla_\kappa F(\kappa_0) \cdot (\kappa_y - \kappa_0)] \, l_t, \tag{6}$$

where $i_t = l_t / |a \times b|$; $\kappa_y$ is the vector drawn to the center of the line $L_t$; $l_t$ is the length of this line. Let the vectors $\kappa^t_m$ and $\kappa^t_n$ define the points of intersection of the line $L_t$ with the faces of the tetrahedron. Evidently,

$$\kappa^t_m - \kappa^t_n = i_t \cdot a \times b. \tag{7}$$

Expressing vectors $\kappa^t_m$ and $\kappa^t_n$ in terms of $\kappa_{10}$, $\kappa_{20}$, $\kappa_{30}$ and taking into account relations $\kappa_{i0} \cdot r_j = \delta_{ij}$, $r_1 \times r_2 = \kappa_{30}/v$, $r_2 \times r_3 = \kappa_{10}/v$, and $r_3 \times r_1 = \kappa_{20}/v$, we obtain

$$i_t = v \left| \frac{y_{\alpha\beta}}{\sigma_{\alpha\beta\gamma} \sigma_{\alpha\beta\zeta}} \right|. \tag{8}$$

Here,

$$y_{\alpha\beta} = (E - E_\xi)(\omega_\alpha - \omega_\beta) - (E_\alpha - E_\beta)(\omega - \omega_\beta);$$
$$\sigma_{\alpha\beta\gamma} = (E_\alpha - E_\gamma)(\omega_\beta - \omega_\gamma) - (E_\beta - E_\gamma)(\omega_\alpha - \omega_\gamma).$$

The indices $\alpha$ and $\beta$ correspond to the edge adjacent to the intersection face of the tetrahedron with the line $L_t$; $\gamma$ and $\delta$ are the remaining indices of the set 0, 1, 2, 3.

The expression for the integral (6) is reduced to the rather simple form

$$I_t(E, \omega) = \frac{v}{2} \left\{ F_\alpha \left( \frac{y_{\beta\gamma}}{\sigma_{\alpha\beta\gamma}} + \frac{y_{\beta\delta}}{\sigma_{\alpha\beta\delta}} \right) + F_\beta \left( \frac{y_{\gamma\alpha}}{\sigma_{\alpha\beta\gamma}} + \frac{y_{\delta\alpha}}{\sigma_{\alpha\beta\delta}} \right) + F_\gamma \frac{y_{\alpha\beta}}{\sigma_{\alpha\beta\gamma}} + F_\delta \frac{y_{\alpha\beta}}{\sigma_{\alpha\beta\delta}} \right\} \left| \frac{y_{\alpha\beta}}{\sigma_{\alpha\beta\gamma} \sigma_{\alpha\beta\delta}} \right|. \tag{9}$$

If we assume that the function $F(\kappa)$ is a constant equal to $F_m$ in each tetrahedron, the last relation is considerably simplified:

$$I_t(E, \omega) = v \cdot F_m \left| \frac{y_{\alpha\beta}}{\sigma_{\alpha\beta\gamma} \sigma_{\alpha\beta\zeta}} \right|. \tag{10}$$

Let us point out some useful relations:

$$\sigma_{ijk} = -\sigma_{jik} = \sigma_{kij}; \quad y_{ij} = -y_{ji}; \quad y_{ij} = y_{ik} + y_{kj} + \sigma_{ijk}.$$

Let us note that ordering the magnitudes $E_i$ and integrating (9) with respect to $\omega$ within the appropriate limits, we obtain expressions [4, 5] describing the contribution of a single tetrahedron to the integral $K(E)$.

Thus, we have expressed the integrals describing the energy distribution of electrons in photoemission in terms of energy values and matrix elements at a regular grid of points in the Brillouin zone; at the same time the calculation of the energy gradient is not required.

LITERATURE CITED

1. G. Gilat and L. J. Raubenheimer, Phys. Rev., 114, 390 (1966).
2. N. W. Dalton and G. Gilat, Solid State Commun., 12, 211 (1973).
3. O. Jepson and O. K. Anderson, Solid State Commun., 9, 1763 (1971).
4. G. Lehmann and M. Taut, Phys. Status Solidi (b), 54, 469 (1972).
5. G. Gilat and N. R. Bharatiya, Phys. Rev. B, 12, 3479 (1975).

# BANDED STRUCTURE OF FILAMENTARY SILICON CRYSTALS

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Filamentary crystals (FC) of silicon are often produced by the sealed-ampul method [1, 2]. The growth mechanism and structure of the FC thus formed have not yet been sufficiently studied and, therefore, the derivation of new experimental data is of considerable interest.

In the present paper, quartz ampuls 20-25 mm in inner diameter and 15-20 cm long were used in the growth of silicon FC. Silicon of KEF, KDB, and EKDB brands with 1-7.5 Ω•cm resistivity served as parent material. After careful cleaning, the ampul was loaded with up to 1-3 g of silicon and a microampul (1 $cm^3$) with bromine and the doping impurity (phosphorus, antimony, boron, indium, etc.). Following evacuation to $10^{-5}$ mm Hg and sealing off, the ampul was placed in a furnace with a temperature gradient of 50 deg/cm. After some time (15-20 min), the transfer of silicon begins from the maximum temperature zone (1150-1250°C) to a colder zone (850-1100°C). The rate of transfer is determined by the temperature difference of the source and crystallization zones as well as by the bromine concentration. Introducing into the ampuls small hangings of gold, platinum, silver, nickel (0.1-0.5 mg) stimulates the formation of silicon FC, which in 5-6 h may attain lengths of 20-30 mm and a diameter of up to 200 or more microns.

Crystallization begins with the formation of randomly arranged polycrystalline silicon islands of irregular shape which in the course of time are bounded by {111} planes. In the subsequent stages, from the surface of faceted islands, fast growth of FC with diameter from a fraction of a micron to a few microns takes place, each island giving at the outset birth to a large number of FC (up to 100 and more). The growth rate of such FC ("leaders" according to the terminology of [3]) may attain at this stage values of $10^3$-$10^4$ μm/min. Most probably their growth proceeds according to the vapor–liquid–crystal (VLC) mechanism [3], and its initiating impurity is gold (or other metals) being introduced in the source zone and transferred by bromine to the crystallization zone.

The growth of "leaders" is completed in a few minutes. We associate the cessation of their growth with the gradual expenditure of gold in the crystallization process, which is due to its inclusion in the crystal lattice. Next, the outgrowing "leaders" begin slowly to thicken, at a rate of 0.1 μm/min.

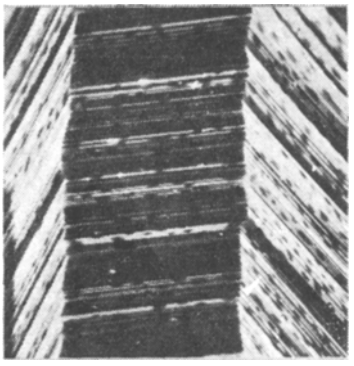

Fig. 1. Growth steps on the side surface of a silicon FC (×1800).

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