# Accurate Lattice Parameter Measurements in a Welded Steel T-Sample

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As part of a project seeking to accurately predict fatigue life of weldments, the Society of Automotive Engineers Fatigue Design & Evaluation Committee (SAE FD&E) has prepared a welded T-sample with substantial residual stress (RS) through its 25 mm thickness [1]. The RS on a through-thickness line in the middle of the T-Joint sample at the weld toe region, where the maximum loading and residual stresses occur, has been measured by several methods. Although the conventional $\sin^2\psi$ RS measurement technique does not require an accurate unstressed lattice parameter ($a_0$) value when evaluating plane stress, high energy x-ray diffraction (HEXRD) and neutron diffraction (ND) techniques do require accurate $a_0$ values. To avoid errors in the RS profile by HEXRD or ND that are potentially introduced by non-uniform $a_0$ values within the sample, the lattice parameter has been measured across a through-thickness cross section in the weld toe region.

In order to obtain the best possible $a_0$ accuracy using a benchtop diffractometer, several unusual steps were taken. Although internal calibration using a reference material (RM) is well known to provide significantly superior results to what can be obtained by external calibration only, the RM cannot be mixed with a solid sample. Instead, the steel specimen was lightly coated with RM from a slurry, thus providing nearly all of the advantages of internal calibration with only a small sample displacement error. No assumption of sample flatness or diffractometer stability is therefore required. The small sample displacement error due to the RM coating thickness, along with other aberrations, is corrected by using the Nelson-Riley (N-R) extrapolation [2]. Since α phase steel has only a few accessible peaks using the standard cobalt anode, a Co tube with spectral contamination was purposely used in order to obtain diffraction patterns with more peaks and thus more data points contributing to the N-R extrapolation. At each data point in the 2θ scan, a full spectrum was saved; then separate diffractograms were generated for each characteristic line of the tube, including Co Kα, Co Kβ, Cu Kα, and Cu Kβ. Even though Kβ peaks do not usually exhibit the splitting observed in Kα peaks at higher angles, Kβ peaks also have multiple contributions which cause noticeable distortion from any of the usual peak profile functions. Therefore, Kβ peaks were fit to sums of peaks based on high resolution spectra of the characteristic emission lines. At each step of the analysis, error propagation is maintained, including using weighted least squares fitting for the extrapolation, thus providing improved estimates of $a_0$ and the uncertainty thereof.

[1] Mach, Justin et al., “FD&E Total Life T-Sample Residual Stress Analytical Predictions and Measured Results,” SAE Technical Paper 2019-01-0528, 2019-, https://doi.org/10.4271/2019-01-0528.

[2] Nelson, J. B., & Riley, D. P. “An experimental investigation of extrapolation methods in the derivation of accurate unit-cell dimensions of crystals.” *Proceedings of the Physical Society, 57*(3), 160-177.