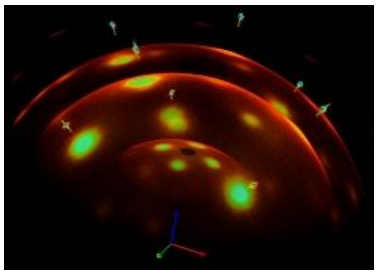
3D Visualization of XRD^3 Texture Data as a Routine Research Tool and an Intuitive Teaching Aid

Victoria M. Jarvis[1], James F. Britten[1], Weiguang Guan[2]
jarvisvm@mcmaster.ca

[1]McMaster Analytical X-ray Diffraction Facility, McMaster University, Hamilton, ON, Canada.
[2]Research and High Performance Computing Support, McMaster University, Hamilton, ON, Canada.

XRD^3 texture analysis is a valuable non-destructive tool for characterizing materials. Full coverage of reciprocal space with texture measurements can now be achieved routinely with the growing availability of rapid data collection and the use of area detectors. Traditional approaches to interpreting texture data involve generating stereographic projections (pole figures) and calculating orientation distribution functions. Although these methods are important sophisticated quantitative tools, they are not always intuitive and don't always tell the full story. Three-dimensional visualization of the data for initial assessment can reveal unexpected scattering behavior in a material. It allows for quick recognition of scattering features including polycrystalline texture, single or twinned crystal diffraction, and diffuse scattering, sometimes observed simultaneously in one sample.

Examples are provided to demonstrate the value of 3D visualization of texture data as a research and teaching tool, using the free MAX3D software package. We present:
(1) GaAs nanowires exhibiting diffuse scattering resulting from stacking faults |
(2) Determination of the orientation matrix of large crystals using single crystal software,
(3) Diffuse lines linking poles on a sphere of reciprocal space,
(4) Isolated 3D pole figures – before stereographic projection,
(5) Illustrations of reciprocal space scan coverage.



Reciprocal space view of InSb nanowires grown on Si (100).