3D Visualization of Textures in Metals and Alloys

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In a separate article, we described how one can use the neo-Eulerian orientation representations to create new 3D visualizations of the Rodrigues Fundamental Zones in homochoric, cubochoric, 3D stereographic, Euler and Rodrigues-Frank orientation representations. In the present article, we use these visualization modes to illustrate how one can represent Orientation Distribution Functions as 3D objects. All renderings available below were created using fortran-90 routines (part of release 3.1 of the EMsoft package) which generate input files for the open source PoVRay rendering program. One rendering was performed with the Chimera visualization package.

For most of the Figures of this paper, we provide here two animations; one a regular animation of the object rotating a full circle, the other a red-blue anaglyph movie for which you will need a pair of red-blue stereo glasses. Below are the figure captions for all the figures that have an associated animation; the link represented by M is the regular movie, A represents the anaglyph movie.

Figure 2: (a) Rodrigues space representation of the cube texture component, along with the outline of the Rodrigues fundamental zone for octahedral rotational symmetry [M, A]; (b) stereographic projection of the cube (blue) and Goss (red) texture components[M, A]; (c) cubochoric representation of the Goss texture component[M, A]; (d) [M, A] and (f) [M, A] are Euler space representations of the cube and Goss components, respectively, along with the mapping of the Rodrigues FZ; in (e), both components are represented in the conventional Euler fundamental zone [M, A].

Figure 3: 3D emission map renderings of the synthetic cube (a) [M, A] and Goss (b) [M, A] textures, showing all equivalent orientations in the standard Euler cell; regions of higher orientation density appear as brighter light sources.

Figure 4: (a) Representation of the *(4 pi,4 pi,4 pi)* monoclinic Euler unit cell; orientations in the blueish octants map onto quaternion *q*, the others on quaternion *-q*. (b) equivalent atom positions (*q* blue, *-q* red) along with regular (*n*) and time-reversing (*n'*) diagonal glide planes and the time-reversing translation vectors **a**'/2, **b**'/2 and **c**'/2. (c) unit cell corresponding to the magnetic space group **P_cc** outlined in purple; the symmetry

elements of this space group are indicated by translation vectors. (d) perspective view of the full *(4pi,4pi,4pi)* unit cell along with the monoclinic cell (outlined in purple) for the traditional representation with beta=90° [M, A] .

Figure 5: (a) [M, A] Euler space representation of the experimental cube texture, along with a traditional (100) pole figure in (b); (c) [M, A] 3D stereographic projection of the cube texture inside the octahedral fundamental zone; (d) [M, A] magnification of the central portion of (c).

Figure 6: (a) [M, A] Euler space representation of the experimental Goss texture; (b) ; (c) [M, A] stereographic projection of the Goss texture inside the octahedral fundamental zone; (d) [M, A] magnification of the central portion of (c).

Figure 9: (a) [M, A] Euler space representation of the Rene 88-DT texture; each unique orientation is represented by a small blue sphere in the octahedral Rodrigues FZ. (b) [M, A] 3D stereographic projection of the Ren'e 88-DT texture represented as an emission map inside the octahedral RFZ.

Figure 12: (a) Rodrigues fundamental zones [M, A] for the octahedral and hexagonal rotational groups **432** and **622** as well as the **432-622** disorientation FZ (green wireframe), drawn on the same scale; (b) **432-622** disorientation FZ [M, A]drawn separately, with the unique disorientations cell outlined in red (c) [M, A], and shown separately (d) [M, A]; (e) equivalent hexagonal Rodrigues fundamental zones represented in a 3D stereographic projection [M, A]; note that the sphere is subdivided into 12 zones, with the vertical zones spanning the sphere surface and connecting on the other side. (f) shows the 24 equivalent FZs for the octahedral rotational group **432** [M, A].

Figure 13: (a) [M] and (b) represent two frames of a movie (rendered using the Chimera package showing an iso-surface rendering of the alpha (pinkish) and beta (light blue) orientation distribution histograms in 3D stereographic projection mode; the projection sphere is not shown. The vertical direction in (a) and (b) corresponds to the hexagonal six-fold rotation axis.

Figure 14: (a) Disorientation histogram for unique $alpha-beta$ interfaces, with the BOR disorientation angle of 45.29° indicated by a dashed vertical line; (b) [M, A] hexagonal Rodrigues fundamental zone scatter plot with the twelve equivalent BORs indicated by red spheres; (c) [M, A] and (d) [M, A] unique disorientation cell scatter plots from two different viewing directions. Note the increased density of points near the BOR locations in (b)-(d).

Finally, here is a link to a zip file containing all the PoV-Ray scene description files for the movies above.