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The X-ray Transform and its Application in Nano-Crystallography

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Abstract: In this article a review on the definition of the X- ray transform and some of its applications in Nano crystallography is presented. We shall show that the X- ray transform is a special case of the Radon transform on homogeneous spaces when the topological group $\boldsymbol{E}(\boldsymbol{n})$ - the Euclidean group - acts on $\mathbb{R}^{\mathbf{2}}$ transitively. First some properties of the Radon transform are investigated then the relationship to texture analysis is briefly illustrated. Finally, some of its applications in material structure detection at the Nano scale are studied.

Keywords: X- ray transform, Nano crystallography, homogeneous spaces.

1. INTRODUCTION

After for almost half of a century, Soviet and American authors [Shtein (1972); Vainshtein and Orlove (1972); Vest and Cormack (1973)] have pointed out Radon's paper in 1917 as the base for solving reconstruction from projections [4]. Then Fritz John revived the subject in important papers during the thirties and found significant applications to differential equations. Now, the appropriate unifying mathematical framework for a large class of reconstruction problems is the Radon transform on the Euclidean space. The X-ray transform as a special case of the Radon transform on homogeneous spaces appears in crystallography and in material sciences. More recent applications to X-Ray (electromagnetic waves with a wavelength of about 10^{-10} meters) technology and tomography have widened interest in the subject. A well-known problem in material sciences is the

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determination of material properties. This method is also known as texture analysis. Texture analysis is the analysis of preferred crystallographic orientation in polycrystalline materials. The analysis of crystallographic preferred orientations by means of orientation density functions and pole density functions is a widely used method in texture analysis. Some more complete introductions into texture analysis and crystallography are presented by many authors [1, 2, 7].

2. RADON TRANSFORM AND X-RAY TRANSFORM

We can have a look at the isometries of space that transform any body into itself. These are called the isometry group or symmetry group of the body. Most bodies in nature are irregular or asymmetrical. In this case, there is no isometry besides the identity, which transforms the body into itself. A group that only consists of the identity is called trivial. Bodies with a trivial isometry group are thus asymmetrical, and bodies with a non-trivial isometry group are called symmetrical. The larger the isometry group of a body, the more symmetrical its appearance. For example, the sphere as a symbol of a symmetrical body is transformed into itself through any isometry, and its symmetry group contains an uncountably infinite number of elements, i.e. as many as there are real numbers (e.g., every rotation around any angle and any axis and every reflection in any plane through the central point).

The isometry group of a crystal is not trivial, but always countable, with the point group itself only. In any case, we have to note that the colloquial terms "symmetric" and "regular" are mathematically described by the concept of the group. In what follows, first we describe the action of isomery group and its relation to the definition of the Radon transform on homogeneous spaces, then it will be specialized to the X-ray transform.

Definition 2. 1. Let G be a locally compact group and S a locally compact Hausdorff space. A left action of G on S is a continuous map $(\mathrm{x}, \mathrm{s}) \mapsto xs$ from $G \times S$ to S such that (i) $s \mapsto xs$ is homeomorphism of S for each $x \in G$, and (ii) $x(ys) = (xy)s$ for all $x, y \in G$ and $s \in S$. A space S equipped with an action of G is called a $G-$space. A $G-$space is called transitive if for every $s, t \in S$ there exists $x \in G$ such that $xs = t$.

Pick s_0 and let $H := \{x \in G \mid xs_0 = s_0\}$, we know from [2] that if G is $\sigma-$compact then S and G/H are homeomprphic. In this case the term homogeneous space is used to S.

Let G be a locally compact group, H and K be two closed subgroups of G, $L := H \cap K$ and also let $X := G/K$ and $Y := G/H$ denote two left coset spaces of G. Assume that $d(kL)$ and $d(hL)$ are two $K-$invariant and $H-$invariant Radon measures on K/L and H/L, respectively. The Radon transform $R : C_c(G/K) \longrightarrow C(G/H)$ was introduced by S. Helgason in 1966 defined by

$$Rf(xH) = \int_{H/L} f(xhK)d(hL) \quad ; \quad (f \in C_c(G/K)). \qquad (3.1.)$$

See [8]. In what follows, we shall show that the X-ray transform (2. 1.) is a special case of (3. 1.).

Let X denotes the plane of $\mathbb{R}^2$ viewed as a subset of $\{(x, y, 1) \mid x, y \in \mathbb{R}\}$. The isometry group $G := M(2)$ of matrices

$$(\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) := \begin{bmatrix} \alpha & \beta & u_1 \\ \gamma & \eta & u_2 \\ 0 & 0 & 1 \end{bmatrix} \in GL(n, \mathbb{R}), \alpha > 0$$

acts transitively on X with the action

$$(\alpha, \beta, \gamma, \eta;\ u_1, u_2) \,\square (a, b) = (\alpha a + \ \beta b + u_1, \gamma a + \ \eta b + u_2\ )$$

The isotropy group of $x_0 = (0, 0)$ is

$$K := \left\{(\alpha, \beta, \gamma, \eta;\ 0, 0\ ) \ \middle|\ \begin{bmatrix} \alpha & \beta \\ \gamma & \eta \end{bmatrix} \in O(2)\right\} = O(2)$$
$$= \left\{\begin{bmatrix} cos\,\phi & sin\,\phi \\ -sin\,\phi & cos\,\phi \end{bmatrix}, \begin{bmatrix} -sin\,\phi & cos\,\phi \\ cos\,\phi & sin\,\phi \end{bmatrix} \,|\theta \in [0, 2\pi)\right\}$$

Let $Y := \{(x, mx + h) : x \in \mathbb{R}\}$ be the space of all lines in the plane of $\mathbb{R}^2$. If we denote the line $y = mx + h$ by (m, h) then the action of G on X induces a transitive action of G on Y as following.

$$(\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) \diamondsuit (a, b) = \left(\frac{\gamma + \ \eta m}{\alpha + \ \beta m}, -\frac{\gamma + \ \eta m}{\alpha + \ \beta m}(\beta h + u_1) + \eta h + u_2\right)$$

Because we have the following

$$(\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) \,\square (a, b) = (\alpha x + \ \beta(mx + h) + u_1, \gamma x + \ \beta(mx + h) + u_2).$$

If we consider $x' := \alpha x + \ \beta(mx + h) + u_1$ then $x = \frac{x' - \beta h - u_1}{\alpha + \beta m}$ and

$$\gamma x + \ \beta(mx + h) + u_2 = \frac{\gamma + \ \eta m}{\alpha + \ \beta m} x' + \frac{(\gamma + \ \eta m)(\beta h + u_1)}{\alpha + \ \beta m} + \eta h + u_2$$

Now, the isotropy group of the X-axis (the point $(0, 0)$) is

$$H := \left\{(\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) : \left(\frac{\gamma}{\alpha}, -\frac{\gamma}{\alpha} u_1 + u_2\right) = (0, 0)\right\}$$
$$= \{(\alpha, \beta, 0, \eta;\ u_1, 0\ ) : (\alpha, \beta, 0, \eta) \in O(2), u_1 \in \mathbb{R}\}$$
$$= \{(\pm 1, 0, 0, \pm 1;\ u_1, 0\ ) : u_1 \in \mathbb{R}\}$$

$$= \mathbb{Z}_2 \times M(1)$$

Thus the group $L := K \cap H = \{\pm I_{2\times 2}\}$ is the trivial group and $H/L = H = \mathbb{R}$ has a Haar measure $dh_{(1,0,0,1;\,u,0)} = \frac{du}{u}$.

Also, if $g = (\alpha, \beta, \gamma, \eta;\ u_1, u_2\ )$, $h = (1, 0, 0, 1;\ s, 0)$ and $K = \left(\alpha', \beta', \gamma', \eta';\ 0, 0\ \right)$ then

$$gK = (\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) \diamond (0, 0) = (u_1, u_2)$$

$$gH = (\alpha, \beta, \gamma, \eta;\ u_1, u_2\ ) \square (0, 0) = \left(\frac{\gamma}{\alpha}, -\frac{\gamma}{\alpha} u_1 +\ u_2\right)$$

$$ghK = (\alpha, \beta, \gamma, \eta;\ \alpha s + u_1, \gamma s + u_2\ ) \square (0, 0) = (\alpha s + u_1, \gamma s + u_2\ )$$

$$gkH = (\alpha\alpha' +\ \beta\gamma', \alpha\beta' +\ \beta\eta', \gamma\alpha' +\ \eta\gamma', \gamma\beta' +\ \eta\eta';\ u_1 +\ u_2\ ) \diamond (0, 0)$$

$$= \left(\frac{\gamma\alpha' + \eta\gamma'}{\alpha\alpha' +\ \beta\gamma'}, -\frac{\gamma\alpha' + \eta\gamma'}{\alpha\alpha' +\ \beta\gamma'} u_1 +\ u_2\right)$$

So the Radon transform is

$$Rf(gH) = \int_H f(ghK)dh.$$

Then

$$Rf(\left(\tfrac{\gamma}{\alpha}, -\tfrac{\gamma}{\alpha} u_1 +\ u_2\right)) = \int_{-\infty}^{+\infty} f(\alpha s + u_1, \gamma s + u_2\ )ds.$$

Now, put $u_1 = p\cos\phi$, $u_2 = \sin\phi$, $\gamma = \cos\phi$ and$\alpha = \sin\phi$ then we have

$$Rf(p, \phi) = \int_{-\infty}^{+\infty} f(p\cos\phi - s\sin\phi, p\sin\phi + s\cos\phi\ )ds.$$

.۲،۲**Example** Here we consider the transform over the unit circle. Let

$$f(x, y) = \begin{cases} \sqrt{1 - x^2 - y^2} & ; \quad x^2 + y^2 < 1 \\ 0 & ; \quad O.W. \end{cases},$$

The transform is given by

$$\check{f}(p, \phi) = \frac{\pi(1 - p^2)}{12}$$

where $-1 \leq p \leq +1$.

3. X-RAY TRANSFORM AS A LINE INTEGRAL

X-ray imaging relies on the principle that an object will absorb or scatter X-rays of a particular energy in a manner dependent on its composition, quantified by the attenuation coefficient μ. The attenuation coefficient μ of a substance is a function in $\mathbb{R}^3$dependent on a variety of factors, but primarily reflective of the electron density of that substance. Therefore, denser substances and substances containing elements with many electrons will have higher attenuation coefficients. This helps explain why bone, which contains high percentages of calcium (20 electrons), potassium (19 electrons), phosphorous (15 electrons), and magnesium (12 electrons), has a much higher attenuation coefficient than soft tissue, which is made up primarily of carbon (6 electrons), nitrogen (7 electrons), and oxygen (8 electrons) [2]. Air is considered to have an attenuation coefficient of zero for simplicity of calculation, so the attenuation coefficient disappears outside the body.

When a beam of X-ray photons emits on texture of homogeneous material, the beam intensity decreases according to the equation

$$I = I_0 e^{-\mu x},$$

where I and I_0 are input and output intensities. The attenuation coefficient μ depends on density of the material ρ and the nuclear composition characterized by the atomic number z. The distance passing a beam through the material is denoted by x. If it passes a x_i's distance through different textures with different attenuation coefficient μ_i's then

$$I = I_0 e^{-\sum \mu_i x_i}.$$

Thus

$$p := -log(\frac{I}{I_0}) = \int_L \mu(\rho, z) ds,$$

indicates inside quality of the texture thus it is called a single projection. The line integral depends on distance of path from the origin and the angle ϕ that it turns left or right. Moving the source and detector together yields a vector of values called profile and various values of p and ϕ yeild sample matrix.

.۳،۱ Definition Let f be a function on some domain $\mathrm{D} \subseteq \mathbb{R}^2$, and let L be a line in the plane, the line integral

$$\check{f} = Rf = \int_L f(x,y) ds$$

is said the Radon transform of f.

Consider Fig. 3.1, to get the line equation. We have $sin\left(\frac{\pi}{2} - \phi\right) = \frac{x}{x_0}$ and $cos\left(\frac{\pi}{2} - \phi\right) = \frac{y}{y_0}$, so $x\, sin\, \phi + y\, cos\, \phi = p$.

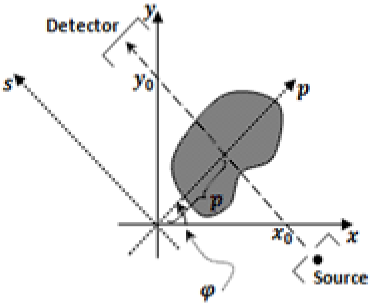

Figure 3.1. Emission-photon Model to Describe line integral

Suppose now a new coordinate system is introduced with axes rotated by the angle ϕ, then we have

$$\begin{bmatrix} p \\ s \end{bmatrix} = \begin{bmatrix} cos\,\phi & sin\,\phi \\ -sin\,\phi & cos\,\phi \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

thus

$$\check{f}(p,\ \phi) = \int_{-\infty}^{+\infty} f(p\,cos\,\phi - s\,sin\,\phi\,, p\,sin\,\phi + s\,cos\,\phi)ds.$$

The first theorem in Radons' 1917 paper asserts that the above integral is well-defined.

Furthermore, if we introduce unit vector $\xi := (cos\,\phi\,,\ sin\,\phi)$ and $X := (x, y)$ then the line equation is $p = \xi \cdot X$ and

$$\check{f}(p,\ \phi) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(X)\delta(p - \xi \cdot X)dxdy, \qquad (2.1.)$$

where δ is the Dirac delta function.

This definition used by Gel'fand, Greav and Vilenkin in 1966. Note that $\check{f}$ is defined on $\mathbb{R} \times S^{n-1}$, where S^{n-1} is the unit sphere. Because $(p,\ \phi)$ and $(-p, -\phi)$ represent the same hyperplane in $\mathbb{R}^n$ ($p = \xi \cdot X$ if and only if $-p = -\xi \cdot X$) thus the Radon transform is not a one to one transform.

Definition3. 2. Let f be a function on some domain $\mathrm{D} \subseteq \mathbb{R}^{\boldsymbol{n}}$, $X = (x_1,\ x_2,\ x_3 \ldots, x_n) \in \mathbb{R}^n$, $dX = dx_1 dx_2\ \ldots\ dx_n$, and more let ξ be the normal vector for hyperplan $p = \xi \cdot X$ in $\mathbb{R}^n$. The Radon transform of f is defined as

$$\check{f} = Rf = \int_{\mathbb{R}^n} f(X)\delta(p - \xi \cdot X)dX$$

is said the Radon transform of f.

In the following theorem we collect some properties of Radon transform.

Theorem 3.3. Let R denotes the Radon transform and $s, \alpha, \beta \in \mathbb{R}$. Assume that f, g are continuous function on $\mathbb{R}^n$. Also consider A as an invertible matrix then we have the following properties

$$\begin{cases} R(\alpha f + \beta g) = \alpha Rf + \beta Rg \\ Rf(sp, s\xi) = |s| Rf(p, \xi) \\ R(f * g) = Rf * Rg \\ Rf = \left(\mathcal{F}_1{}^{-1} \mathcal{F}_n\right) f \end{cases}$$

Where $\mathcal{F}_1$ *and* $\mathcal{F}_n$*denote the one dimensional and denotes the* n*-dimensional Fourier transforms on* $\mathbb{R}^n$.

4. X-RAY TRANSFORM AND CRYSTALLOGRAPHY

Functional properties of various materials used in different areas such as life sciences, electronics, mechanics, mining engineering, food industry and etc. depend on their atomic and molecular structure. Knowledge of the internal structure and texture analysis of materials give us applicable technical properties. Unfortunately, the limitations in human power of vision blocked scientists' sight to have enough information about the internal parts of tissues. A variety of tools and techniques aimed to solve this issue. Usage of the various methods such as magnetic resonance imaging (MRI), computerized tomography scan (CT-scan), X-ray diffraction in the crystalline materials analysis is very common. Crystallography can be referred as the study of the atomic positions via measuring the distribution of diffracted X-rays. The history of crystallography is as long as the discovery of the X-ray by Wilhelm C. Rontgen in 1895. The first experiment to identify the nature of the crystalline by using distribution of the diffracted radiations was conducted by Laue and showed that when radiation strikes with a crystal, they disperse in different directions and at various intensities. Stereographic projection technique has been found to measure and collect data of all intensities, it also help us to read out the angular relationships between different planes and directions in the crystal or unit cell in a lattice, this data set is called pole distribution density function (P. D. F).

Some methods have been introduced to obtain the orientation distribution function (ODF) in a polycrystalline sample from pole figures, one can see more details in [2, 9, 12]. In this paper we suppose that a pole figure data set there exists and we want to use a family of harmonic function in order to derive the ODF function.

Let start with some notations and definitions, consider K_s and K_c as Cartesian coordinate systems fixed on specimen and a crystal in it. These two coordinate systems can be coincided with the appropriate orientations, see Fig. []. According to the scheme proposed by Bunge, a set of $(\varphi_1, \varphi, \varphi_2)$ are need to be coincide two coordinate systems, these angles are called Euler angles. The crystallographic orientation $(\varphi_1, \varphi, \varphi_2)$ of an individual crystal gives us an orthogonal transformation $g = g(\varphi_1, \varphi, \varphi_2) \in O(3)$ which brings K_s into coincidence with K_c.

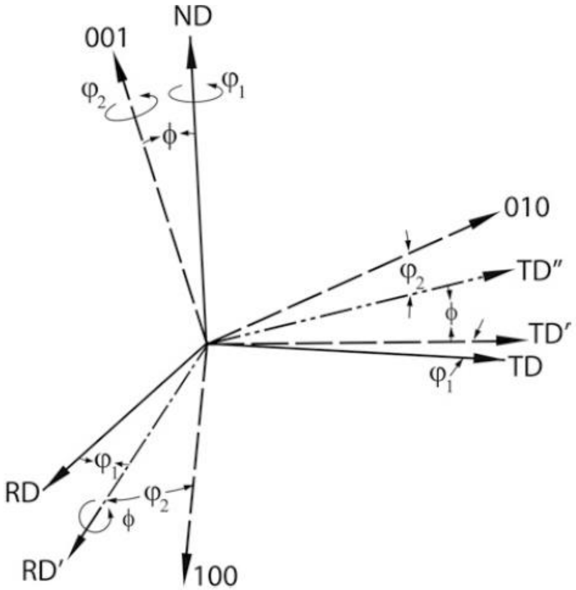

Figure 4.1. Two coordinate systems can be coincided by Euler angles rotation

It is noted that, owing to the symmetry of unit cell and the textures, the orientation space (or the Euler space), however, is restricted to a smaller region. This restriction is also valid for all texture components in the polycrystalline. The common way to describe the regularity of an atom lattice is to extend it periodically to the three–dimensional Euclidean space $\mathbb{R}^3$ and to consider its symmetries. Symmetries are isometric mappings of the three–dimensional space that leave the extended atom lattice invariant. The set of all symmetries of the extended atom lattice forms a group, the so called space group $S_{space} \subseteq O(3) \otimes T(3)$ of the crystal. Here $O(3)$ and $T(3)$ are the orthogonal group and the group of all translations in $\mathbb{R}^3$. The orthogonal part $H = S_{point} = S_{space}/T(3) \subseteq O(3)$ of the space group is called point group or isotropy group of the crystal. A crystallographic point group is a set of symmetry operations, like rotations or reflections that leave a central point fixed while moving other directions and faces of the crystal to the positions of features of the same kind. For a periodic crystal.

A direction specified by coordinates relative to a crystal coordinate system is called crystal direction. Following the general convention we denote crystal directions by $h \in \mathbb{S}^2$. Two crystal directions $h_1, h_2 \in \mathbb{S}^2$ are called crystallographically equivalent if there exists a symmetry $g \in S_{space}$ of the crystal such that $h_1 = gh_2$. We denote by

$$hS_{space} = \{ hq \mid q \in S_{space}\}$$

the class of all crystal directions crystallographically equivalent to a given crystal direction $h \in \mathbb{S}^2$ and by $\mathbb{S}^2/S_{space}$ the set of all classes of crystallographically equivalent directions.

A direction specified by its coordinate vector relative to the specimen coordinate system is called specimen direction and is usually denoted by the letter $r \in \mathbb{S}^2$.

Crystal directions and specimen directions are connected via the coordinate transformation $g = g(\varphi_1, \varphi, \varphi_2) \in O(3)$ from the crystal coordinate system to the specimen coordinate system. With this notation a crystal direction $h \in \mathbb{S}^2$ and a specimen direction $r \in \mathbb{S}^2$ represent the same physical direction if and only if $r = gh$. Let $g_1, g_2 \in O(3)$ be two coordinate Also, two transformations g_1 and g_2 are crystallographically equivalent orientations if and only if there exists a symmetry $q \in S_{point}$ such that $g_1 = g_2 q$. The class

$$gS_{point} = \{gq \mid q \in S_{point}\} = O(3)/S_{point}$$

of all coordinate transformations that are crystallographically equivalent to a given coordinate transformation $g \in O(3)$ is called crystal orientation and the factor group $O(3)/S_{point}$ of all crystal orientations is called orientation space. Let $gS_{point} \in O(3)/gS_{point}$ be a crystal orientation, $hS_{point} \in \mathbb{S}^2/S_{space}$ a class of crystallographically equivalent crystal directions and $h \in \mathbb{S}^2$ a specimen direction. Then r represents a direction identical to one of the directions represented by the class hS_{space} if and only if

$$hS_{point} = \left(gS_{point}\right)^{-1} r$$

Consider a one–type, polycrystalline specimen, i.e. a compound of identical crystals all possessing the same point group $S_{point} \subseteq O(3)$. Next we assume that each crystal has a well-defined crystal orientation $gS_{point} \in O(3)/gS_{point}$ relative to the specimen thus neglecting e.g. internal crystal defects. Then, if one denotes dV the volume elements of the sample which possess the orientation g within the element of orientation dg, and denotes the V the total sample volume, then, an orientation distribution function $f(g)$, is defined by $f(g) = \frac{dV/V}{dg}$ where $dg = 1/(8\pi^2)\ sin\phi d\varphi_1 d\phi d\varphi_2$.

. More abstractly we define

Definition 4.1. Let $O(3)/S_{point}$ be a point group and let $f\colon O(3)/S_{point} \longrightarrow \mathbb{R}^{+}$ a non–negative, integrable function on $O(3)/S_{point}$ normalized to1

$$\frac{1}{16\pi^2}\int_{O(3)} f\big(gS_{point}\big)dg = 1.$$

Then f is called orientation density function (ODF).

Beside the distribution of crystal orientations within a specimen one can also ask for the distribution of crystal directions that are in line with a certain specimen direction modulo crystal symmetry. To be more precise let us fix a specimen direction $r \in \mathbb{S}^2$. Then any distribution of crystal orientations $gS_{point} \in O(3)/gS_{point}$ constitutes by virtue of the mapping $gS_{point} \longmapsto \big(gS_{point}\big)^{-1}r$ a distribution on the classes of crystallographically equivalent crystal directions $\mathbb{S}^2/S_{spoint}$.

Lemma 4.2. (fundamental equation of texture analysis)**.** Let $S_{point} \subseteq O(3)$ be some point group and let $f \in L^1\big(O(3)/S_{point}\big)$ be the ODF of a probability measure μ on $O(3)/S_{point}$. Then the mapping

$$\pi\colon O(3)/S_{point} \longrightarrow \mathbb{S}^2/S_{point}, \quad gS_{point} \longmapsto \big(gS_{point}\big)^{-1}r$$

is measurable for any $r \in \mathbb{S}^2$ and the induced measure $\mu \circ \pi^{-1}$ on $\mathbb{S}^2/S_{point}$ has the probability density function

$$xf(.\,,r) \in L^1\big(O(3)/S_{point}\big),$$

where the operator x is defined as following

$$x\colon C\big(O(3)\big) \longrightarrow C(\mathbb{S}^2 \times \mathbb{S}^2)$$

$$xf(h,r) = \frac{1}{2}\big(\mathcal{R}f(h,r,Id) + \mathcal{R}f(h,r,-Id)\big)$$

.

And $\mathcal{R}$ denotes the Radon transform on $O(3)$.

Definition 4. 3 . Let $f \in L^1\big(O(3)/S_{point}\big)$ be an ODF. Then the function

$$xf \in L^1\big(\mathbb{S}^2/S_{spoint} \times \mathbb{S}^2\big)$$

is called pole density function (PDF) corresponding to f. For any $h, r \in \mathbb{S}^2$ the trace functions $xf\big(S_{spoint}h,.\big) \in L^1(\mathbb{S}^2)$, $xf(.\,,r) \in L^1\big(\mathbb{S}^2/S_{spoint}\big)$ are called pole figure and inverse pole figure, respectively. The PDF defined by an ODF $f \in L^1\big(O(3)/S_{point}\big)$ is commonly denoted by the letter $p = xf$. This relationship between an ODF and its PDF is known as the fundamental equation of texture analysis and is due to Bunge (1965), Roe (1965) and others.

Remark 4. 4. Although the ODF and the PDF are defined on the factor spaces $xf \in L^1(\mathbb{S}^2/S_{spoint} \times \mathbb{S}^2)$ $O(3)/S_{spoint}$ and $\mathbb{S}^2/S_{spoint} \times \mathbb{S}^2$, respectively, we will treat them sometimes as functions defined on $O(3)$ and $\mathbb{S}^2 \times \mathbb{S}^2$ possessing for any $g \in O(3), h, r \in \mathbb{S}^2$ and $q \in S_{spoint}$ the symmetry properties $f(g) = f(gq)$ and $P(h,r) = P(qh,r)$, respectively. While the ODF of an specimen is not directly accessible, the PDF $P(h,r)$ of a specimen can be determined for specific crystal and specimen direction $h, r \in \mathbb{S}^2$ by diffraction techniques.

If one denotes dV the volume elements of the sample which possess the orientation g within the element of orientation dg, and denotes the V the total sample volume, then, an orientation distribution function $f(g)$, is defined by $f(g) = \frac{dV/V}{dg}$ where $dg = 1/(8\pi^2)\ sin\phi d\varphi_1 d\phi d\varphi_2$. The function $f(g)$, which depends on the orientation g, can be developed in a series of generalized spherical harmonics

$$f(\varphi_1, \varphi, \varphi_2) = \sum_{l=0}^{\infty} \sum_{n=-l}^{+l} \sum_{m=-l}^{+l} w_{lmn} z_{lmn}(\varphi)\, e^{-i(m\varphi_1 + n\varphi_2)}.$$

Where w_{lmn} are the coefficients of the series of generalized spherical harmonics. $z_{lmn}(\varphi)$ are the certain generalizations of the associated Jacob function. Mathematical methods have been developed that allow an ODF to be calculated from numerical data obtained from several experimental pole figures.

The problem of estimation of the true ODF from PDF is known as the PDF–to–ODF inversion problem. In the next work we will introduce an efficient family of harmonic function to solve the PDF–to–ODF inversion problem.

Serial femtosecond X-ray crystallography has created new opportunities in the field of structural analysis of protein. Contrary to conventional protein crystallography, recent experiments are performed 1) on multiple crystals with random sizes and orientations delivered via a liquid jet, rather than on a single mounted rotating crystal, and 2) with the crystals immersed in a large-diameter beam, rather than the beam being confined to the interior of the input facet. In the future research we will propose an algorithm to estimation of the true ODF from PDF in the Nano crystallography framework.

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