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Heeding Anisotropic "Powder" Diffraction Patterns. Rob Grothe, Molecular Biology Inst., Univ. of California, Los Angeles.

The fundamental difficulty in solving structures from polycrystalline samples can be overcome by reaping the angular variations from anisotropic diffraction images. Most crystallographers willfully destroy this fruit by grinding the sample into powder to facilitate analysis.

An isotropic powder consists of grains sampling all orientations uniformly. Its Fourier transform has spherical symmetry. Thus, reflections with similar Bragg plane spacings cannot be distinguished. Overlap of peaks obscures individual intensities. Systemic overlap often limits the resolution of pattern interpretation.

In this talk, I will demonstrate how the texture (distribution of grain orientations) of an anisotropic sample determines the angular intensity profile of each reflection (ring). I will show how to estimate texture from profiles observed in non-overlapped rings and how to use the texture estimate to reconstruct profiles obscured in overlapped rings.

Finally, I will discuss two ways to convert anisotropic patterns into solved structures: 1) a data reduction process where profile-derived filters extract intensities and 2) a refinement strategy which minimizes differences between calculated and observed angular Fourier coefficients.