

Zirconium-based alloys such as Zircaloy-4 is used as nuclear fuel cladding material and in other parts like pressure tubes and fuel spacer grids. Even though Zircaloy-4 has many desirable properties in these applications, its sensitivity to changes in phase distribution (e.g., hydride formation) and chemistry can influence materials properties. For example, α -annealed Zircaloy-4 (α -Zry-4) in its base metal condition has four different preferred orientations (POs) with (002) being the most prominent one. While tungsten inert gas (TIG) welding preserved these POs (Figure 1) of α -Zry-4, hydrogen charging decreased the level of (002) PO and adding two more POs of high reflection angles {(112) and (201)} to the material. These changes in texture can affect the properties of the material. Therefore, chemical phase analysis using X-ray powder diffraction (XRD) is implemented in this study to understand effects of the Zr hexagonal closed-packed unit cell parameters and materials texture on the mechanical property changes. In this endeavor, the full profile fitting of XRD patterns using of general structure analysis system (GSAS) softwareⁱ using the Rietveld method is applied. Due to the influence of many different processing variables that effect the materials chemistry, XRD pattern fitting of Zr-based alloys is challenging. For this reason, many cycles of refinement and the use of different fitting parameters have to be applied in the Rietveld analysis—the profile fit shown in Figure 1a was completed after 902 refinement cycles. These changes in Zr-based alloys chemistry and the Rietveld refinement of the XRD patterns will be discussed in detail in this presentation.

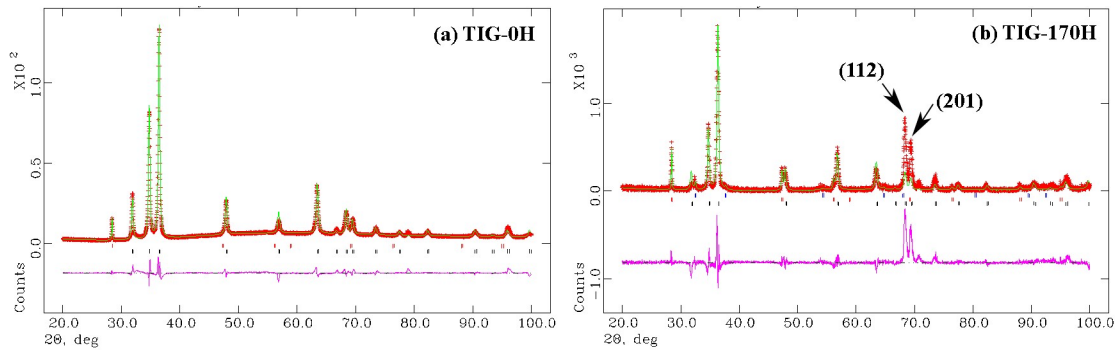


Figure 1. Rietveld analysis of TIG-welded α -Zry-4 samples. (a) Nonhydrogen-charged and (b) hydrogen-charged (170 wppmH). The χ^2 of the fits are 0.21 and 3.63 for TIG-0H and TIG-170H patterns, respectively. The (112) and (201) POs are not added to the profile fits to show their existence in TIG-170H sample. The red, green, and pink color patterns represent the experimental, calculated fit, and the difference patterns, respectively. Red and black color tick marks indicate Si 640d (or 640b) internal standard and Zr-hcp reflection peak positions, respectively.

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ⁱ A.C. Larson and R.B. Von Dreele, "General Structure Analysis System (GSAS)", Los Alamos National Laboratory Report LAUR 86-748 (2000).