# Mathematical descriptions of Fourier Symmetrization

The Fourier symmetrization consists of two steps. One is correcting distortion of an original FFT image, and the other is folding and rotating a corrected image based on a crystal symmetry. This note gives mathematical descriptions about each step.

## Correcting distortion

An FFT image is usually distorted due to various reasons such as piezo creep, thermal drift, and difference of piezo constants in $x$ and $y$ directions. This section describes mathematical basis of correcting such distortion. Here we think about uniform distortion constant in time: expansion, shrinkage, and shear in $x$ and $y$ directions (Fig. 1). Such distortion results in deviation of FFT peak locations from ideal ones. Our goal is to find how to correct the deviation.

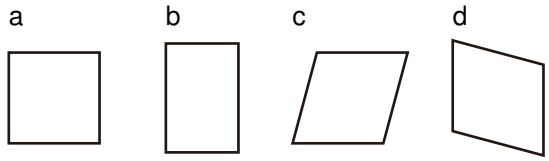


Figure 1: Distortion. (a) ideal, (b) expansion and shrinkage, (c) $x$-shear, (d) $y$-shear.

Let coordinates of atomic peaks observed in an FFT image $\boldsymbol{q}_1 = (q_{1x}, q_{1y})$ and $\boldsymbol{q}_2 = (q_{2x}, q_{2y})$. Due to the distortion, these peaks are shifted from the ideal locations, $\boldsymbol{q}_1{}'$ and $\boldsymbol{q}_2{}'$. This shift is expressed by a $2 \times 2$ matrix $M$, $\boldsymbol{q}_i{}' = M\boldsymbol{q}_i$. Our goal is nothing but getting the matrix $M$.

When shear direction is $x$, $M$ is given as a product of matrices of shear and expansion (or shrinkage),

$$M = \begin{pmatrix} m_1 & m_2 \\ 0 & m_3 \end{pmatrix} = \begin{pmatrix} 1 & m_2/m_3 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} m_1 & 0 \\ 0 & m_3 \end{pmatrix}. \tag{1}$$

To get these three parameters of $M$, we solve the following three equations: $|\boldsymbol{q}_i{}'| = 1/a_i$ and $\boldsymbol{q}_1{}' \cdot \boldsymbol{q}_2{}' = |\boldsymbol{q}_1{}'||\boldsymbol{q}_2{}'| \cos\theta$, where $a_i$ is the distance[1] between atomic rows corresponding to $\boldsymbol{q}_i$ and $\theta$ is the angle between $\boldsymbol{q}_1{}'$ and $\boldsymbol{q}_2{}'$ determined by a crystal symmetry. Given $\boldsymbol{q}_i{}' = M\boldsymbol{q}_i$, these three equations are

$$(q_{1x}m_1 + q_{1y}m_2)^2 + (q_{1y}m_3)^2 = 1/{a_1}^2, \tag{2}$$

$$(q_{2x}m_1 + q_{2y}m_2)^2 + (q_{2y}m_3)^2 = 1/{a_2}^2, \tag{3}$$

$$(q_{1x}m_1 + q_{1y}m_2)(q_{2x}m_1 + q_{2y}m_2) + q_{1y}q_{2y}{m_3}^2 = \cos\theta/(a_1a_2). \tag{4}$$

These equations can be rewritten as

$$\begin{pmatrix} {q_{1x}}^2 & 2q_{1x}q_{1y} & {q_{1y}}^2 \\ {q_{2x}}^2 & 2q_{2x}q_{2y} & {q_{2y}}^2 \\ q_{1x}q_{2x} & q_{1x}q_{2y} + q_{2x}q_{1y} & q_{1y}q_{2y} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 1/{a_1}^2 \\ 1/{a_2}^2 \\ \cos\theta/(a_1a_2) \end{pmatrix}, \tag{5}$$

where $A = {m_1}^2, B = m_1m_2$, and $C = {m_2}^2 + {m_3}^2$.

When shear direction is $y$, $M$ is given as

$$M = \begin{pmatrix} m_1 & 0 \\ m_2 & m_3 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ m_2/m_1 & 1 \end{pmatrix} \begin{pmatrix} m_1 & 0 \\ 0 & m_3 \end{pmatrix}. \tag{6}$$

We can get equations for $y$-shear case in the same manner to get Eq. (5). The resultant equations have the same form as Eq. (5), but $A = {m_1}^2 + {m_2}^2, B = m_2m_3$, and $C = {m_3}^2$.

Now we find that equations to be solved are Eq. (5) with respect to $A$, $B$, and $C$. By solving the equations, we finally get the matrix as

$$m_1 = \sqrt{A}, \quad m_2 = \frac{B}{\sqrt{A}}, \quad m_3 = \sqrt{C - \frac{B^2}{A}} \qquad (\text{for } x\text{−shear}), \tag{7}$$

[1]This is the $d$ value in terms of X-ray diffraction. It depends on the symmetry of lattice whether this is the same as the lattice constant $a_0$. For example, $a_i = a_0$ for 4mm and $a_i = \sqrt{3}a_0/2$ for 3m.

$$m_1 = \sqrt{A - \frac{B^2}{C}}, \quad m_2 = \frac{B}{\sqrt{C}}, \quad m_3 = \sqrt{C} \qquad \text{(for } y\text{−shear)}, \tag{8}$$

where

$$A = \frac{{q_{2y}}^2/{a_1}^2 + {q_{1y}}^2/{a_2}^2 - 2q_{1y}q_{2y}\cos\theta/(a_1a_2)}{(q_{1x}q_{2y} - q_{1y}q_{2y})^2}, \tag{9}$$

$$B = -\frac{q_{2x}q_{2y}/{a_1}^2 + q_{1x}q_{1y}/{a_2}^2 - (q_{1x}q_{2y} + q_{1y}q_{2x})\cos\theta/(a_1a_2)}{(q_{1x}q_{2y} - q_{1y}q_{2y})^2}, \tag{10}$$

$$C = \frac{{q_{2x}}^2/{a_1}^2 + {q_{1x}}^2/{a_2}^2 - 2q_{1x}q_{2x}\cos\theta/(a_1a_2)}{(q_{1x}q_{2y} - q_{1y}q_{2y})^2}. \tag{11}$$

In actual process with Igor Pro, the wave scaling is changed to correct expansion or shrinkage in $x$ and $y$ directions ($m_1$ and $m_3$). You may want to change aspect ratio of a window to plot a symmetrized FFT image. Parameters used to correct distortion ($m_1$, $m_2$, and $m_3$) are saved as wave note of a resultant symmetrized wave.

## Folding and rotating an FFT image

Folding and rotating an FFT image are done based on mirror and rotational symmetries of a crystalline lattice, respectively. Important properties of an FFT image for this purpose are that amplitude of an FFT image has

1. mirror symmetry same as that of an original real-space image,
2. rotational symmetry same as that of an original real-space image,
3. $C_2$ symmetry.

We make sure these properties in the following sections. Let $f(x, y)$ and $F(q_x, q_y)$ are a real-space image and its Fourier transform, respectively,

$$F(q_x, q_y) = \int f(x, y)e^{-i(q_x x + q_y y)}dxdy. \tag{12}$$

### mirror symmetry

When $f(x, y)$ has mirror symmetry with respect to $x$-axis, $f(x, y) = f(-x, y)$,

$$F(q_x, q_y) = \int f(-x, y)e^{-i(q_x x + q_y y)}dxdy \tag{13}$$

$$= -\int f(x, y)e^{-i(-q_x x + q_y y)}dxdy \tag{14}$$

$$= -F(-q_x, q_y). \tag{15}$$

Therefore, $|F(q_x, q_y)| = |F(-q_x, q_y)|$.

### rotational symmetry

When $f(x, y)$ has rotational symmetry, $f(x, y) = f(x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta)$,

$$F(q_x, q_y) = \int f(x\cos\theta - y\sin\theta, x\sin\theta + y\cos\theta)e^{-i(q_x x + q_y y)}dxdy \tag{16}$$

$$= \int f(x, y)e^{-i(q_x(x\cos\theta + y\sin\theta) + q_y(-x\sin\theta + y\cos\theta))}dxdy \tag{17}$$

$$= F(q_x\cos\theta - q_y\sin\theta, q_x\sin\theta + q_y\cos\theta). \tag{18}$$

### $C_2$ symmetry

Since $f(x, y)$ is a real function,

$$F^*(q_x, q_y) = \int f^*(x, y) e^{i(q_x x + q_y y)} dxdy \tag{19}$$

$$= \int f(x, y) e^{-i(-q_x x - q_y y)} dxdy \tag{20}$$

$$= F(-q_x, -q_y). \tag{21}$$

Therefore, $|F(q_x, q_y)| = |F(-q_x, -q_y)|$.

### Symmetrization

Fig. 2 shows equivalent points in FFT space, which are averaged by symmetrization. $p$3m1 and $p$31m have different sets of equivalent points. Due to $C_2$ symmetry described above, however, eventually they have the same set of equivalent points. Consequently, atomic peaks can be available to indicate high-symmetry direction for all symmetries. Half of the equivalent points are used for actual calculation to reduce amount of calculation. Effective multiplicity is 2, 6, and 4 for 2mm, 3m, and 4mm, respectively.

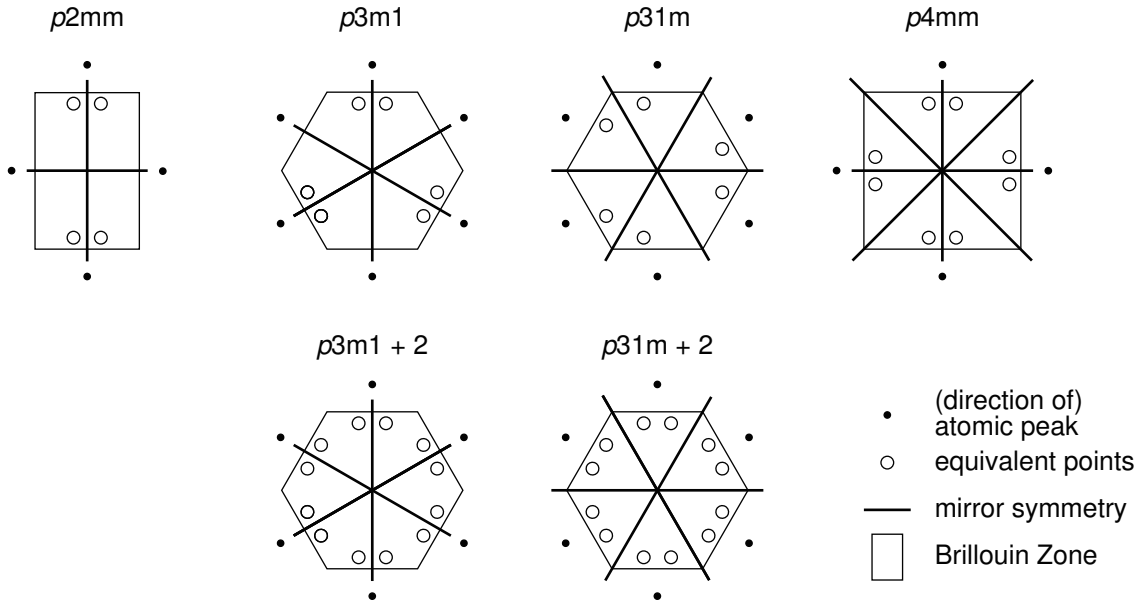


Figure 2: Equivalent points in FFT space for each symmetry.