DETERMINATION OF THE STRESS DISTRIBUTION FUNCTION BY X-RAY DIFFRACTION USING FOURIER ANALYSIS

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Abstract. *The residual stress has a large influence on the mechanical behavior of the alloys and composite. The modern surface treatment techniques introduce residual stress, which may be characterized by strong stress gradient. Therefore, in order to measure and to control such stress gradients, new and reliable experimental methods have been developed worldwide.*

The X-ray diffraction method is widely used in the stress measurement; however, as a drawback, some difficulties may arise in the interpretation of the experimental data when the depth of the X-ray penetration is of the same order of magnitude of the variation of the stress caused by the gradient. Such misinterpretation is mainly due to the non-linearity of the $\theta_{\varphi,\psi}$ vs. $\sin^2\psi$ *dependency in the gradient presence. Therefore the* $\mathrm{sen}^2\,\psi$ *method cannot be used in the calculation of the stress distribution function in the material surface.*

The Fourier Transform is a powerful mathematical tool in the crystallography diffraction methods. It is used in the research and analyses of crystalline materials. In this work we presented a methodology for the calculation of the stress distribution function using Fourier analysis and the convolution/deconvolution functions.

Keywords*: X-ray diffraction, residual stress, Fourier transform, convolution, deconvolution*

1. Introduction

One of the most important factors that determines the mechanical behavior of the materials are the mechanical stress that act in the materials in the absence of external loads and/or temperature gradient, knowing as residual stress. Most of the characteristics of this behavior depend essentially of the values and distribution of the residual stress in the material.

The modern material surface treatments, as laser, ionic implantation among others, create stresses, located in the surface layers and characterized by strong gradient (Assis J. et al, 2003). The residual stresses that appear after these processes can improve the performance of the materials front to the aggressiveness of environment and reduce the fatigue failure (Martins C. O. D et al, 2004). For that reasons became necessary to incorporate information regarding the residual stress and to develop reliable methods for its determination (Lu J.). The most common method to measure residual stress is the X-ray diffraction. The traditional method of X-ray tensomety is known as “$\sin^2\psi$ method” This method presents limitations in the interpretation of the experimental data when the depth of the X-ray penetration is comparable with the variation of the stress caused by the gradient. The principal equation of this method comes from the theory of elasticity, and is known as “deformation - $\sin^2\psi$” dependence (Timoshenko S.P., 1980):

$$\sigma_\varphi = -\frac{E}{1+\nu} ctg\theta_0 \frac{\partial\theta_{\varphi,\psi}}{\partial\sin^2\psi} \qquad (1)$$

Where, ν and E are the elasticity constants, ψ and φ are the angular coordinates in the spherical system, σ_φ is the stress that acts in the φ direction and $\frac{\partial \theta_{\varphi,\psi}}{\partial \sin^2 \psi}$ is the inclination angle tangent of this function. If the material is stressed close to the surface with a gradient ($\hat{\sigma} = f(z)$), each layer (dz) in a depth (z) will produce its own displacement of diffraction peak ($\Delta\theta = g(z)$). Then, the $\theta_{\varphi,\psi}$ vs.$\sin^2 \psi$ relation became non linear, since the value $\frac{\partial \theta_{\varphi,\psi}}{\partial \sin^2 \psi}$ is not a constant. Each layer contributes in the experimental diffraction profile with its own displacement value and with its own intensity value. If the inclination angle ψ is altered, it is also varied the penetration depth, causing a different contribution from each layer in the final profile, and the linearity of the dependence is lost. For that reason, turns impossible to use this method in the determination of the stress gradient. Another process, such as the introduction of textures, also causes non-linearity in this relation but will be not discussed in this work.

In this paper we present a new technique of measurement the residual stress by the X-ray diffraction method in the presence of strong gradients close to the material surface. Firstly we discussed a computational solution to obtain the diffraction profile line with strong gradient stress. With this solution we can obtain a stress gradient existence criterion. Then applying a signal processing techniques (the Fourier analysis and the concepts of convolution and deconvolution) we developed a methodology that allows the simulation of the diffraction profile broadened by the stress gradient. This simulation permits the resolution of the inverse problem; obtain the stress distribution function having the diffraction profile line broadened by the presence of a stress gradient.

2. Direct simulation of diffraction profile

In the presence of stress gradient, every layer (dz) produces its own displacement value ($\Delta\theta(z)$), then when the inclination angle of the incident beam change the total profile won't dislocate lineally. We can express the diffraction profile $I(\theta,\varphi,\psi)$, as the sum of the contribution of each layer in the profile:

$$I(\theta,\varphi,\psi) = \int_0^\infty I(\theta) e^{-\mu t(\varphi,\psi,z)} dz \tag{2}$$

The attenuation of the radiation in each layer is expressed as:

$$I_{dif} = \alpha I_0 e^{-\mu z} = \alpha I_0 e^{-\mu t\left(\frac{1}{\cos(\psi+90-\theta)}+\frac{1}{\cos(\psi-90+\theta)}\right)} \tag{3}$$

where α is the proportionality coefficient containing all the factors of the diffracted intensity, as the Lorentz polarization factor, the structural factor and of multiplicity among others. The diffraction angle of the profile (θ), depends of the layer depth and the stress distribution function given for:

$$\sigma(t) = \sigma_0 f(kt) \tag{4}$$

where σ_0 is the material surface stress, k is the parameter of the stress gradient and f is the function that represents the distribution form.

Using the “deformation - $\sin^2 \psi$” dependence applied in the case of uniaxial stress, and the Bragg law, that relates the diffraction angle and the deformation, we can obtain the diffraction angle as a function of the stress.

$$\theta_\psi = \theta_0 - \frac{\sigma(t)\left(\sin^2\psi - \nu\cos^2\psi\right)}{E \quad ctg\theta_0} \tag{5}$$

Then we can calculate the position of the peak of each component of the diffraction profile and we can obtain the function $I_{\theta,\varphi,\psi}$. This profile is approximating by a Gauss or Cauchy function. Using this methodology, through the computational modeling, the simulated diffraction profile is calculated, knowing the distribution of the stress gradient. The computational simulations of this numerical methodology are shown in figs. 2-4 for the functions shown in fig.1.

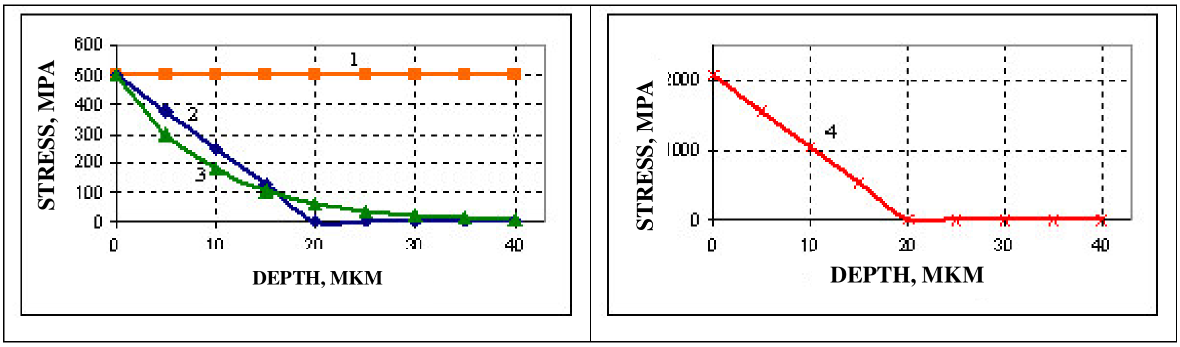
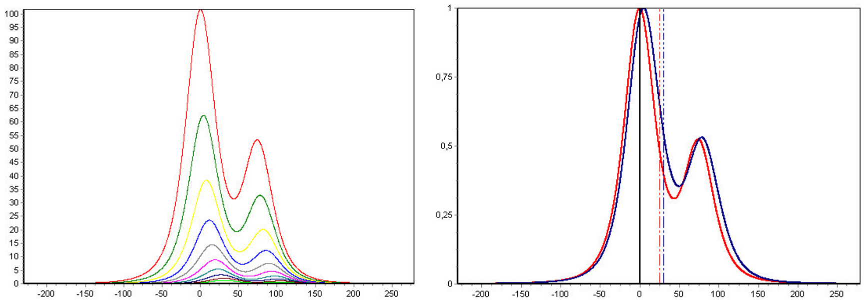
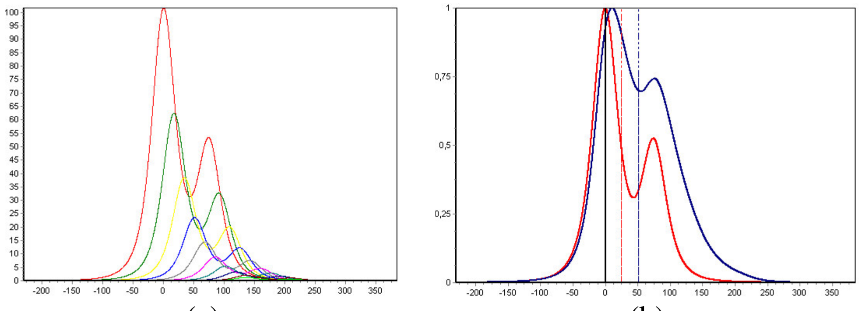


Figure 1 Patterns function using in the simulations 1- $\sigma = 500 Mpa$, 2- $\sigma = 500 - 25t$, 4- $\sigma = 500e^{-0.103t}$ 4- $\sigma = 2075 - 103t$



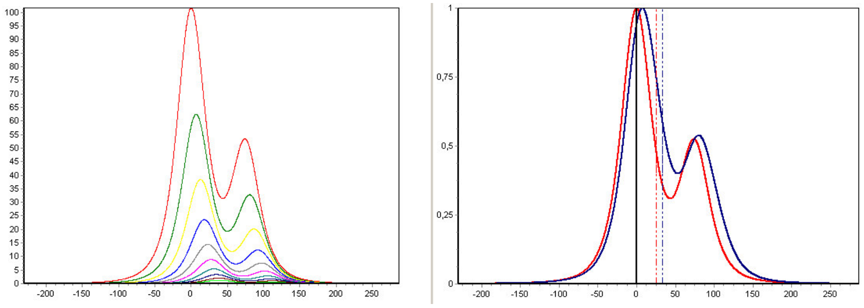
(a) (b)

Figure 2. Diffraction line profile simulation for linear stress ($\sigma = 500 - 25t$), Inclination angle ($\psi = 60^0$), Mesh $1\mu m$ (a) Individual Profiles (b) Broadening profile and free stress profile (Integral breadth $B_{stand.} = 8{,}2;\ B_{total} = 8.7$).



(a) (b)

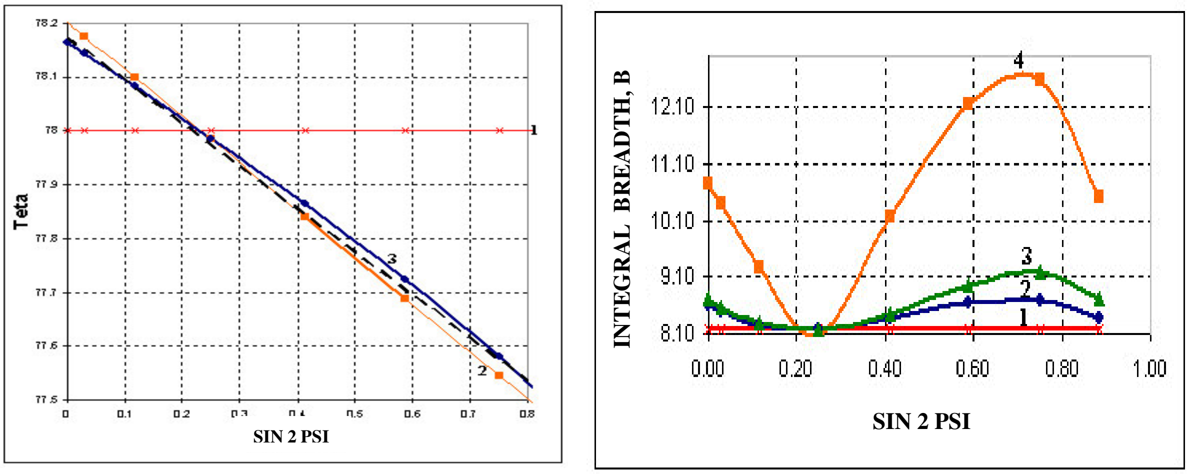
Figure 3. Diffraction line profile simulation for linear stress ($\sigma = 2075 - 103t$), Inclination angle ($\psi = 60^0$), Mesh $1\mu m$ (a) Individual Profiles (b) Broadening profile and free stress profile (Integral breadth $B_{stand.} = 8{,}2;\ B_{total} = 9.2$).



(a) (b)

Figure 4. Diffraction line profile simulation for exponential stress ($\sigma = 500e^{-0.103t}$), Inclination angle ($\psi = 60^0$), Mesh $1\mu m$ (a) Individual Profiles (b) Broadening profile and free stress profile (Integral breadth $B_{stand.} = 8,2;\ B_{total} = 12.9$).

With this methodology it is possible to obtain the diffraction profile and verify the distortion produced by the presence of a known stress gradient. This fact is an indication of the existence of this stress gradient. Then the integral breadth can be used as an existence stress gradient criterion instead the non-linearity of the θ vs. $\sin^2\psi$ relationship. We can observe in Fig. 5, that the non-linearity is not enough market to used as a good criterion. However this methodology don't solve our first problem, the determination of the stress distribution function from a distorted diffraction profile (experimental or simulated).



(a) (b)

Figure 5. (a) θ vs. $\sin^2\psi$ Relation. Angles ($0^0 - 90^0$). 1-Stress free ($\sigma = 0$) 2- Constant stress ($\sigma = 500MPa$), 3-Stress with gradient ($\sigma = 500 - 25t$), --- Linear Regression. (b) Integral Breadth vs. $\sin^2\psi$ Relation. Angles ($0^0 - 90^0$) 1-Constant stress ($\sigma = 500Mpa$), 2-Gradient ($\sigma = 500 - 25t$), 3-Gradient ($\sigma = 500e^{-0.103t}$), 4-Gradient ($\sigma = 2075 - 103t$).

3. Simulation of diffraction profile using Fourier analysis

The Fourier Transform is an important and well succeed applied tool in the diffraction methods for the research and analyses of crystalline materials. This tool has been used in applications in the study of structural distortions (Warren, B. E., 1969) and in diffraction problems as the separation of the X-ray K_α peaks describing the profile with Fourier coefficients (Gangulee, A., 1970).

In agreement with the Fourier Transform theory, the experimental diffraction line $h(x)$, can be expressed by the convolution of the pattern function $g(x)$ and the distortion function $f(x)$:

$$h(x) = \int_{-\infty}^{+\infty} g(\tau) f(x-\tau) d\tau \tag{6}$$

In terms of the Fourier transformation this situation can be expressed as:

$$H(\tau) = G(\tau) * F(\tau) \tag{7}$$

where $H(\tau)$, $G(\tau)$ and $F(\tau)$ are them Fourier Transform of the corresponding previous functions. For the case of the broadening of the diffraction line caused by the stress gradient, the distorting function $f(x)$ depends of the attenuation of the X-ray beam in the material $I(x)$ and the stress distribution $\sigma(x)$. Analyzing the influence of these two factors we can consider:

$$f(x) = I(x)\sigma(x) \tag{8}$$

Being x the angular coordinate of the diffraction line. The limitation of this approach is that the involved functions doesn't depend directly on the angular coordinate (θ), however depends of the depth of the material (t). This limitation is solved in the numeric calculation process when we transform t in θ, using Eq. (5) and substituting in Eq. (3), then we obtain the intensity depending of the diffraction angle. The Figs. 6-8, represents the simulations of the diffracted profiles using the convolution procedure. The comparison of the integral breadth of the two simulations, (see Table 1), validates the results for the use of the Fourier Transform, in the solution of this problem. This validation allows use the inverse procedure for the determination of the stress distribution.

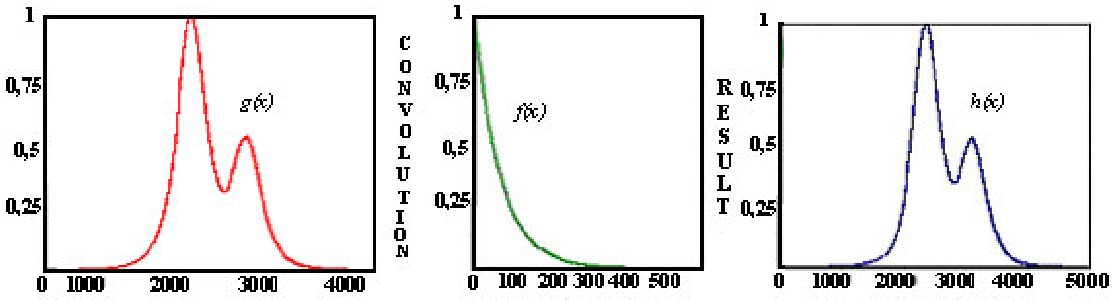


Figure 6. Diffraction line profile simulation using Fourier analysis for linear stress ($\sigma = 500 - 25t$) (Integral breadth B_{total} =*8.6)*.

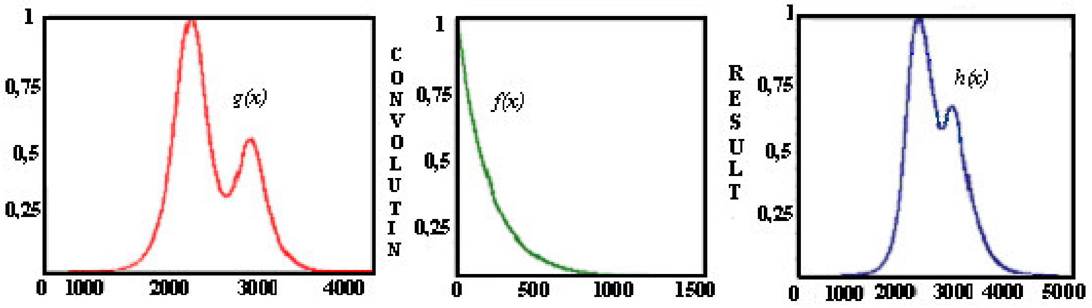


Figure 7. Diffraction line profile simulation using Fourier analysis for exponential stress ($\sigma = 500e^{t0.103}$) (Integral breadth B_{total} =*10.1)*.

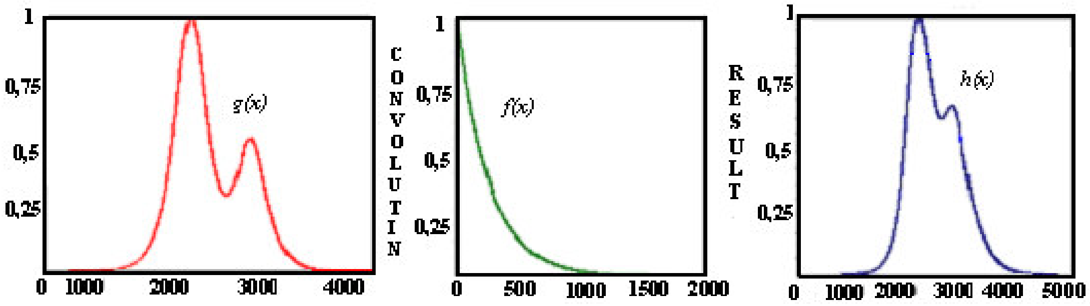


Figure 8. Diffraction line profile simulation using Fourier analysis for exponential stress ($\sigma = 1025 - 103t$) (Integral breadth B_{total} =*11.8).*

Table 1. Integral Breadth obtained in Direct Simulation and Simulation by Fourier analysis

Gradient	Integral Breadth		Standard Deviation	%
	Direct Sim.	Fourier Sim.		
$\sigma = 500 - 25t$	8.7	8.6	0.01	1.15
$\sigma = 1025 - 103t$	12.6	11.8	0.06	6.35
$\sigma = 500e^{t0.103}$	9.2	9.8	0.07	6.52

The inverse procedure, applied in the calculation of the gradient distribution function is given by the Eq.(9), when we obtain distortion function, and then using Eq.(8) is we compute the stress distribution function:

$$F(x) = \frac{H(x)}{G(x)} \tag{8}$$

The results of this procedure are presented in the figures 9-11. The restored stress functions are in the right of the figures.

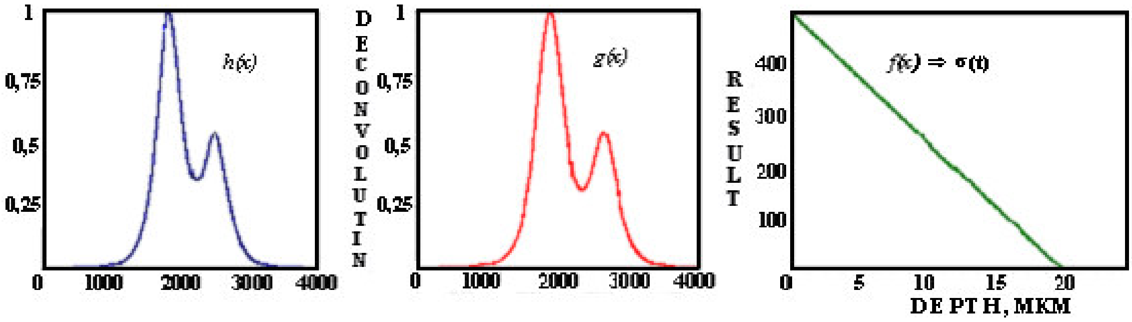


Figure 9. Stress distribution function restoration by the deconvolution of the final profile and the distortion function. Stress gradient $\sigma = 500 - 25t$

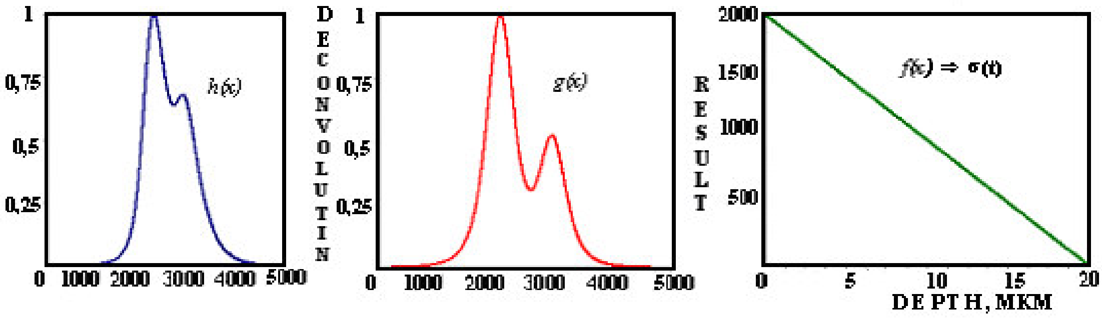


Figure 10. Stress distribution function restoration by the deconvolution of the final profile and the distortion function. Stress Gradient $\sigma = 1025 - 103t$

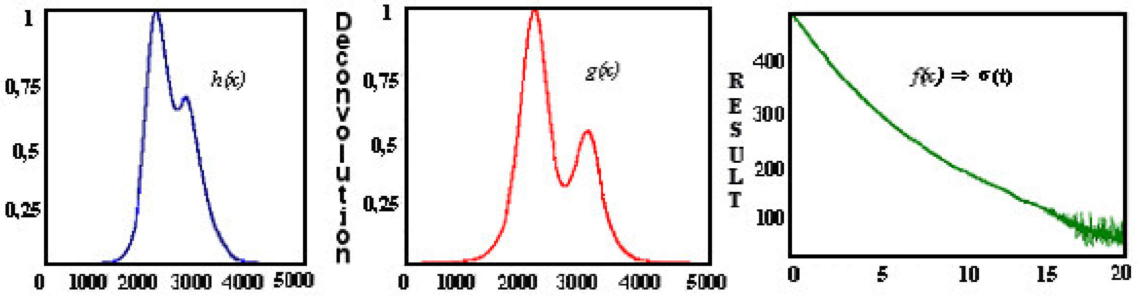


Figure 11. Stress distribution function restoration by the deconvolution of the final profile and the distortion function. Stress Gradient $\sigma = 500e^{t0.103}$

In these figures the match among the restored functions and de analyzed stress gradients, can be observed. In the exponential case is possible to observe, the noise due to numerical divisions of close zero values.

4. Conclusions

In this paper we use a simulation of diffraction profile in order to prove that the integral breadth is a criterion for the existence of stress gradient.

Also we developed a methodology for the determination of the stress distribution function using the Fourier Transform Method. This methodology was tested with the direct simulation of the diffraction profile. Three functions of stress distribution were used, with different gradients and it was obtained a match among the initial stress distributions and the restored distributions. This work will continue with the comparison of experimental values.

5. References

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6. Responsibility notice

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