RESIDUAL STRAIN DETERMINATION BY RIETVELD REFINEMENT OF TOF NEUTRON-DIFFRACTION MEASUREMENTS ON DEFORMED URANIUM

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Since recently, an alternative approach to the $\sin^2\Psi$ method of strain determination is becoming more frequently used. It includes the refinement of strain and stress related parameters in Rietveld refinement program. An advantage of this approach is that all available Bragg reflections are used simultaneously to obtain the strain tensor. However, for a successful application in the Rietveld refinement, the challenge lies in the accurate modeling of strain and stress dependence on the crystallographic direction and the ability to handle arbitrary crystal symmetry. A recently published model (N. C. Popa and D. Balzar, *J. Appl. Cryst.*, 34 (2001) 187) allows for accurate modeling of diffraction-line shifts in Rietveld-refinement for all Laue symmetries without making Voigt or Reuss approximations. This is accomplished by expanding strain and stress tensor components in series of spherical harmonics, similarly to the texture modeling. The method yields the texture-weighted strain orientation distribution function (WSODF) and average strain and stress tensors that are usually of engineering interest.

We conducted the neutron TOF measurements on the SMARTS instrument at the Los Alamos Neutron Science Center. The neutron time-of-flight diffraction measurements yield the whole diffraction pattern for Rietveld refinement at every sample orientation. A comparable experiment with constant-wavelength neutrons or x-rays would require an order of magnitude longer data collection time in order to scan through at least several Bragg peaks to provide a sufficient number of data points for Rietveld refinement. Multiple data banks of SMARTS yielded $hkl$-dependent strains for different crystalline and sample directions, which provided us with the required data to fit the spherical harmonics coefficients describing the strain state. The measurements were collected on two samples of uranium (undeformed and plastically deformed), which allowed us to determine changes in the residual strain state after plastic deformation. A particular advantage of the determination of strain tensor through Rietveld refinement is that multiphase components and low crystalline symmetry systems with overlapping reflections can be reliably analyzed. That is one of the reasons why we selected pure uranium for the measurements because of its orthorhombic crystalline structure. Another expected outcome is to shed more light on the elastic-plastic behavior of uranium, a strategically important, although relatively poorly studied material. A comparison of results obtained by a traditional $\sin^2\Psi$ method will also be given.