Multiscale fatigue modelling of additively manufactured metallic components

T.D. Dinh\textsuperscript{1,2}, J. Vanwalleghem\textsuperscript{1,2}, H. Erdelyi\textsuperscript{3}, S. Cornelissen\textsuperscript{4}, T. Craeghs\textsuperscript{4}, W. Van Paepegem\textsuperscript{1}

\textsuperscript{1}Department of Materials, Textiles and Chemical Engineering, Ghent University, Technologiepark 46, B-9052 Zwijnaarde, Belgium
\textsuperscript{2}SIM vzw, Technologiepark Zwijnaarde 48, B-9052 Zwijnaarde, Belgium
\textsuperscript{3}Siemens Industry Software NV, Interleuvenlaan 68, B-3001 Leuven, Belgium
\textsuperscript{4}Materialise NV, Technologielaan 15, B-3001 Leuven, Belgium

ABSTRACT
Additively manufactured metallic components have been used in medical and aerospace applications. In these components, surface roughness and porosity are integral features that might significantly reduce their fatigue lives, especially in the high cycle fatigue regime. Thus, to precisely estimate the fatigue life of an additively manufactured component, these defective features are incorporated into our proposed fatigue model. To capture the local plasticity caused by the defects, a nonlinear isotropic-kinematic hardening elasto-plasticity model is employed in our finite element (FE) models. Additionally, the gas-entrapped pores are modeled as circles whilst the surface topography, which was measured using stylus-based profilometer, is explicitly modeled in the FE models. The finite element results are post-processed by our in-house software to extract the Smith-Watson-Topper (SWT) fatigue indicator parameter. This parameter is calculated at each element centroid of the FE mesh, i.e., the local indicator. Afterward, an average value of the SWT parameter over a so-called critical area whose center is located at the considered centroid is also calculated, i.e., the nonlocal indicator. The results show that the local SWT indicator is too conservative in predicting the fatigue life of the component while the nonlocal SWT one can provide good results.

INTRODUCTION
Additive manufacturing (AM) is a rapidly developing technology that can allow manufacturers to produce metallic components with complex geometries within a short period of time. AM can contribute to resource saving and production cost reduction. At present, there are many different methods for metallic AM, among them selective laser melting (SLM) and selective electron beam melting (EBM) are mature and enable to manufacture near net-shape parts. Nevertheless, it is commonly known that AM processes can induce unwanted features that can be considered as AM-associated defects, e.g., porosity, tensile residual stress, and high surface roughness in the resultant parts [1]. These defects act as internal stress raisers and shorten the fatigue crack initiation life drastically, especially, in the high cycle regime (HCF) [1]. As such, to facilitate the industrialization of AM, especially, for fatigue critical load bearing applications, mastering the influence of AM-associated defects, in particular, the surface roughness and the gas-entrapped pores, to fatigue performance is crucial [2]. Moreover, Ti6Al4V, or Ti64 in short, is the material of choice for many fatigue critical applications in the aviation industry [2]. Thus, prediction of the fatigue initiation life at high cycle regime of AM Ti64 is the subject of the present study.
To reduce the number of experimental tests and to gain a better understanding about the fatigue damage mechanisms of AM materials, several models have been employed to predict the fatigue properties of AM parts and most of them can only handle a single type of defect. Recently, Biswal et al. [3] proposed a mechanistic model to predict the fatigue life of AM Ti64 accounting for the effects of isolated gas-entrapped pores. Those authors utilized a nonlinear isotropic kinematic hardening plasticity model for AM Ti64 to simulate the material behavior in the plastic deformation regime and AM Ti64 material parameters were utilized in the strain life relation to account for the influence of microstructure on the fatigue crack initiation. The gas-entrapped pores were modeled as spheres embedded in a cubical block that is subject to uniaxial far field stress. The resultant stress-strain fields are then utilized to calculate the Smith-Watson-Topper (SWT) fatigue damage parameter. The predicted results are in good agreement with the experimental data. However, because in their model, the SWT parameter was extracted at a local point, it cannot account for the size effect of the gas-entrapped pore. Nevertheless, that work has been encouraging enough to merit further investigation.

In the present paper, we propose a mechanistic fatigue model in which the effects of high surface roughness and gas-entrapped pores on the fatigue crack initiation life of AM Ti64 can be investigated simultaneously. In the finite element models presented in this paper, the gas-entrapped pores were modeled as circles, and the surface roughness was created based on measured surface texture data. The model was then discretized using axisymmetric elements in the FE software. Additionally, the nonlinear isotropic kinematic hardening plasticity was employed to model the behavior of AM Ti64 and the non-local SWT fatigue parameter was utilized to calculate the fatigue crack initiation life of AM Ti64 materials.

The outline of this manuscript is as follows. In the next section, the experimental data, including material properties of AM Ti64 and surface texture measurement, are presented. Afterwards, the theoretical background of the proposed model is described. Subsequently, calibration and validation of the model are shown. The manuscript ends with some concluding remarks.

EXPERIMENTAL DATA

The stable cyclic stress-strain relationship of Ti64, fabricated by SLM [4] and direct laser deposition (DLD) [1], is very similar compared to the wrought Ti64 counterpart. It thus enables the employment of a single cyclic stress-strain relationship of AM Ti64 for fatigue analyses. The relationships between the total strain range and the stress range, i.e., the Ramberg-Osgood relationship, is as follows (cf. Eq. (1)):

\[
\frac{\Delta \varepsilon}{2} = \frac{\Delta \sigma}{E} + \left(\frac{\Delta \sigma}{K}\right)^{\frac{1}{n}}
\]  

(1)

where \(\Delta \varepsilon\) and \(\Delta \sigma\) are respectively the strain and stress ranges, \(E\) is the material elastic modulus, \(K\) is the cyclic strength coefficient and \(n\) is the cyclic strain hardening exponent. Before quantifying the effects of AM defects to the fatigue performance, we need to define a reference stress-life, or S-N, curve which is obtained from the machined, heat-treated, HIPed specimens. Such data are obtained from refs. [5]. From the reference S-N curve and the Ramberg-Osgood relationship, the strain-life can thus be obtained as follows:
\[
\frac{\Delta \varepsilon}{2} = \varepsilon_a = \frac{\sigma_f'}{E} (N_f)^b + \varepsilon_f'(N_f)^c
\]  
(2)

where \(\varepsilon_a\) is the strain amplitude. Based on this strain-life equation, Smith, Watson, and Topper proposed the SWT model to account for the mean stress effects (cf. Eq. (3)).

\[
\sigma_{\text{max}} \varepsilon_a = \left(\frac{\sigma_f'}{E}\right)^2 (N_f)^{2b} + \sigma_f' \varepsilon_f'(N_f)^{b+c}
\]  
(3)

Herein \(\sigma_{\text{max}} = \sigma_m + \sigma_a\), where \(\sigma_m\) is the mean stress and \(\sigma_a\) is the stress amplitude.

The focus of the present work is on HCF of AM Ti64, thus, the applied load level is much lower than the material yield stress. However, the AM defects can act as stress raisers and local plasticity can occur at the valley of the surface roughness or at the root of the gas-entrapped pores. In [3], Biswal et al. utilized the nonlinear isotropic kinematic hardening plasticity model to simulate the mechanical behavior of AM Ti64 under cyclic loading. That plasticity model was calibrated with the experimental data provided in ref. [4] such that the stable cyclic behavior is reached at 20 cycles to reduce computational expense without affecting to the prediction of HCF. The results showed that the model could successfully capture the cyclic softening behavior of AM Ti64. That model is thus also employed in the present work to enhance the precision of the calculated SWT parameter.

To construct the FE models, the characterization of the gas-entrapped pores needs to be done to identify the size, shape, and relative position with respect to the free surface of the considered AM component. For this purpose, experimental data from different sources have been collected in Biswal et al. [3]. In addition, the present authors also performed fatigue tests of nine hourglass-shaped Ti64 samples with as-built surface quality that were subject to uniaxial constant amplitude tension-compression tests at three different load amplitudes. The surface roughness texture of one sample for each load amplitude was measured utilizing a surface profilometry (Perthometer S5P). Each specimen was measured twice at different locations with the spatial resolution of 4 \(\mu m\) and a measured length of ca. 12.5 mm.

**METHODOLOGY**

To create the FE model from the measured surface roughness data, the present authors first created a smooth sample and meshed it with rectangular elements. Then, an auxiliary linear simulation has been performed in which the measured surface roughness data were imposed as displacements to the nodes located in the smooth surface. The material model utilized in this simulation is fictitious and we utilized a linear elastic model with the Young’s modulus of 200 MPa and the Poisson’s ratio of 0.3. Afterward, the resultant deformed mesh was directly utilized for subsequent simulations in which the model was subject to different load cases and the cyclic behavior of AM Ti64 was modeled by the nonlinear isotropic kinematic hardening plasticity model, as mentioned in the previous section. Subsequently, the calculated stress and strain fields were utilized to calculate the SWT fatigue damage parameter.

All samples considered in the present work were subject to constant amplitude uniaxial tension-compression loads. However, the local stress state at the defects has a multiaxial nature. In addition, the mechanical behavior of Ti64 is orthotropic, thus, the maximum principal stress and the maximum principal strain at a material point are not coaxial. To compute the SWT parameter in a fatigue load cycle for such cases, we first solved an eigenvalue problem of the stress field in the loading stage of the fatigue cycle to find the maximum principle stress, \(\sigma_{\text{max}}^i\), and the orientations of principal normal stresses. These orientations constitute the rotation matrix, \(R\), which
was utilized to project the corresponding strain field, both in the loading and unloading stages, onto
the principal normal stress directions (cf. Eq. (4)).

\[ \bar{\varepsilon} = R^T \varepsilon R \]  

where \( \varepsilon \) is the strain field either in the compression or tension loading stages, and \( \bar{\varepsilon} \) is its
counterpart in the principal directions. The SWT fatigue damage parameter can then be calculated
utilizing Eq. (5).

\[ SWT = \frac{\sigma_{\text{max}}}{2} \left( \varepsilon_{\text{tension}} - \varepsilon_{\text{compression}} \right) \]  

All the aforementioned operations on stress/strain fields and the calculation of the SWT parameter
were performed at the centroid of the axisymmetric elements. This SWT is referred to as local
fatigue parameter. Subsequently, an average value of the SWT parameter over a so-called critical
area whose center is located at the considered element centroid is also calculated, i.e., the nonlocal
indicator \( SWT \) (cf. Eq. (6)).

\[ SWT = \frac{1}{A_{\text{crit}}} \iint SWT \, dA \]  

where \( A_{\text{crit}} = \pi r_{\text{crit}}^2 \) and \( r_{\text{crit}} \) is the radius of the critical area. In [6], Susmel and Taylor proposed
a modified version of theory of critical distances (TCD), in which the characteristic length, i.e., \( r_{\text{crit}} \)
in our case, is assumed to be a power function of the number of fatigue cycles, \( N_f \). We employed
that model here, as such, the relationship between \( r_{\text{crit}} \) and \( N_f \) can be expressed in Eq. (7).

\[ r_{\text{crit}} = A N_f^B \]  

Herein, \( A \) and \( B \) are fatigue model parameters and are determined from fatigue life data of an AM
component that contains defects. From Eqs. (3), (6) and (7), the fatigue life at a certain load
amplitude can be determined.

MODEL CALIBRATION AND VALIDATION

The proposed fatigue model was utilized to predict the fatigue lives of AM Ti64 components
with the AM inherent defects in case of uniaxial constant amplitude tension-compression cyclic
loads. The load amplitude, load ratio, and the corresponding fatigue lives of the components are
presented in Table 1. Whilst the data for the samples that failed because of the gas-entrapped
pores were extracted from [1], [3], [7], the counterparts for the samples that failed because of the
high surface roughness were obtained from the experiments performed by the authors of this paper.
To provide the local stress/strain fields in the samples so that the fatigue damage parameters can
be computed, nonlinear finite element analyses were performed. In [3], Biswal et al. distinguished
three types of pores depending on their relative locations to the free surface. If the pore is located
at the surface of the sample, i.e., surface pore, it is modelled as a hemisphere. Those authors also
performed numerical studies and found that if the distance-to-pore-diameter ratio is equal or greater
than four, the stress concentration factor is constant. Thus, the pores that satisfy this condition are
deemed as internal pores. The remaining type of pores is treated as the subsurface pores. Moreover, Biswal et al. also found that the stress concentration factors, obtained from the internal pore and the surface one, are almost the same because the stress state at the hot spots between the two cases is nearly identical. Therefore, in the present study, the authors did not distinguish
between the surface pores and internal pores. Both types were modelled as circles with the
distance to the free surface of the component is equal to four times of their diameters. The
subsurface pores were also modelled as circles and their distance to the free surface are obtained from experiments. Thus, the width of the employed FE models is adjusted according to the radius of the considered pore and its distance to the free surface of the component.

<table>
<thead>
<tr>
<th>Location</th>
<th>Distance to the free surface (µm)</th>
<th>Diameter (µm)</th>
<th>Max. applied load (MPa)</th>
<th>Applied load ratio</th>
<th>Predicted fatigue life cycles (experiments)</th>
<th>Predicted fatigue life cycles based on SWT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface</td>
<td>-</td>
<td>72</td>
<td>575</td>
<td>0</td>
<td>7.34 x 10^4</td>
<td>8.5 x 10^4</td>
</tr>
<tr>
<td>Subsurface</td>
<td>88</td>
<td>45</td>
<td>356</td>
<td>-1</td>
<td>1.6 x 10^6</td>
<td>2.2 x 10^6</td>
</tr>
<tr>
<td>Subsurface</td>
<td>95</td>
<td>58</td>
<td>470</td>
<td>-1</td>
<td>4.5 x 10^6</td>
<td>1.5 x 10^6</td>
</tr>
<tr>
<td>Surface</td>
<td>-</td>
<td>100</td>
<td>415</td>
<td>-1</td>
<td>5 x 10^6</td>
<td>4.5 x 10^6</td>
</tr>
</tbody>
</table>

Samples that failed due to the gas-entrapped pores

To determine the fatigue model parameters, A and B in Eq. (7), the authors utilized the data for which Nf is respectively equal to 1.27 x 10^4 and 3.93 x 10^4 cycles to find the corresponding value of r_{crit}. As a result, A = 1.9358 and B = -0.6083 were obtained. The remaining data in Table 1 were then utilized to validate the model.

The predicted and experimental fatigue life cycles of AM specimens with different types of defects are presented in Table 1. Overall, our predicted fatigue lives based on the local SWT are in slightly better agreement with the experimental data compared to the counterparts from Biswal et al. Indeed, Biswal et al. employed quadratic tetrahedron elements in their FE models and calculated the SWT parameter based on the stress and strain along the loading direction (i.e., σ_{22} and ε_{22} in their study), while in this work the authors employed linear rectangular axisymmetric elements in the FE models and calculated the SWT parameter based on the maximum principal normal stress and its energetic conjugate strain range. Nevertheless, there is still one predicted result that is out of the error band two, i.e., the predicted result is more than two times different compared to the experiment.

Moreover, the local SWT yields over-conservative results in prediction of the fatigue lives of AM Ti64 components that failed because of the high surface roughness (cf. Table 1). The nonlocal SWT, however, yields better results for these components, which manifests itself in the very good agreement between the predicted fatigue life of sample S2, 2.05 x 10^4, and the counterpart from the experiment, 1.91 x 10^4. Indeed, it is a well-known fact that the high surface roughness causes a very high stress gradient around the surface valleys. As such, only the nonlocal fatigue damage parameters, i.e., ST in our case, which can take into account the stress gradient, can precisely capture the fatigue behavior of these components. Moreover, the predicted fatigue lives obtained by utilizing the nonlocal SWT parameter are also in good agreement with...
the experimental data in case the samples failed because of the gas-entrapped pores. Especially, all the predicted fatigue lives obtained from the nonlocal $\overline{SWT}$ are within error band two of the experimental data.

**CONCLUSIONS**

In this article, a mechanistic model for fatigue crack initiation of AM Ti64 is proposed. To account for the influence of microstructure on the fatigue crack initiation, the authors utilized the nonlinear isotropic kinematic hardening plasticity model for AM Ti64 to model the material behavior at the plastic deformation regime and the AM Ti64 material parameters in the strain life relation. Additionally, the nonlocal $\overline{SWT}$ fatigue damage parameter, which can account for the stress gradient at the hot spot, was utilized to estimate the fatigue lives of the AM Ti64 components that were subject to constant amplitude uniaxial tension compression tests with different mean stress ratios. The results show that the nonlocal $\overline{SWT}$ can robustly predict the fatigue lives of AM Ti64 components that failed due to either high surface roughness or gas-entrapped pores. The proposed model will be utilized to predict the fatigue lives of AM Ti64 under multiaxial load cases in future works.

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**REFERENCES**


