Reconstruction of Single-Grain Orientation Distribution Functions for Crystalline Materials -
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Reconstruction of Single-Grain Orientation Distribution Functions for Crystalline Materials
A fundamental imaging problem in microstructural analysis of metals is the reconstruction of local crystallographic
orientations from X-ray diffraction measurements. This work develops a fast, accurate, and robust method for the
computation of the three-dimensional orientation distribution function for individual grains of the material in consideration.
We study two iterative large-scale reconstruction algorithms, the algebraic reconstruction technique (ART) and conjugate
gradients for least squares (CGLS), and demonstrate that right preconditioning is necessary in both algorithms to provide
satisfactory reconstructions. Our right preconditioner is not a traditional one that accelerates convergence; its purpose is to
modify the smoothness properties of the reconstruction. We also show that a new stopping criterion, based on the
information available in the residual vector, provides a robust choice of the number of iterations for these preconditioned
methods.

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