

Comparison of Residual Stress Measurement Techniques and Implementation Using X-Ray Diffraction

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Abstract. Regardless of the particular residual stress (RS) measurement technique being used, all are based on the same basic principles when using x-ray diffraction (XRD). Every technique has both its advantages and disadvantages, many of which are well known to engineers and scientists however, some of the important “finer points” are unfortunately not widely discussed or known by those not well versed in the subject. This paper will try to bring to light many of these commonly misunderstood issues by comparing the different techniques and attempt to illuminate the associated problems a user may encounter when measurements become challenging i.e. when RS measurements are to be performed in tight grooves or on textured materials for example. In this study, different techniques including the: $\text{Cos}\alpha$ technique, MET (used in Psi, Omega, or Modified Psi mode) have been evaluated and tested on a variety of materials and geometries.

Introduction

RS measurements using XRD techniques were first performed as early as 1925 [1]. Since then, measurement techniques and equipment slowly evolved in the following decades and major improvements were realized in the 1970s and the 1980s. Many RS measurement techniques based on XRD have been developed and implemented on a variety of instruments that are widely used in industry and academia today. As the use of XRD became more widespread in the 1950s, a technique called the Single Exposure Technique (SET) was commonly used however, it had very limited accuracy and did not work well on materials that did not possess a near random grain orientation distribution. Furthermore, the SET used only 1 data point, and relied on precise knowledge of the unstressed lattice spacing which was often difficult to determine experimentally with sufficient accuracy on the actual components or samples under investigation. As such, the quality of the data was very difficult to assess because non-linear relationships cannot be observed with only 2 data points. Due to the inherent limitations of the SET, scientists and engineers developed a new technique called the Multiple Exposure Technique (MET) which uses many more data points resulting in high confidence RS measurement results that do not rely on knowing the unstressed lattice spacing a priori [2]. Since then, many related standards have been developed, accepted and applied to the measurement of RS via XRD worldwide.

In this study, different techniques including the: $\text{Cos}\alpha$ technique, MET (used in Psi, Omega, or Modified Psi mode) will be evaluated and tested on a variety of materials and geometries. This paper will emphasize the different findings and the limitations associated with each of the techniques evaluated.

Principles

Generalized technique: these principles apply to MET when used in either Omega or Psi mode. The XRD technique uses the distance between crystallographic planes, i.e. d-spacing, as a strain gage and can only be applied to crystalline, polycrystalline and semi-crystalline materials [2]. When the material is in tension, the d-spacing increases and when the material is in compression, the d-spacing

decreases. The presence of RS in the material produces a shift in the XRD peak angular position that is directly measured by the detector [3]. For a known x-ray wavelength λ and n equal to unity, the diffraction angle 2θ is measured experimentally and the d-spacing is then calculated using Bragg's law:

$$n\lambda = 2d \sin \theta \tag{1}$$

Where λ is the wavelength of the radiation. Once the d-spacing is measured for unstressed (d_0) and stressed (d) conditions, the strain is calculated using the following relationship:

$$\varepsilon = (d - d_0)/d_0 \tag{2}$$

For the $\sin^2\psi$ method where a number of d-spacings are measured, stresses are calculated from an equation derived from Hooke's law for isotropic, homogeneous, fine grain materials:

$$\varepsilon_{\phi\psi} = \frac{1}{2} S_2 (\sigma_{\phi} - \sigma_{33}) \sin^2 \psi + \frac{1}{2} S_2 \sigma_{33} - S_1 (\sigma_{11} + \sigma_{22} + \sigma_{33}) + \frac{1}{2} S_2 \tau_{\phi} \sin 2\psi \tag{3}$$

Where, $\frac{1}{2} S_2$ and S_1 are the x-ray elastic constants of the material, σ_{ϕ} is the stress in the direction of the measurement ϕ , ψ is the angle subtended by the bisector of the incident and diffracted x-ray beam and the surface normal, and $\varepsilon_{\phi\psi}$ is the crystallographic strain at a given ψ tilt, see figure 1.

The main difference between the Omega and Psi modes can be seen in the defocusing effects observed at high ψ angles. RS measurements performed in Psi mode are relatively insensitive to defocusing errors when compared to Omega mode. The increased defocusing effect and associated errors observed in Omega geometry can be mitigated by employing two detectors which can be used to minimize the magnitude of negative ψ angles employed in a RS measurement and thus minimize defocusing errors. At the same time, care must be taken in the selection of the incident x-ray beam size to limit both defocusing and beam divergence errors [2]. Moreover, Psi mode offers a constant absorption of x-rays for all ψ tilts due to the constant x-ray path whereas, in Omega mode the absorption varies with the ψ tilt angle and requires a correction. The depth of penetration is very similar for both modes except at high ψ tilt angles [4].

Modified Psi. When working in Modified Psi mode which is a special geometry set-up convenient for vertical beam direction, the x-ray

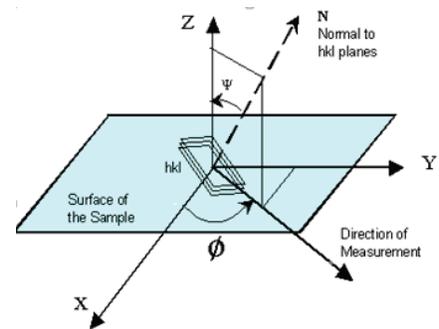


Figure 1: Definition of the axis and the direction of measurement.

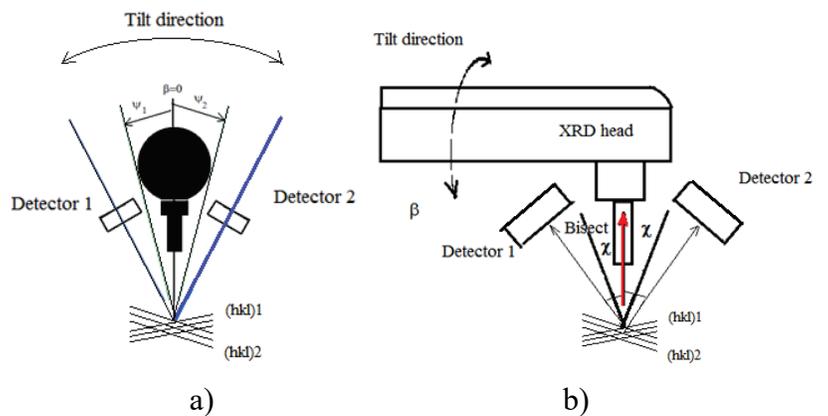


Figure 2: Goniometer geometries: a) Omega mode and b) Modified Psi mode.

beam is perpendicular to the surface of the sample and the diffracting {hkl} planes lie in a plane with an angular offset of $(180-2\theta)/2$ and the ψ angles for each plane vary with the inclination, see figure 2. In this case, for each normal to the {hkl} plane, the ϕ and ψ are a function of the goniometer tilt angle as shown in Eq. 4. The relationship between the β , χ , ψ , and ϕ angles are shown in Eq. 4 and Eq. 5.

$$\cos \psi = \cos \beta \cdot \cos \chi \tag{4}$$

$$\cos \phi = \frac{\sin \beta \cdot \cos \chi}{\sin \psi} \tag{5}$$

Where β is the tilt angle and χ is the offset angle between the incident beam and the bisector of incident and diffracted beams. The derived Eq. 6 is shown as follows:

$$\begin{aligned} \varepsilon = & \frac{1}{2} S_2 (\sigma_{11} \sin^2 \beta \cos^2 \chi + \sigma_{22} \sin^2 \chi) \\ & + \frac{1}{2} S_2 (\tau_{12} \sin \beta \sin 2\chi + \tau_{13} \sin 2\beta \cos^2 \chi + \tau_{23} \cos \beta \sin 2\chi) + C \end{aligned} \tag{6}$$

The technique does not provide a direct measurement of the shear stress which is necessary when dealing with curved surfaces and non uniform processes applied to heterogenous materials. This technique also requires two detectors at opposite ϕ angles [5]. The most accurate measurement for this configuration is a triaxial measurement where tilt angles ψ , ϕ can be correctly used as in the $\text{Sin}^2\psi$ method [6].

Cos(α) method. This method uses the diffraction ring (also called the Debye Ring) where the position of the peak at each angle α around the ring is measured [7]. This special set-up which doesn't required any change in the incident angle. Using the relationship between the derived strains in Eq. 7 and Eq. 8, one can plot the strain as a function of $\cos \alpha$ to calculate the normal stress σ_{11} and as a function of $\sin \alpha$ to calculate the shear stress σ_{12} .

The constitutive equations are as follows:

$$\varepsilon_{\alpha 1} = \frac{1}{2} [(\varepsilon_{\alpha} - \varepsilon_{\pi+\alpha}) + (\varepsilon_{-\alpha} - \varepsilon_{\pi-\alpha})] = \frac{1}{2} S_2 \cdot \sigma_{11} [\sin^2(\psi_0 - \eta) - \sin^2(\psi_0 + \eta)] \cos \alpha \tag{7}$$

$$\varepsilon_{\alpha 2} = \frac{1}{2} [(\varepsilon_{\alpha} - \varepsilon_{\pi+\alpha}) - (\varepsilon_{-\alpha} - \varepsilon_{\pi-\alpha})] = \frac{1}{2} S_2 \cdot 2\tau_{12} \cdot (\sin 2\eta \sin \psi_0) \sin \alpha \tag{8}$$

Where ψ_0 is the inclination of the sample relative to the goniometer, 2η is the angle subtended by the incident beam and diffracted beam, and ε_{α} , $\varepsilon_{\pi+\alpha}$, $\varepsilon_{-\alpha}$ and $\varepsilon_{\pi-\alpha}$ are the measured strains from sectors of the ring as shown on figure 3.

When using Eq. 7 and Eq. 8, it is necessary that symmetrically opposite peaks are available on the Debye Ring. It should be noted that $\psi_0 \neq 0^\circ$ when using this technique. It is recommended to tilt the head in such a way that one side of the Debye Ring represents ψ angles close to 0° , and the other side of the ring

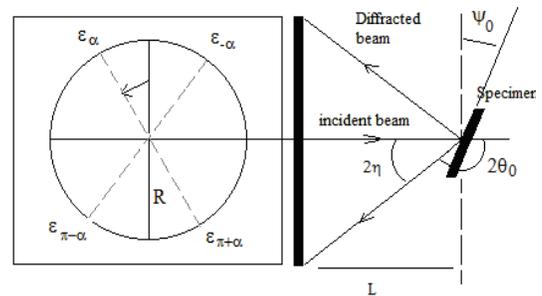


Figure 3: Principle of Cos α method using Debye Ring

represents ψ angles as high as possible to better represent the strains present. The shear stress σ_{12} provided by this technique is not of interest at this moment.

Experiments

Three samples were selected for RS measurement on the surface employing all of the aforementioned techniques. The samples were as follows: 1) a shot peened flat steel sample with a grooves that were flat at the bottom with nominal stress of -450 ± 35 MPa, 2) an aluminum plate with low stress that exhibits some preferred orientation, and 3) a flat shot peened Ni-base alloy sample with a nominal stress of -1040 ± 50 MPa. No measurements were performed with Psi and Modified Psi modes on this sample. The error reported is only 1 Standard deviation.

In the case of the steel sample, RS measurements were collected in both the axial direction parallel to the grooves, and in the direction transverse to the grooves. The groove dimensions were as follows: Groove 1 (GR1): 2 mm wide by 1.5 mm deep, and Groove 2 (GR2): 2 mm wide by 2 mm deep. The most important parameters that determine the capability of any measurement technique and associated goniometer hardware to successfully measure RS in confined areas such as grooves are: 1) the angular opening between the incident beam and diffracted beam, and 2) the direction of ψ tilting associated with the RS measurement. RS measurements were performed employing 4 different goniometers thus using all available geometries.

All of the RS measurements on the steel and aluminum samples were performed using Cr α ($\lambda=2.291\text{\AA}$) x-radiation diffracting from the {211} plane at $156^\circ 2\theta$, and the {222} plane at $157^\circ 2\theta$ respectively. RS measurements on the Ni-base alloy sample were performed using Cr β ($\lambda=2.08487\text{\AA}$) x-radiation diffracting from the {311} plane at $149^\circ 2\theta$ when using the $\text{Cos}(\alpha)$ technique, and Mn α ($\lambda=2.10314\text{\AA}$) x-radiation diffracting from the {311} plane at $152^\circ 2\theta$ when using the other techniques. Table 1 lists the available angular tilt range ψ for each technique using the diffraction conditions reported above. The aperture size used in the experiment was 1 mm except the cos α where the aperture was 2 mm. A mask is applied on the top around the grooves to avoid any diffraction from those surfaces.

Table 1: Goniometer capability and ranking for GR1:W:2 mm x D:1.5 mm, GR2:W:2 mm x D:2 mm

Goniometer Geometry/Mode	Technique	Angular opening ($^\circ$)	Angle GR1 @ $\psi=0$ ($^\circ$)	Angle GR2 @ $\psi=0$ ($^\circ$)	Selection (Groove)
PSI	$\text{Sin}^2\psi$	24	33.7	26.5	Transverse
Omega	$\text{Sin}^2\psi$	48	33.7	26.5	Axial
Modified PSI	$\text{Sin}^2\beta$	48	33.7	26.5	Transverse
Debye Ring	$\text{cos}\alpha$	48	33.7	26.5	None

As such, when measuring RS in the bottom of grooves it is desirable to have a goniometer (or 2 goniometers) that work in both Psi and Omega modes so as to enable RS measurements in two directions.

Results and Discussions

RS measurements were performed employing the 4 different goniometers. The results reported in table 2 indicate that the RS measurements in the axial direction were performed relatively easily in GR1 using all of the techniques. RS measurements performed in the transverse direction in GR1 were possible using Psi and Modified Psi with reduced accuracy due to the limited ψ tilt range available. RS measurements in the transverse direction of GR1 were not possible using $\text{Cos}\alpha$ and Omega because of the very limited ψ tilt range available in these geometries. Any result not within 2 standard deviation for each material is considered failed.

Table 2: RS measurement results on different head goniometer geometries and techniques.

Goniometer Geometry/Mode	Technique	Direction	Steel sample GR1 (-470±70 MPa)	Steel sample GR2 (-450±70 MPa)	Al sample Low stress <50MPa	Ni-Base alloy sample (-1040±100MPa)
PSI	Sin ² ψ	Axial	-524±19	-228±36*	+28±8	N/A
		Trans	-526±15*	-204±26 ^F	+1±10	
OMEGA	Sin ² ψ	Axial	-435±8	-475±5	+12±13	-1070±50
		Trans	F	F	-21±6	
Modified PSI	Sin ² β	Axial	-443±5	-596±11 ^F	+18±12	N/A
		Trans	-386±19*	-188±46 ^F	+13±8	
Debye Ring (2D detector)	Cosα	Axial	-485±42	-642±234 ^F	-29±31	-719±50 ^F
		Trans	F	F	-86±10 ^F	

Note: * indicates results were corrected after removing bad data points, F indicates a failed measurement
 N/A indicates data not available

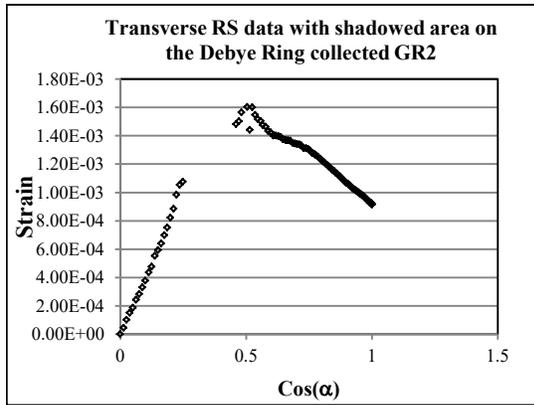


Figure 4: Strain vs. Cosα data plot observed measuring RS in the groove area

angle. For Cosα, because of the ψ tilt angular range necessary to perform a reliable RS measurement, a portion of the Debye-Ring is masked (or shadowed) and the data obtained is rendered unusable i.e., when using the Cosα technique on GR2, high ψ angles are not an option so the data missing from the Debye-Ring renders the strain calculation useless (see Figures 4 and 5). As an analogy, this is equivalent to attempting to use Psi or Omega Modes to calculate the shear stress when all of the positive (or negative) ψ tilts are not available for the calculations.

One approach to making all the above techniques successful is to remove the material around the location of interest (i.e. the bottom of the groove) so as to expose the location of interest. The disadvantage to this approach is that the part must be sacrificed at the expense of the RS measurements and as such only non-production parts would be analyzed.

For GR2, the RS measurements failed in all directions in all Modes except using Omega Mode in the axial direction. Omega-Mode is the only one that is capable of accurately measuring RS in the bottom of a very narrow, deep groove in the axial direction. In such cases, the beam size must be selected carefully and in some instances, a mask on top of the groove may be used to obtain reliable RS results. The success of Psi-Mode in the axial direction is related to the narrow angle opening between the beam and the detector (i.e. the high back reflection {hkl} selected in this particular instance). The Psi-Mode data was corrected after removing bad points at high ψ tilt

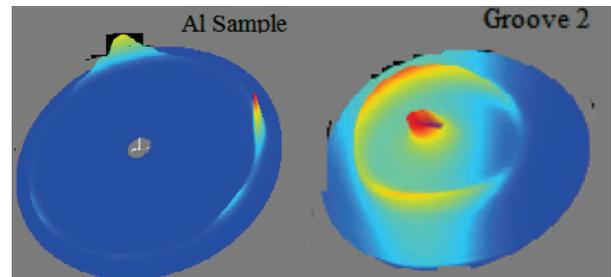


Figure 5: Debye Ring data measured in the groove 2 and Al sample

For the aluminum sample, all methods were capable of producing RS results within an acceptable range however, some scatter was observed due to the texture present in the material only, no size effect was observed during the measurements. The $\text{Cos}\alpha$ technique had more difficulties and the measurements were repeated few times before a stress value could be calculated [8]. This is because of spotty data on the Debye Ring. This confirms the problem with the shadowing effect observed in the grooves. When looking at the slope of the data curve for a given RS value, the $\text{Cos}\alpha$ technique has a reduced slope when compared to the other techniques [9]. This explains the high experimental errors in the RS values.

When perform RS measurements on the Ni-Base alloy sample, the $\text{Cos}\alpha$ technique failed due to the weak peak intensity collected using $\text{Cr}_k\beta$ line. RS measurements using the Omega technique worked well however no measurements were performed with Psi and Modified Psi modes on this sample .

Summary

The results obtained indicate that amongst the various techniques applied to RS measurement, the MET using $\text{Sin}^2\psi$ was capable of measuring RS on a wide variety of materials with different geometries and material conditions whereas the $\text{Cos}\alpha$ technique was limited to isotropic materials and near flat surfaces. Moreover, the Omega-Mode was the only one that was capable of measuring RS in deep grooves in the axial direction. The use of Psi-Mode may be advantageous when tight constraints related to the geometry of the test specimen become an issue. The Psi-mode goniometer is preferred when compared to the Modified Psi-mode goniometer because the latter is more limited in terms of sample geometry constraints and the scattering vector is offset from the ψ tilt plane. For successful RS measurements on a wide variety of components as well as in confined spaces and complex geometries, a combination of Psi and Omega Modes are ideal. For the $\text{Cos}\alpha$ technique to be viable for RS measurement, more development would be required to deal with scattered data on the Debye Ring and its various geometric limitations.

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