RENDERING OF CRYSTALLOGRAPHIC ORIENTATIONS, ORIENTATION AND POLE PROBABILITY DENSITY FUNCTIONS

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Insightful rendering of a multivariate function f is a serious problem, which becomes still more delicate if the domain of the multivariate function is not Euclidean. In the latter case, the projected graph of the function will usually be distorted. Displaying sequences of cross—sections through the domain is the most simple method which generalizes to define instructive projections onto lower—dimensional manifolds as e.g. provided by the spherical X—ray or Radon transform.

Since our particular interest is to render crystallographic orientations and/or their probability density function f defined on $SO(3)$ or, equivalently, on the sphere S^3 of unit quaternions in 4 dimensional real space R^4, spherical projections or spherical means with respect to lower—dimensional manifolds apply. A mathematically distinguished projection is provided by the spherical X—ray transform Xf of a real—valued function f defined on a sphere, which associates with f its mean values Xf along one—dimensional circles with the origin O of the coordinate system as center and spanned by two unit vectors. Crystallographic pole probability density functions are the sum of two spherical X—ray transforms.

Our suggested family of views is parameterized by (i) the orientation of an external coordinate system and (ii) a crystallographic direction h. These two parameters define a projection which is the directional pole probability density function of h. Then sections of the orientation space such that their superposition yields the user—specified h pole probability density function are uniquely defined by choosing (i) a second crystallographic direction h_0, (ii) a distinguished specimen direction r_0 with respect to the external coordinate system, and (iii) an angle γ representing the azimuth of h_0 with respect to r_0. Thus the relation of h and h_0 to the specimen coordinate system is simultaneously visualized.

The kind of spherical projection of the specified sections and the selected projections onto the unit disk determines the distortion of the display. Commonly, the spherical projections preserving either volume or angle are favoured.

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 and knows which views he/she is actually rendering. The only prerequisite to understand the views is to know the spherical projection and the geometrical interpretation of the defining parameters h, h_0, r_0, and γ.

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