MAX3D: Routine Reciprocal Space Mapping

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Abstract

When we use an area detector to collect diffraction data for single crystal structure analysis or polycrystalline solid or film texture analysis we rotate the sample around the $\phi$ or $\omega$ diffractometer axis and store the 3D pattern as distorted slices of reciprocal space. MAX3D is a visualization program which allows us to compile and view the data as a single object – a 3D plot of intensity vs. radial $2\theta$. Seeing the full diffraction pattern allows us to better determine crystal or film quality, identify weak super-lattice reflections or twinning, observe the details of diffuse or incommensurate scattering, monitor phase changes, enhance student understanding, etc. A variety of examples will be presented.