RENDERING OF CRYSTALLOGRAPHIC ORIENTATIONS, ORIENTATION AND POLE PROBABILITY DENSITY FUNCTIONS

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ABSTRACT

Since the domain of crystallographic orientations is three-dimensional and spherical, their insightful rendering or rendering of related probability density functions requires (i) to exploit the effect of a given orientation on crystallographic axes, (ii) to consider spherical means of the orientation probability density function with respect to lower–dimensional manifolds, and (iii) to apply projections from the two–dimensional unit spheres \( S^2 \subset \mathbb{R}^3 \) onto the unit disk \( D \subset \mathbb{R}^2 \). The familiar crystallographic “pole figures” are actually the sum of two spherical X–ray transforms which associate with a real–valued function \( f \) defined on a sphere its mean values \( Xf \) along one–dimensional circles with centre \( O \), the origin of the coordinate system, and spanned by two unit vectors. The family of views suggested here defines generalized cross–sections in terms of simultaneous orientational relationships of two different crystal axes with two different specimen directions such that their superposition yields a user–specified pole probability density function. Thus, the spherical averaging and the spherical projection onto the unit disk determine the distortion of the display. Commonly, the spherical projection preserving either volume or angle are favored. This rich family displays \( f \) completely, i.e. if \( f \) is given or can be determined unambiguously, then it is uniquely represented by several subsets of these views. A computer code enables the user to specify and control interactively the display of linked views which is comprehensible as the user is in control of the display.

INTRODUCTION AND MOTIVATION

A crystallographic orientation is basically the rotation \( g^* \) in \( SO(3) \) which maps a right–handed coordinate system \( K_S \) fixed to the specimen onto another right–handed coordinate system \( K_C \) fixed to the crystal. It may be parameterized by three conventionally defined Euler angles, e.g. \( g^* \in G \subset SO(3) : g^* = g^*(\alpha, \beta, \gamma) \) where the first rotation by \( \alpha \in [0, 2\pi) \) is about the \( Z \)-axis, the second by \( \beta \in [0, \pi] \) about the (new) \( Y' \)-axis, and the third by \( \gamma \in [0, 2\pi) \) about the (new) \( Z'' \)-axis of the crystal coordinate system \( K_C \). Then \( (\alpha, \beta) \) are the spherical coordinates of the direction \( Z'' = Z_C = z_{K_C} \) with respect to \( K_S \). There exist 11 other ways to define Euler angles, and they are all in use, somewhere [3].

The coordinates of a unique direction denoted \( h \) with respect to the crystallographic coordinate system \( K_C = g^* K_S \) and \( r \) with respect to the specimen coordinate system \( K_S \) are related to each other by \( h = M((g^*)^{-1}) r =: M(g) r \) with

\[
M(g) = \begin{pmatrix}
cos \alpha \cos \beta \cos \gamma - \sin \alpha \sin \gamma & \sin \alpha \cos \beta \cos \gamma + \cos \alpha \sin \gamma & -\sin \beta \cos \gamma \\
-\cos \alpha \cos \beta \sin \gamma - \sin \alpha \cos \gamma & -\sin \alpha \cos \beta \sin \gamma + \cos \alpha \cos \gamma & \sin \beta \sin \gamma \\
\cos \alpha \sin \beta & -\sin \alpha \sin \beta & \cos \beta
\end{pmatrix}.
\]
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Obviously, 
\[ M^t(g) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_{K_C} = \begin{pmatrix} \cos \alpha \sin \beta \\ \sin \alpha \sin \beta \\ \cos \beta \end{pmatrix} =: r_{K_S} \text{ for all } \gamma \in [0, 2\pi), \] (1)
and
\[ M(g) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}_{K_S} = \begin{pmatrix} \cos(\pi - \gamma) \sin \beta \\ \sin(\pi - \gamma) \sin \beta \\ \cos \beta \end{pmatrix} =: h'_{K_C} \text{ for all } \alpha \in [0, 2\pi). \] (2)

Let \( f : SO(3) \mapsto IR^1 \) denote an orientation probability density function. Then,
\[ \frac{1}{2\pi} \int_{[0,2\pi]} f(g(\alpha, \beta, \gamma))d\gamma = \frac{1}{2\pi} \int_{\{g \in SO(3) | e_2 = gr\}} f(g)dg = (Xf)(z_{K_C}, r_{K_S}), \] (3)
which is the probability density function of the crystallographic direction \( z_{K_C} \), and
\[ \frac{1}{2\pi} \int_{[0,2\pi]} f(g(\alpha, \beta, \gamma))d\alpha = \frac{1}{2\pi} \int_{\{g \in SO(3) | h' = ge_3\}} f(g)dg = (Xf)(h'_{K_C}, z_{K_S}), \] (4)
which is the probability density function of the specimen direction \( z_{K_S} \). Analogous relations hold for differently defined Euler angles.

In these instances, averaging may be thought of as being provided by projections of \( f : D \times [0,2\pi] \mapsto IR^1 \) onto the unit disk \( D \subset IR^2 \). If \( f \) is rendered in sections of fixed \( \gamma \), then their superposition is the spherical distribution of the crystallographic \( z_{K_C} \) direction. Analogously, if \( f \) is rendered in sections of fixed \( \alpha \), then their superposition is the spherical distribution of the specimen \( z_{K_S} \) direction.

Generally, the X-ray transform \( X : L(SO(3)) \mapsto L(S^3 \times S^3) \) of an orientation probability density function \( f \) defined on \( SO(3) \) is defined as [5]
\[ (Xf)(h, r) := \frac{1}{2\pi} \int_{\{g \in SO(3) | h = gr\}} f(g)dg. \] (5)

The basic crystallographic X-ray transform, i.e. the pole density function projection, is provided by
\[ (Af)(h, r) = \frac{1}{2}\left((Xf)(-h, r) + (Xf)(h, r)\right), \] (6)
and \( Af \) is referred to as bi-axial probability density function. Considering \( h \) rather a parameter than a variable, \( Af \) is called pole density function, considering \( r \) a parameter, it is called “inverse” pole density function.

**RENDERING GENERALIZED SECTIONS OF ORIENTATION SPACE**

Plots of conventional sections orthogonal to an coordinate axis of the Euler space thought of as being spanned by three orthogonal axes suffer from serious distortions [4, 2]; since the volume/area is not preserved, the visual inspection, especially the interpretation of local maxima, may be misleading. Slightly more involved are \( \sigma \)-sections [1, 4], which preserve and
display the same volume portion of the orientation space. They add up to the \( c \)-pole density plot according to eq. (3), but other axes or their distributions, respectively, cannot visually be inferred.

More appropriately defined generalized sections of the orientation space should satisfy some specific properties to provide a comprehensive insight, such as

- the sections should preserve volume, respectively area;
- the direction of any given axis with respect to the reference frame should be geometrically visible,
- the parameters defining a section should have a simple geometrical interpretation,
- the user should be enabled to choose the most informative sections in a fast and interactive way,
- the sections should add up to a user–specified pole probability density function,
- the set of sections should visualize the complete information of the orientation probability density function.

Then, dynamically linked views [6, 7, 8] of such sections and their superposition will provide easy–to–read and instructive simultaneous displays of the orientation data, their probability density function and corresponding pole probability density functions with respect to given crystallographic or specimen directions.

Therefore, a generalized \( \gamma \)-section of the orientation space is defined by

1. the parameter \( g_0 \) defining the orientation of the specimen coordinate system \( K_S \) with respect to some external coordinate system \( K \);
2. a crystallographic direction \( h_0 \) characterizing the pole point or pole density plot, which is the superposition of all sections. An orientation \( g \) is generally displayed at location \( r = g^{-1} h_0 \) and at all locations corresponding to crystal–symmetrically equivalent directions of \( h_0 \) when projected onto the unit disk;
3. a second crystallographic direction \( h_1 \) not parallel to \( h_0 \), a specimen direction \( r_1 \), an angle \( \gamma \in [0, 2\pi] \), and an angular tolerance \( \Delta \gamma \). An orientation is actually displayed if and only if the angle of \( h_1 \) and \( r_1 \) projected onto the tangential plane of the \( h_0 \)-pole sphere at \( r_0 \) is in \([\gamma - \Delta \gamma, \gamma + \Delta \gamma]\), i.e.

\[
\angle (r_1 - (r_1 \cdot r) r, \ g^{-1} h_1 - (g^{-1} h_1 \cdot g^{-1} h_0) g^{-1} h_0) = \angle (r_1 - (r_1 \cdot r) r, \ g^{-1} h_1 - (h_1 \cdot h_0) r) \in [\gamma + \Delta \gamma, \gamma - \Delta \gamma].
\] (7)

If \( \gamma = 0 \), then all orientations are actually displayed for which \( h_1 \) is perfectly aligned with \( r_1 \) and \( h_0 \) coincides with the direction \( r \) displayed in the pole point plot. If \( \gamma = \pi/2 \) or \( \gamma = \pi \), then all orientations are displayed for which \( h_1 \) is largely misaligned with \( r_1 \) and \( h_0 \) coincides with the direction \( r \) displayed in the pole point plot.

The angle \( \gamma \) enclosed by \( h_1 \) and \( r_1 \) when looking at the tangential plane from outside the pole sphere is also visualized in an angular display. Continuously varying \( \gamma \) along the circle
The view is complete in the sense that two different data sets are not rendered in the same way. The superposition of all sections is the $h_0$–pole point or pole density plot.

Figure 1: (111)–pole sphere displaying $h_0 = (111)t$, and the associated tangential plane with the orthogonal projection of the crystal direction $h_1 = (100)t$, represented by $g^{-1}h_1$ with respect to the specimen coordinate system $K_S$, and its crystal–symmetrically equivalents, and the orthogonal projection of the specimen direction $r_1$ enclosing the angle $\gamma$ (Figures by courtesy of Heiko Kost, KPMG InfoDesign, Saarbrücken, Germany).

Figure 2: Top view of tangential plane with the orthogonal projection of the crystal direction $h_1 = (100)t$, represented by $g^{-1}h_1$ with respect to the specimen coordinate system $K_S$, and its crystal–symmetrically equivalents, and the orthogonal projection of the specimen direction $r_1$ enclosing the angle $\gamma$ (Figure by courtesy of Heiko Kost, KPMG InfoDesign, Saarbrücken, Germany).

Generalized $\gamma$–sections could be especially appropriate for exploratory data analysis like "how
does a given crystal direction $\mathbf{h}_1$ relate with a given specimen direction $\mathbf{r}_1$, e.g. second principal stress direction?”.

Instead of varying $\gamma$, it could be fixed to $\gamma = 0$, or $\gamma = \pi/2$, respectively. If $\mathbf{h}_1$ is kept fixed, then varying $\mathbf{r}_1$ over the whole pole sphere corresponds to exploring “where is $\mathbf{h}_1$ headed to?” The answer is provided by the most dense clusters of orientations. As before, the sections sum to the $\mathbf{h}_0$–pole point plot and display the entire orientation space, each with equal area and in the same amount of cpu–time. The view is complete in the sense that two different data sets are not rendered in the same way. For every set of parameters with $\gamma \in \{0, \pi/2, \pi, 3\pi/2\}$ the user can easily infer the $\mathbf{h}_1$–direction of every displayed orientation due to its simple relationship with respect to the direction $\mathbf{r}_1$.

Exchanging the roles of $\mathbf{r}_1$ and $\mathbf{h}_1$ allows exploring the data according to “which crystallographic direction heads to $\mathbf{r}_1$?”. This sectioning has the same properties as the previous one. It is not recommended to vary $\mathbf{h}_0$ and keep all other parameters defining sections fixed. Varying $\mathbf{h}_0$ has totally different effects; the corresponding sections do not sum to pole point or pole density plots, but to a uniform distribution instead. They do not display the entire orientation space, neither in equal area nor in the same time, and the view is not complete.

A computer program allows to change the parameters interactively by a single mouse click or drag, and displays the parameters of the plot within the plot. This behavior is important since it allows to explore the data by changing the projections and sections rapidly in a well controlled way and with minimum eye movement. The approach is driven by actively displaying specific regions of the orientation space.

APPLICATION TO ORIENTATION AND POLE PROBABILITY DENSITY FUNCTIONS

Given any generalized section and a location $\mathbf{r}$ in the $\mathbf{h}_0$–pole density plot, with $\mathbf{h}_0$ not parallel to $\mathbf{h}_1$ and with $\mathbf{r}$ not parallel to $\mathbf{r}_1$, the set of orientations

$$G(\mathbf{h}_0, \mathbf{r}, \mathbf{h}_1, \mathbf{r}_1) = \{ g | \mathbf{h}_0 = g \mathbf{r} \text{ and } \angle(\mathbf{r}_1 - (\mathbf{r}_1 \cdot \mathbf{r}) \mathbf{r}, g^{-1} \mathbf{h}_1 - (\mathbf{h}_1 \cdot \mathbf{h}_0) \mathbf{r}) = \gamma \}$$

in the section which is displayed at that specific point contains a single orientation $g \in G$. Then just the density $f(g)$ at that point is rendered using contour level lines and/or shaded iso-planes.

LINKED VIEWS OF ORIENTATION DENSITY FUNCTIONS

When highlighting shall be applied to display an orientation probability density functions, a display of the $\mathbf{h}_0$-pole density of a selected set of orientations in a view already rendering the $\mathbf{h}_0$-pole density of all orientations is required. A set of orientations (which is now an infinite set) is selected in one view of orientations with specific pole directions and the other views shall display, which specimen directions are preferred by other crystallographic directions for that set. The conditional density $\mathbf{h}_0$ given $g$ is in the selected set provides the required information. The idea is to use contouring and rendering of iso-planes of the two densities with two totally different color scales. The unselected density is displayed with a gray-level
The conditional density of the selected set is displayed in a colored scale. Thus the two sets can easily be distinguished. At every point of the pole density plot the larger density is displayed. Optionally, one of the displays may be switched off or the contour lines may be added on top of the other iso–planes which would allow for numerical comparison of two pole densities.

CONCLUSIONS

Any information concerning the location of contributing grains or orientational relationships of neighboring grains would require different data and different experimental techniques than X–ray diffraction, and eventually methods of orientation mapping. The display of orientation and pole probability density conveys only summary information about the texture. Therefore, an orientation probability density function should be displayed in the most sensible possible way, revealing the best possible insight by exhibiting simultaneous orientational relationships of two different crystal axes with two different specimen directions in generalized $\gamma$–sections such that their superposition yields a user–specified pole probability density function.

REFERENCES