



## Application Report XRD 16

## DIFFRAC.DQUANT: Norm compliant quantification of retained austenite

The Ratio Method implemented in DIFFRAC.DQUANT and precise intensities measured with the D2 PHASER benchtop diffractometer allow the accurate determination of retained austenite levels in steel. This helps in optimizing heat treatment which is key for tuning the mechanical properties of the steel.

Quantitative phase analysis by X-ray diffraction is one of the most accurate and established methods for the determination of the amount of austenite in steel. Austenite (or gamma-iron) is a high-temperature form of iron. Upon quenching it incompletely transforms to martensite (alphairon, or ferrite) during the production of carbon steels. This transformation process is crucial for the strength and other mechanical properties of steel. Subsequent heat treatment during steel production may further change the austenite concentration. Furthermore the cooling conditions influence the microstructure of the steel. This is resembled in the degree of texture (or preferred orientation) of the austenite/ martensite crystallites.

XRD data were collected using a D2 PHASER benchtop diffractometer, equipped with a LYNXEYE linear detector and cobalt radiation. The size and shape of the samples is limited for the D2 PHASER, whereas the D8 series of instruments allows for much more flexibility in sample dimensions and geometry. The Ratio Method is used for calculating concentrations directly from the ratio of intensities of phases without the need for calibration. Protocols such as ASTM E 975 or SAE SP-453 provide standardized procedures for obtaining results with an accuracy level of 0.5% or better. The intensity of an X-ray powder diffraction peak is, amongst others, directly proportional to the concentration of the phase, and trigonometric intensity factors. Those factors are constant for a given experimental setup (geometry and wavelength), diffraction peak and crystal structure. The trigonometric factors can be taken from literature, or can be directly calculated from available crystallographic data. Using the respective trigonometric factors, the ratios of the intensities therefore directly yield the concentrations.

Figure 1 shows the graphical definition of the peak ranges for the intensity determination. From these intensities and the respective trigonometric factors ratios are defined in the expression editor (see Figure 2). Those ratios correspond to the concentration of retained austenite in the martensite matrix. In the method, multiple pairs of peaks are used. If differences in concentration calculated from different pairs are observed, this is indicative of texture in the material.



Figure 1: Standard scan chart in DIFFRAC.DQUANT. The orange and green colors represent the integration ranges for austenite and martensite, light blue ranges correspond to background areas.



Figure 2: Concentration/Intensity chart in DIFFRAC.DQUANT. The lower panel represents the background corrected integral intensities as defined graphically (see Figure 1). The upper panel shows the austenite concentrations expressed as intensity-ratio modules, which are defined in the expression editor.



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