Development of Orientation Quantification for Single Crystal and Textured Polycrystals from Neutron Transmission Data

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It is conventional knowledge that microstructures govern the properties of material and can change dramatically during different stages of material of processing. A detailed understand of the relationship between materials properties and their microstructures is essential for the design and manufacturing of new materials. That relationship motivated the development of numerous techniques to quantify the microstructures in materials. Most of those techniques employ a diffraction technique which measure the intensity of diffraction peaks which depend on the volume fraction of crystals in a sample that are in a diffracting position. Diffraction technique using x-ray can be used to determine the bulk averaged texture in specimen, while technique employing optical microscopy, scanning electron microscopy with electron backscatter diffraction (SEM-EBSD) and X-ray diffraction (XRD) imaging can be used to map grains and their orientation within the sample. The techniques mentioned above are limited by the penetration depth of the radiation - sub-micrometers (SEM-EBSD), and micrometers (XRD imaging). Neutrons generally have a higher penetration depth than both electrons or X-rays, and this expanded penetration depth provides new opportunities for studying bulk samples.

Time-of-Flight (TOF) neutron transmission spectra of single crystal or multi-grain samples are characterized by dips at wavelengths where Bragg's law is being fulfilled for distinctive crystal orientations, which can be used to determine, the number of grains in the sample, the orientation of the grains in the sample, and the size of the mosaic block per grain in the sample. While TOF neutron transmission spectra through ideally random textured polycrystalline samples (small grains and random orientation) are characterized by sudden well-defined step increase in intensity (so-called Bragg-edges) at neutron wavelength locations that exceed the Bragg condition for coherent scattering at that corresponding lattice spacing. For cases, in which the grains orientations are not random (i.e., nearly all manufactured materials), the preferred crystallographic orientation results in TOF neutron transmission spectra characterized by "deformed" Bragg-edges at the location of these "non-random oriented" planes.

In this presentation, I will discuss efforts to recover the orientation matrix of a single crystal using data from neutron transmission measurements. The map of the recovered orientation matrix is validated using Sinpol, which is a collection of routines for calculation of the total cross section that determines the attenuation of neutron beam by crystalline specimen. A similar effort to determine the preferred crystallographic orientation in textured polycrystalline samples is explored.

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