Utilization of symmetry of solids in some experiments

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Abstract. It is known that some anisotropic quantities, that describe the properties of solids, can be determined, to a reasonable accuracy, by a limited number of data along the "special directions" (SD). SDs are very useful in various theoretical and experimental investigations. Among other things, they define projections which are the most efficient to reconstruct three-dimensional (3-D) electron momentum densities from Compton scattering spectra. The concept of SDs and their power is illustrated by comparing an isotropic average of the function based on either three high--symmetry directions or even only one, but SD.

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In crystalline solids, having periodicity of the lattice, various physical quantities are invariant under an appropriately selected projection operator, which is a sum (with relevant coefficients) of transformations of the point group of the crystal. In the paper reciprocal lattices and quantities with the full symmetry of the Brillouin zone (BZ) are considered. Examples of such quantities are electronic densities, Fermi surfaces, the effective mass and associated quantities as, e.g. Compton scattering spectra [3, 4]

$$(1) \qquad N(p_z) = \int\int \rho(\mathbf{p}) dp_x dp_y$$

where $\rho(\mathbf{p})$ is the electron density in the extended momentum space $\mathbf{p}$. All these quantities can be expressed as a series of lattice harmonics $F_{l,v}(\theta,\phi)$ of a given symmetry [8, 12]

$$(2) \qquad f(\mathbf{p}) = \sum_{l,v} f_{l,v}(p) F_{l,v}(\theta,\phi)$$

where the index v distinguishes harmonics of the same order, (θ,ϕ) are the azimuthal and polar angles of the direction $\mathbf{p}$ with respect to the reciprocal lattice coordinate system and the $f_{l,v}(p)$ are the radial coefficients of the function $f(\mathbf{p})$. The idea of such an expansion was proposed by Houston [8] and then applied in many papers, e.g. [14], at the beginning to get the isotropic component $f_0(p)$. The task of this paper is quite different. Knowing values of $f(\mathbf{p})$ along a limited number of directions $\mathbf{p}$, reconstruction of $f(\mathbf{p})$ in the whole three--dimensional (3-D) space $\mathbf{p}$ is essential – sometimes its anisotropy is more important than the isotropic part.

This is the case when, e.g. one wants to reconstruct anisotropy of the Fermi surface from a few measured Compton profiles.

As it was discussed in Refs. [5, 6, 12] (which deal with cubic structures), the maximum number of $f_{l,\nu}(p)$ that can be fitted to $f(\mathbf{p})$ without undue loss of precision is equal to the number of data $f(\mathbf{p'})$ only if the $\mathbf{p'}$ are chosen along very particular directions $\mathbf{p'}(\theta,\phi)$, which we call special directions SDs. Such a treatment is approximately equivalent to applying Gaussian quadrature in calculations of the radial functions that occur in the expansion of data into lattice harmonics.

The idea of SDs was introduced by Bansil [1] to reduce 3-D integration of a periodic function of a wave vector $\mathbf{k}$ to one-dimensional (1-D) integral. The next papers [2, 5, 6, 9, 10] were devoted to finding such sets of SDs which allow to reproduce an anisotropy of $f(\mathbf{p})$ too and in all of them, except for Ref. [9], only cubic structures were considered.

In Ref. [10] (also in the present paper) the results were compared with those published in Refs. [1, 2, 5, 6, 9] in the following way. On the basis of functions $f(\mathbf{p})$, known for a limited number of directions $\mathbf{p}(\theta,\phi)$, we are able to determine only a limited number of the expansion coefficients, i.e.

$$(3) \qquad f(\mathbf{p}) = \sum_{l,\nu=0}^{(l,\nu)_{max}} f_{l,\nu}^a(\mathbf{p}) F_{l,\nu}(\theta,\phi)$$

where $f_{l,\nu}^a(p)$ denote the approximated coefficients, which, except for a few functions $f(\mathbf{p})$ used for their determination, describe arbitrary $f(\mathbf{p})$ only with some approximation.

The correctness of their determining, depending on the choice of directions $\mathbf{p}(\theta,\phi)$, can be estimated by interdependencies between a $f_{l,\nu}^a(p)$ and true $f_{l,\nu}(p)$ in the following form:

$$(4) \qquad f_{l,\nu}^a = f_{l,\nu} + \sum_{n,\mu} d_{n,\mu} f_{n,\mu}(p)$$

where the indices $(n,\mu) > (l,\nu)_{max}$ and coefficients d define a deviation of $f_{l,\nu}^a(p)$ from its true value $f_{l,\nu}(p)$ (more details in Ref. [10]). This is illustrated on the example of determining the isotropic component based on three high-symmetry directions, HSD (in the experiment such profiles are usually measured) and three sets of 1-, 2- and 3-SDs, displayed in Fig. 1. In the case of 1-SD all authors ([1, 2, 9]) proposed the same solution – the cross-cut of zeros lines of two first anisotropic harmonics F_4 and F_6, while for 2- and 3-SDs results from Ref. [5] were used.

In the case of three HSD ([100], [110] and [111]), the isotropic average $f_{l,\nu}^a(p)$ was estimated either from
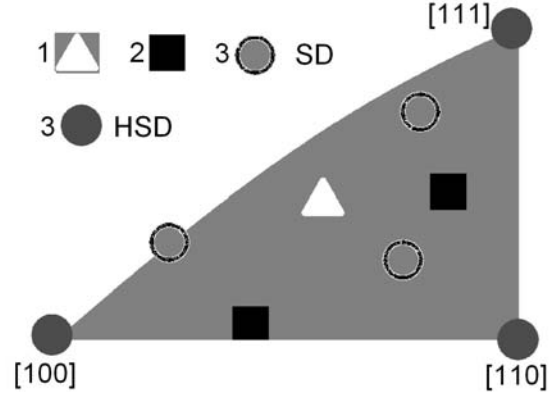

Fig. 1. Stereogram of three sets of SDs described by the following angles (θ,ϕ) 1-SD – (74.54, 26.00); 2-SD – (73.40, 37.99) and (88.24, 19.08); 3-SD – (64.49, 35.34); (79.01, 11.30) and (81.00, 33.68); and three high-symmetry directions marked in the irreducible part of the BZ (in the crystallography so-called asymmetric unit of the BZ).

Eq. (3) (by using standard inversion technique):

$$(5) \qquad f_0^a(p) = [10f_{[100]}(p) + 16f_{[110]}(p) + 9f_{[111]}(p)]/35$$

or the average over these directions was made, i. e.

$$(6) \qquad f_0^a(p) = [f_{[100]}(p) + f_{[110]}(p) + f_{[111]}(p)]/3$$

denoted in Table 1 as 3-HSD$_3$ and 3-HSD$_1$ in connection with using, in Eq. (3), three and one lattice harmonics, respectively.

On the example of 3-HSD we show the way of calculating coefficients $d_{l,\mu}$ defined in Eq. (4) and presented in Table 1. Functions $f_{[100]}(p)$, $f_{[110]}(p)$ and $f_{[111]}(p)$ are expanded into infinite lattice harmonics series according to Eq. (2)

$$f_{[100]}(p) = f_0(p) + 2.2913\,f_4(p) + 1.2748\,f_6(p) \\ + 2.9607\,f_8(p) + 1.8854\,f_{10}(p) + 3.4775\,f_{12.1}(p) + \ldots$$

$$f_{[110]}(p) = f_0(p) - 0.5728\,f_4(p) - 2.0715\,f_6(p) \\ + 1.6654\,f_8(p) - 0.0589\,f_{10}(p) - 0.6419\,f_{12.1}(p) + \ldots$$

$$f_{[111]}(p) = f_0(p) - 1.5275\,f_4(p) + 2.2662\,f_6(p) \\ + 0.8772\,f_8(p) - 2.9794\,f_{10}(p) + 0.2743\,f_{12.1}(p) + \ldots$$

and next inserted into Eqs. (5) and (6).

As can be seen, when anisotropy is such that even the component f_{14} is important, knowing $f(\mathbf{p})$ along 3-SDs [5] allows to reproduce the isotropic component $f_0(p)$ perfectly. Moreover, the results presented in Table 1 show that:

Table 1. Values of the coefficients $d_{l,\mu}$ from $l = 4$ up to $l = 14$ (defined in Eq. (4)) describing the deviations of f_0^a from their true values for two cases of using 3-HSD and three sets of SDs presented in Fig. 1

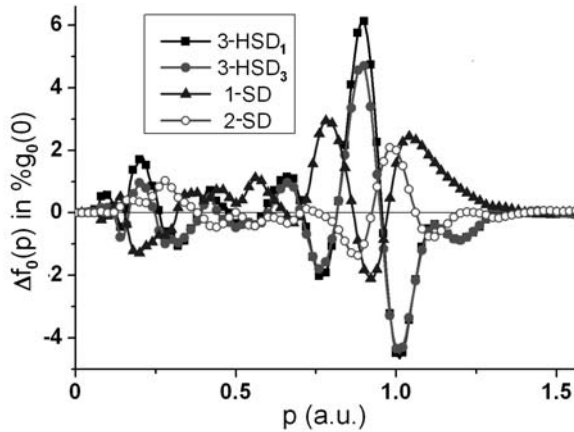| l, μ	3-HSD$_1$	3-HSD$_3$	1-SD	2-SD	3-SD
4	0.064	–	–	–	–
6	0.490	–	–	–	–
8	1.834	1.833	–1.466	–	–
10	–0.384	–0.254	0.977	–	–
12.1	1.037	0.771	0.502	–0.701	–
12.2	–1.663	–1.869	–0.667	1.358	–
14	1.073	0.566	0.784	–0.572	–

Fig. 2. $\Delta f_0(p)$ for the cases described in Table 1 where radial functions $f_{l,\mu}(p)$ correspond to the radial components of electron-positron momentum densities in ErGa$_3$.

1^0 – $f_0(p)$ should be described by the lattice harmonic, i.e. by Eq. (5) instead of (6);

2^0 – 1-SD leads to the same $f_0(p)$ as 3-HSD.

It is worth emphasizing that the way of checking the accuracy of describing any function $f(\mathbf{p})$ by the lattice harmonics series, proposed in Ref. [10] and demonstrated on the example of $f_0(p)$ in Table 1 of this paper is the most objective, because it does not depend on the choice of the approximated function $f(\mathbf{p})$. In order to demonstrate how it may look for real data, in Fig. 2 the quantity $\Delta f_0(p)$ which reads

$$\Delta f_0(p) = f_0^a - f_0 = \sum_{n=4}^{n=12} d_{n,\mu} f_{n,\mu}(p)$$

is shown with using $d_{l,\mu}$ from Table 1 and functions $f_{l,\mu}(p)$ which correspond to radial components of electron-positron momentum densities in ErGa$_3$ presented in Fig. 3 and in Ref. [10]. In this particular case, the use of 1-SD reproduces the isotropic component $f_0(p)$ exceptionally well.

The method of finding SDs, applied in the paper [10], is demonstrated in Fig. 3 on the example of 7-SD. The previous proposal [9] (triangles in Fig. 3) was based on the assumption that the best way of determining SDs is to choose such zeros of the first omitted harmonic which, first of all, are more or less equally spaced and secondly are close to zeros of the second neglected
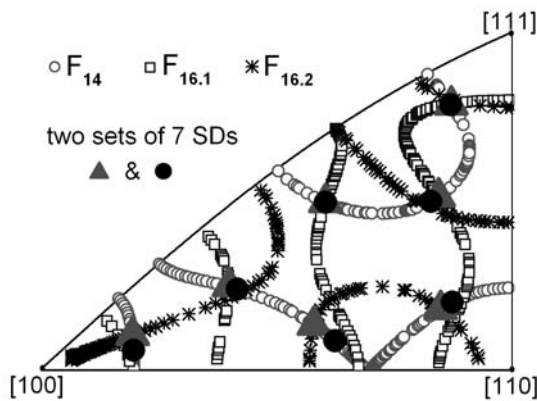

Fig. 3. Lines of zeros of cubic harmonics F_{14}, $F_{16.1}$ and $F_{16.2}$ together with two sets of 7-SD: determined in Ref. [9] – triangles and in this paper – circles. HSDs are in the corners of the stereogram.

harmonic. Such a choice was suggested by the results of the tests performed for some models [9]. However, as it was pointed before, the results of such tests may depend on the behaviour of higher components $f_{n,\mu}(p)$ of a particular model, while a procedure of determining $d_{n,\mu}$ coefficients is univocal. Proceeding as in [10], a slightly another solution than in Ref. [9] is found. Being on lines of zeros of the first harmonic, omitted in Eq. (3) (in this case of F_{14}), a trial to eliminate contributions from both $F_{16.1}$ and $F_{16.2}$ was undertaken – such a choice is indicated in Fig. 3 by the full circles. As it is seen, in this case two sets of 7-SDs (determined in Ref. [9] and in this paper) are very similar.

Summarizing

The proper choice of SDs optimizes the description of various physical quantities, having symmetry of the lattice as well as defines (to minimize experimental time and costs) which projections should be measured in, e.g. Compton [7] or neutron scattering [13] and positron annihilation [11] experiments. As far as we know, there are two quite different opinions that one should measure spectra along: 1 – main symmetry and intermediate directions [7]; 2 – only intermediate directions [11] (however, the author did not define them). Results found in papers [1, 2, 5, 6, 9, 10] and examples presented above clearly indicate that they are not only low-symmetry directions, but they also must be very particular. Of course, their number depends on the anisotropy of $f(\mathbf{p})$ and the symmetry of the lattice, i.e. on the volume of the irreducible part of the BZ.

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