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Physics-Informed Uncertainty Quantification in Modeling of Machining-Induced Residual Stress

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Abstract

Machining processes involve various sources of uncertainty which lead to inaccurate interpretation of results in the surface integrity of machined products. This work presents a physics-informed, data-driven modeling framework for achieving comprehensive uncertainty quantification (UQ) of the impact of process and material variability on machining-induced residual stress (RS). Uncertainty due to the variation in bulk material properties and model input parameters in machining are considered. Preliminary results showed that variations in calibration parameters have a substantial effect on modeling RS, while the variation in material properties has a smaller effect. Further research directions for UQ in machining are also outlined.

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1. Introduction

Machining-induced residual stress (RS) is known to be a key influence on the fatigue life or crack propagation within machined structures [1]. In general, tensile RS is undesirable because it can increase the fatigue crack growth, whereas compressive RS is desirable because it can reduce it. Therefore, it is very important to accurately quantify RS in machining of life-limited components such as turbine blades and biomedical implants.

The mechanism of machining-induced RS has been investigated experimentally since 1950s [2]. Often, analytical and computational modeling approaches have been employed to predict the machining-induced RS which requires a physics-based understanding of the relationships between RS and influential factors such as cutting conditions, operation, tool geometry, material properties, etc. Although computational models and simulations are very promising to understand the physics of machining-induced RS, the lack of quantitative representation of their prediction accuracy deters further application in process control and optimization [3]. Furthermore, due to the numerous sources of uncertainty and variability, measuring and predicting machining-induced RS often appears to be random

in nature. Therefore, understanding the uncertainty in the output of machining simulations is important for careful decision-making [3].

Modeling of RS requires several input parameters including material properties and process parameters to represent the physical behavior of the process. For example, modeling of RS typically requires a model or data of thermo-mechanical loads imposed on the workpiece material's subsurface during machining. Measurement of these loads is experimentally challenging, and numerical methods are likewise limited in their ability to accurately predict the magnitude and scale of thermal and mechanical loads. With respect to material properties, there are inherent variations exhibited by any commercially available material due to minor variations in chemistry and pre-processing history, as well as due to the inherent microstructural anisotropy of common metallic alloys. For example, Ti-6Al4V alloy consists of both alpha and beta grains, which may furthermore vary in size and texture/orientation, as well as their degree of strain hardening. Even carefully measured material properties, such as Young's modulus and yield strength, will vary for a given material depending on the pedigree (pre-processing methods and history), as well as the inherent uncertainty of materials characterization techniques (e.g., stress and strain uncertainties in tensile testing).

With respect to process parameters, cutting speed and feed rate (i.e., the cross section of the uncut chip), as well as tool geometry (rake and flank angles) are typically well-defined during cutting with geometrically-defined tools (e.g., single-point machining rather than grinding). However, the key process variable that changes with time is the wear condition of the cutting tool, i.e., flank/rake wear and cutting edge radius. While the effects of tool condition, and associated uncertainties with respect to the machining-induced residual stress can be quite large, the present study is primarily concerned with the effects of uncertainties in the workpiece material properties. Additionally, physics-based models make several assumptions and simplifications regarding the physical phenomena which causes model error. Solving the model numerically also causes numerical approximation error [4]. In general, based on the sources of uncertainty, it can be classified into two categories: aleatory and epistemic [5]. Aleatory uncertainty originates from sources that are inherently random and cannot be eliminated through modeling. Epistemic uncertainty arises from the incomplete or lack of knowledge of modeling of a physical system. In this paper, the case of epistemic uncertainty in the context of RS modeling is considered.

In recent years, UQ in machining has become a popular topic of many researchers because of the need to optimizing the process for improving the product's service performance and life cycle. With an aim to quantify the uncertainty in peak tangential force, Gul et al. [6] implemented in-situ simulator models inside the local regions of interest defined by the uncertain parameters of two solid end-milling processes. Using Bayesian inference, Schmitz et al. [7] explored input parameter uncertainties such as depth of cut, tool geometry, spindle speed, and force model coefficients in the milling process. Sánchez et al. [8] employed uncertainty methods to investigate the variability of locators in machining. Ren et al. [9] modeled the uncertainty of acoustic emission (AE) signal to filter the raw AE signals directly from sensors in a turning process. Rao et al. [10] proposed a coupled uncertainty model to determine optimal machining conditions. However, systematic UQ through experiments is typically time consuming, expensive, and an inefficient use of material and computational resources. As a result, current UQ analysis in the field of machining simulation is still in its infancy. Most UQ research in the machining field has been applied for stability and tool-wear predictions, such as cutting force and modal parameter estimations [11] and chatter prediction in milling [12]. To the best of the authors' knowledge, UQ in machining due to the uncertainty in material properties has yet to be undertaken. It is crucial to assess and quantify sources of uncertainty to achieve quality control in surface finishing. The present work seeks to address this gap by providing initial insights into the effects of calibration parameters with respect to machining-induced RS, specifically for nickel-based superalloy Inconel 718. In this study, inputs previously characterized with an in-situ RS model for Inconel 718 [1] were leveraged to study the effect of experimental model input parameter uncertainty.

This work focuses on uncertainty due to model input parameters and bulk material properties at the macro scale. Relevant model parameters include the peak normal pressure (P_0)

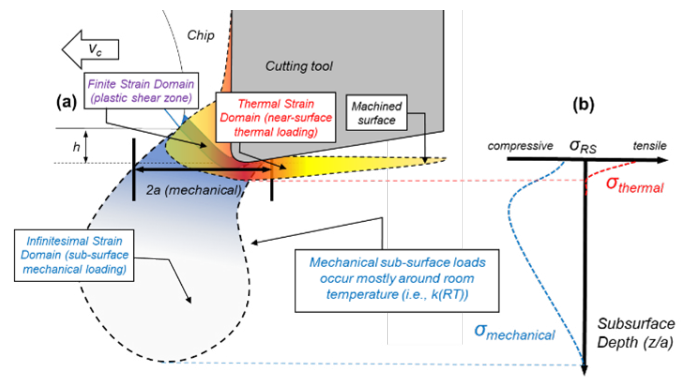


Fig. 1. Schematic illustration of (a) mechanical and thermal effects on RS formation; (b) relative depth of magnitude of mechanical and thermal domain RS contributions.

and the effective friction coefficient (μ_{eff}) were considered as uncertainty sources. The latter of which is a ratio of the feed forces to the cutting forces, rather than a purely tribological phenomenon. The overall source of uncertainty considered here are (i) the inherent variability of material properties and (ii) the statistical nature of μ_{eff} .

2. Methods

The starting point of UQ in machining-induced RS simulation is based on several steps which are demonstrated below:

2.1. Physics-Informed Model of Machining-induced RS

Based on modified tractional sliding contact Hertz theory and experimental observations, a semi-analytical model of the machining process was established to predict the residual stress directly caused by mechanical load. A multi-domain modeling framework, which is based on coupled (thermomechanical) calculations in the elastic, plastic, thermal, and thermodynamic domains was employed to generate the RS distribution [13]. As can be seen in Fig. 1, there are four major domains associated with thermomechanical finishing processes. This semi-analytical method consists of calibrating the contact width ($2a$) through pattern-matching with model generated von Mises plots which demonstrated in Fig. 2. The state of stress beneath a sliding cylinder can be calculated using Hertz theory which can be defined with parameters such as contact width (a), contact pressure (P_0), tractional pressure (q_0) and friction coefficient (μ_{eff}) [13]. Following Merwin and Johnson's [14] approach, the Prandtl-Reuss incremental relations were employed to model the RS distribution along the depth of the sample. Further details on the theoretical background and experimental calibration may be found in Ref. [1].

The main input parameters of this semi-analytical model are the equivalent elastic contact width (a), cutting speed (v_c), the effective friction coefficient (μ_{eff}), and peak normal pressure (P_0) from experimental calibration, as well as material properties.

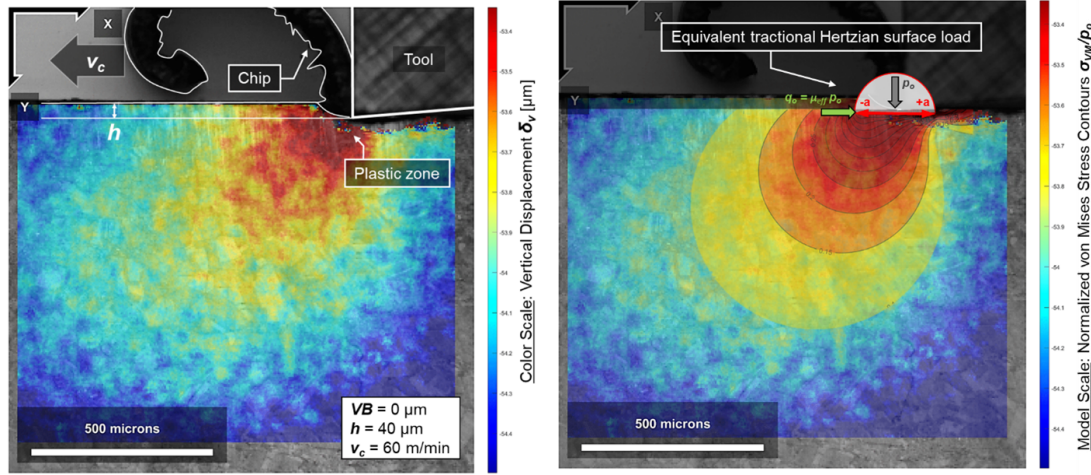


Fig. 2. Displacement field from DIC analysis (left) and illustration of sub-surface stress model calibration (right).

2.2. Sources of Uncertainty

While there are several sources of uncertainty in machining-induced RS, this paper focuses on uncertainty based on variation of (i) material properties and (ii) model input parameters.

2.2.1. Variation of Material Properties

Theoretically, materials exhibit deterministic behavior, but in practice they are inherently random. By invoking Information Theory and Maximum Entropy Principle, Guillemot and Soize [15] suggested that the Young's modulus (E) and Poisson ratio (ν) are not independent, and they are more likely statistically dependent Gamma-distributed random variables. Detailed theoretical derivation of statistical dependency between E and ν are given in Ref. [16]. In order to address the UQ due to variations in material properties, the statistical nature of E and ν was employed. Additionally, materials yield strength (YS) were also considered uncertainty due to the material's texture, i.e., preferential crystallographic orientation induced during pre-processing (e.g., rolling, forging, additive, etc.).

2.2.2. Variation of Model Input Parameters

In this physics-based model, the peak normal pressure (P_0), which is a function of the cutting forces (F_f and F_c) and effective half-width of contact (a), were calibrated experimentally, and thus carry experimental uncertainties that compound for both the effective friction coefficient (μ_{eff}) and the peak normal pressure (P_0). It is noted that μ_{eff} might change or be uncertain with tool coatings, coolants/lubricants, or due to measurement uncertainties. Cutting forces differ due to the varying strength of individual grains being cut and cyclical/serrated chip formation, as well as progressive (minor) tool-wear. Likewise, the effective half-width of contact (a) varies slightly at different points during steady-state chip formation due to cyclical chip formation and inherently uncertain grain-scale displacements, which form the basis for experimental measurement of a [1]. Based on typical experimental standard deviations (95% confidence intervals

for dozens of measurements) for force and contact width measurements of approximately 10%, both μ_{eff} and P_0 carry experimental uncertainties of approximately 20%. μ_{eff} varies significantly with uncut chip thickness, which is demonstrated in Ref. [1]. It is important to note that a varies approximately 10–15% and P_0 varies 10–20% around its mean value. Therefore, it is important to choose the proper distribution of μ_{eff} .

2.3. Modeling Based on Uncertainty in Material Properties

According to Ahmed and Kopsaftopoulou [17], the random Young modulus (E) and Poisson ratio (ν) associated with the isotropic random elasticity tensor can be defined as

$$E = \frac{9C_1C_2}{(3C_1 + C_2)}, \quad \nu = \frac{(3C_1 - 2C_2)}{(6C_1 + 2C_2)} \quad (1)$$

where C_1 and C_2 are the random bulk and shear moduli, respectively, that are statistically dependent Gamma-distributed random variables, with parameters $(1 - \lambda, \underline{c}_1/(1 - \lambda))$ and $(1 - 5\lambda, \underline{c}_2/(1 - 5\lambda))$. Here, $\underline{c}_1$ and $\underline{c}_2$ are the mean values of bulk moduli C_1 and shear moduli C_2 , and $\lambda \in [-\infty, 1/5]$ is a model parameter controlling the level of statistical fluctuation [15]. The mean value of the bulk modulus $\underline{c}_1$ and shear modulus $\underline{c}_2$ can be calculated using the following equations:

$$\underline{c}_1 = \frac{\underline{E}}{3(1 - 2\nu)}, \quad \underline{c}_2 = \frac{\underline{E}}{2(1 + \nu)} \quad (2)$$

where $\underline{E}$ is the mean value of the Young's modulus and $\underline{\nu}$ is the mean value of the Poisson's ratio. Although the Young's modulus and Poisson's ratio are statistically dependent Gamma-distributed random variables, they can be realized through two independent Gamma-distributed random variables: namely, the bulk modulus and shear modulus [15]. The mathematical details can be found in Ref. [17].

There are several methods to randomize YS like the log-normal distribution, the Weibull distribution. However, a log-normal distribution is considered to be a preferred distribution to randomize the yield strength [18].

Lognormal Distribution: If a random variable X is a log-normal distribution, then a normal distribution would be $Y = \ln(X)$. Similarly, $X = \exp(Y)$ is a log-normal distribution of a normal distribution Y . The general formula of a log-normal distribution of a random variable (RV) X with mean μ_X and standard deviation σ_X is defined as:

$$f_X(x) = \frac{e^{-\frac{1}{2}\left(\frac{\ln(x)-\mu_Y}{\sigma_Y}\right)^2}}{\sigma_Y \sqrt{2\pi}}, 0 < x < \infty \quad (3)$$

where $f_X(x)$ is the probability density function (PDF) of a RV X , and

$$\sigma = \sqrt{\ln\left(\left(\frac{\sigma_X}{\mu_X}\right)^2 + 1\right)} \quad (4)$$

and

$$\mu_Y = \ln(\mu_X) - \frac{1}{2}\sigma_Y^2 \quad (5)$$

are the standard deviation and expected value, respectively, for the normal distribution variable $y = \ln(x)$.

2.4. Modeling Based on Uncertainty in Model Input Parameters

There are several model input parameters which were described in Section 2.2.2. Most of them were calibrated from experiments, and those are a function of μ_{eff} . Therefore, only μ_{eff} was randomized to model the input parameters. Joo et. al [19] proposed an algorithm to model the distribution of friction factor where it can be modeled using Gamma, log-normal, Weibull, and normal distribution. Various attempts have been taken to fit the data points with different distributions, however, in this model, μ_{eff} can be randomized properly using the log-normal distribution. Steele [20] also proposed that coefficients of friction can be treated as having a log-normal distribution instead of a normal or uniform distribution since μ_{eff} only includes positive real numbers. The log-normal distribution is a popular choice for characterizing the coefficient of friction because it is a probability distribution of logarithmic values from a related normally distribution. Schoop et al. [1] mentioned that μ_{eff} varies between 0.7 to 0.85 for an uncut thickness 75 μm . It is important to note that the uncertainty caused by μ_{eff} results in uncertainty on the macroscale.

2.5. Uncertainty Quantification

Once the model input probability distributions are available, it is necessary to pass those input parameters into the model to estimate the output probability distributions. The goal of this study is to compute the statistical properties of input variables such as mean, standard deviation, and confidence interval for each model prediction. This can be done by using the Monte Carlo method, which entails drawing samples from the input random distributions and evaluating the deterministic model with the selected inputs.

3. Results and Discussion

Four model input parameters: Elastic Modulus (E), Poisson's ratio (ν), Yield strength (YS) and effective friction μ_{eff} are considered the main uncertain parameters. Along with these, the half-width of contact (a), the peak normal pressure (P_0), and cutting forces (F_c and F_f) are considered to be uncertain only to their respective degrees of experimental measurement uncertainty of 10% for each, and 20% for coupled metrics such as μ_{eff} and P_0 . At the first step, this paper investigates the uncertainty propagation considering material properties E , ν , YS driving random parameters. In the next step, the effective friction μ_{eff} is considered as a random parameter. It is noted that RS is normalized with the yield limit (k) and only cutting direction (xx) was considered.

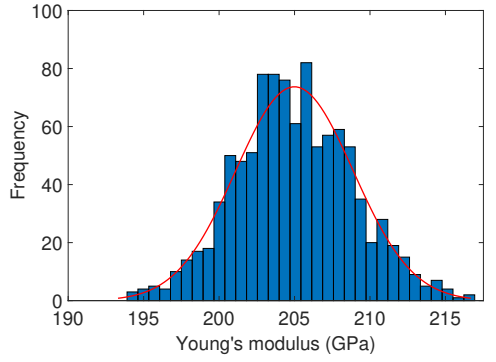
3.1. UQ Due to the Variation of Material Properties

In order to investigate the effects of variation in material properties on the propagation of RS, E , ν , and YS were considered as random variables. From a theoretical perspective, it was deduced that E and ν are dependent random variables and they jointly follow Gamma distribution. Considering statistical dependency between E and ν , 1000 samples were generated using the Gamma probability distribution. From Ref. [17], the mean value of E was taken as 205 GPa with a standard deviation of 1.332 GPa. The mean and standard deviation of ν was taken to be 0.284 and 0.007, respectively. The modeling parameter that controls the statistical fluctuation, λ , was taken as -450 from Ref. [17].

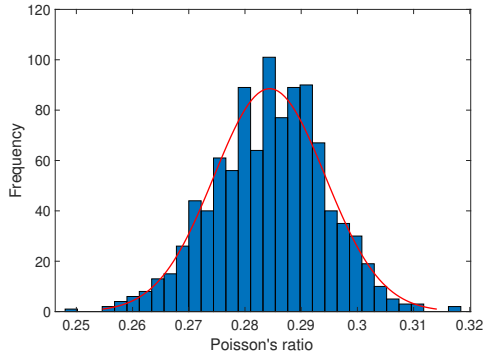
Fig. 3 shows the distribution of material properties for 1000 samples using statistically dependent Gamma distribution. Fig. 4 shows the results of RS distribution and their 95% confidence interval. It can be seen that the material properties have a negligible effect of uncertainty propagation. Since E and ν has negligible effect of RS distribution, therefore, variation of yield stress (YS) needs to be properly investigated in various scale to determine the effect of material properties in RS profile. In order to investigate uncertainty propagation due to the variation of YS, YS was randomized using log normal distribution. 1000 samples were generation based on the mean value of 1035MPa and 10% standard deviation. Fig. 5a shows the distribution of $\frac{P_0}{k}$ for 1000 samples. It is important to note that YS was normalized with the peak normal pressure (P_0). RS distribution due to the variation of YS is shown in fig. 5b. YS has significant impact on residual stress distribution in machining.

3.2. UQ due to the variation of calibration parameters

Due to the lack of experimental data, it is a challenging task to model the uncertainty of μ_{eff} . Using mean value and approximate standard deviation, Fig. 6(a) shows the distribution of μ_{eff} where 1000 samples were drawn from the log-normal distribution with shape and scale parameters of 11.776 and 4.532, respectively. The next step was to obtain the distribution of RS with the Monte Carlo simulation. Fig. 6(b) demonstrated the RS profile for randomly distributed μ_{eff} . It can be seen from the

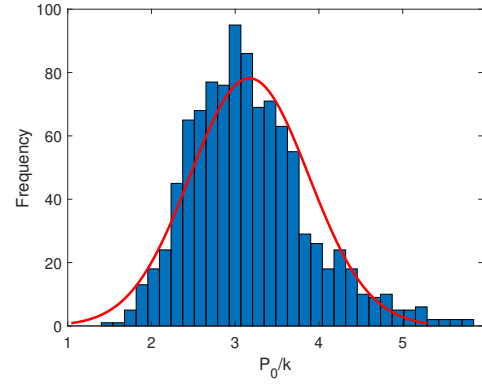
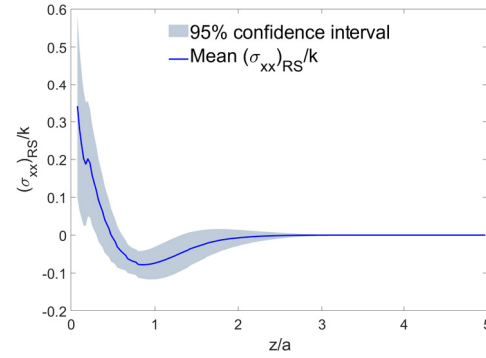


(a) Distribution of Young's Modulus with a mean of 205 GPa.



(b) Distribution of Poisson's ratio with a mean of 0.285.

Fig. 3. Distribution of material properties used in the simulation.

(a) Distribution of P_0/k 

(b) RS profile

Fig. 5. Uncertainty quantification due to the variation of YS.

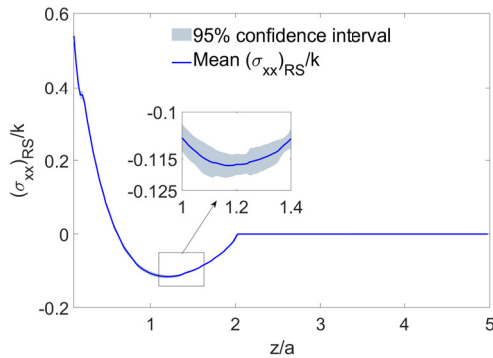
Fig. 4. Uncertainty quantification due to the variation of E and ν .

Figure 6(b) that μ_{eff} has significant impact on the machining-induced RS profile.

4. Conclusion

In this study, a preliminary investigation on machining-induced RS on the variability of material properties and effective friction coefficient (μ_{eff}) was presented. A physics-based, computationally efficient method was constructed to generate the RS profile. High-fidelity Monte Carlo simulations were performed for the variation of E , ν , YS and μ_{eff} . This study represents an introductory study aiming to tackle the significant

challenges of uncertainty in RS measurement. Based on the preliminary results, the following conclusions can be drawn:

- The effect of material properties, particularly the variation of Young's modulus and Poisson's ratio, carry a smaller impact on machining-induced RS, with resulting uncertainties of around $\pm 1\%$ in the model-predicted RS. Thus, the macro-scale anisotropy in these elastic properties may be negligible for a given workpiece material.
- The effect of uncertainty in the effective friction coefficient (μ_{eff}), which was estimated to be uncertain on the order of $\pm 20\%$ due to experimental uncertainties in process force measurements, led to an uncertainty of $\pm 5\%$ for the model-predicted RS profile. Therefore, the physics-informed model can be considered somewhat sensitive to experimental uncertainties in μ_{eff} .
- Analysis showed that uncertainty in YS due to microstructural anisotropy and bulk crystallographic texture plays a vital role for RS distribution, with resulting uncertainties in RS that may exceed $\pm 100\%$ of the predicted value.

The present study should be considered preliminary and will require detailed experimental validation. Future studies of uncertainty in RS measurements and model-based prediction should expand this preliminary analysis to better understand the degree to which various sources of uncertainty com-

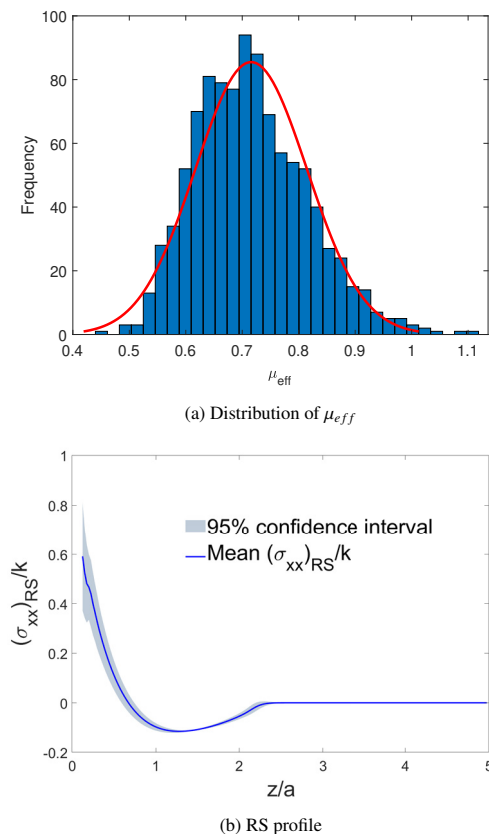


Fig. 6. Uncertainty quantification due to the variation of μ_{eff} .

pound. Moreover, future work should focus on further elucidating the importance of microstructural anisotropy on machining-induced RS, including the potential for major deviations between average and local RS, which may have profound implications for the fatigue performance of machined surface layers.

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Declarations

Conflict of Interest: The authors declare no conflicts of interest.

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