The Effects of Notch Size and Material Microstructure on the Notch Sensitivity Factor for Notched Components

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Abstract

Nickel base superalloys are used in hot sections of gas turbine engines due to its high strength and good creep, fatigue, and corrosion resistance at high temperature. In this paper, a new probabilistic approach based on weakest-link theory that accounts for the effects of the microstructure, notch size and notch acuity is described and applied to nickel base superalloy to determine the fatigue notch factor, notch sensitivity index and the probability of forming microstructurally small crack from the notch root. The simulation results obtained from this framework are compared with experimental results and results obtained using existing classical methods for notched polycrystalline nickel base superalloys for the different notch root radii and acuities considered.

Keywords: nickel base superalloy, non-metallic inclusions, probabilistic framework, fatigue notch factor, crystal plasticity

1. Introduction

Nickel base superalloy is a high performance material subjected to severe operating conditions. It is widely used in aero engine components and power-plants because of its high strength and good creep, fatigue and corrosion resistance at high temperatures [1-2]. Fatigue failure is of great importance for these components for the catastrophic consequence caused by cyclic stresses and strains. Fatigue failure of nickel-base superalloy is a limiting factor for their reliable use in many engineering applications. Most of the prior research studies on the fatigue behavior of nickel-base superalloy are focused on higher length-scale phenomena and on direct experimental observation of the fatigue damage processes [3]. Under high cycle fatigue (HCF) situation, crack nucleation and microstructurally small crack growth is highly heterogeneous at the grain scale and the influence of

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microstructure on small crack formation and growth has been shown to play a significant role [4].

Microstructure features such as inclusions, pores, the grain size distribution, the grain boundaries, the precipitate size distribution, and volume fraction often have main influences in determining the crack formation and growth in both low cycle fatigue (LCF) and HCF in nickel-base superalloys [5]. Since polycrystalline IN 100 is prepared by powder metallurgy (PM) technique, inclusions and pores in microstructure always provide crack nucleation sites [5]. The presence of inclusions within a grain or near grain boundaries and pores in a polycrystalline material can significantly reduce the number of cycles to form a fatigue crack because the incompatibility of deformations between the inclusions and the surrounding materials leads to local plasticity [6]. Hyzak and Bernstein [7] and Deybal et. al. [8] have established the important roles played by inclusions in the formation and propagation of fatigue crack in nickel base superalloys while considering two PM nickel base superalloys.

One major problem common with fatigue research of these materials with complex microstructures is the scatter in fatigue life or fatigue strength for similar experiments conducted under the same operating conditions. Prior studies have shown that larger amount of scatter exists in the early stages of crack growth due to the microstructural variability and relatively little scatter in the large crack growth stage [9]. Due to this inherent scatter involved in HCF, numerous probabilistic approaches have been developed in HCF lifing strategies. Deyber et al. [10] proposed a probabilistic framework using statistical distribution of particle size. The authors considered two different modes of fatigue crack initiation in the DA 718: Fatigue micro-crack formation on second phase particles (carbides and nitrides) of less than 10 μ m grain size and transgranular stage I initiation of fatigue crack along favorably oriented slip bands. The resulting probability of failure based on crack formation at particle interfaces is given as:

$$P_f(\sigma_d) = 1 - \exp\left(-\left[\frac{\Sigma_1 + \lambda\langle\sigma_{eq} - \sigma_y\rangle}{\sigma_0}\right]^m\right) \quad (1)$$

where Σ_1 is the maximum principal stress, λ is the particle shape factor, σ_{eq} is the equivalent Mises stress, σ_y is the yield stress, and σ_0 is the scaling parameter. Deyber et. al. [10] also proposed a model for crack propagation based on Tomkins model [11] given as:

$$\frac{da}{dN} = \alpha \cdot a, \text{ where } \alpha = \frac{\pi^2}{8} \frac{\Delta\epsilon_p \Delta\sigma^2}{(2T)^2} \left(1 + \frac{\pi^2}{8} \left(\frac{\Delta\sigma}{2T}\right)^2\right) \quad (2)$$

where T is the ultimate tensile stress in the damage process zone of the crack, $\Delta\varepsilon_p$ is the plastic strain amplitude, $\Delta\sigma$ is the maximum principal stress amplitude. Based on the model, the probability that a particle of diameter D_0 will propagate, in a potential number of cycles (N_0), was determined. The probability of failure is assumed to be equal to the probability of finding a particle of size greater than the potential particle size, D_0 . The overall global probability of failure is taken as the combined product of the probabilities of failure at the surface, subsurface and within the bulk of the material and given as:

$$P_f = 1 - \left\{ \prod_{n=1}^{N_{el,surf}} \left[\left(1 - P_f(\sigma_d) P(D \geq D_0) \right)^{N_{p,surf}} \right] * \prod_{n=1}^{N_{el,subsurf}} \left[\left(1 - P_f(\sigma_d) P(D \geq D_0) \right)^{N_{p,subsurf}} \right] * \prod_{n=1}^{N_{el,bulk}} \left[\left(1 - P_f(\sigma_d) P(D \geq D_0) \right)^{N_{p,bulk}} \right] \right\} \quad (3)$$

Where $P_f(\sigma_d)$ is given in Eq. (1), N_p and N_{el} are the number of particles contained in the meshed elements in each location (surface, subsurface and bulk).

Based on known microstructure of PM nickel base superalloy, Pineau [12] proposed a probabilistic framework that employs the statistical distribution of inclusion sizes to determine probability of failure of different components. The proposed model considers both surface and volume defects and the propagation of defects to a critical size. The resulting probability that any one inclusion intercept a free surface for uniform size distribution of spherical inclusion is given as [12]:

$$P_{surf}(D, n, S, V) = 1 - \left(1 - \frac{DS}{V} \right)^{nV} \quad (4)$$

where D is the inclusion diameter, S is the highly stressed surface area, V is the volume of the specimen, and n is the number of inclusions per unit volume. However, for varying inclusion sizes grouped into classes, the probability that inclusion of size class k intercept a free surface for distribution of inclusions sizes is given as:

$$P_{k,surf}(D_k, n_k, S, V) = 1 - \left(1 - \frac{D_k S}{V} \right)^{n_k V} \quad (5)$$

Pineau [12] used the model to estimate the probability of failure of three different sized components made from Rene 95 and established that probability of failure is highly size dependent.

Existing probabilistic framework models account for stress heterogeneity effect using the concept of effective volume. Doudard et al. [13] extended this concept to account for multiaxial loading histories in HCF by introducing a factor to represent the distribution of activated slip directions and also captures the variability of the activation level. In this approach, it is assumed that slip directions become active when the shear stress amplitude T_a exceeds the critical yield strength. Doudard et al. [13] used Poisson point process [14-15] to describe the activation and the average density of active sites λ is given as:

$$\lambda = \frac{1}{V_0 S_0^m} \int (2T_a)^m d\Theta \quad (6)$$

where m , V_0 is the reference volume and $V_0 S_0^m$ are material-dependent parameters. Equation (6) is integrated over all possible angles to account for all the space directions defined by the solid angle Θ . Doudard et al. [13] defined the probability P_k , (within a domain Ω of volume V) of finding k active sites as:

$$P_k = \frac{[N(\Omega)]^k}{k!} \exp[-N(\Omega)] \quad (7)$$

Where $N(\Omega)$ is the average number of active sites given as:

$$N(\Omega) = \lambda V \quad (8)$$

The resulting probability of failure P_f is given as:

$$P_f = 1 - \exp \left[-\frac{1}{V_0} \int \left(\frac{2T_a}{S_0} \right)^m \cos(\zeta) d\Theta dV \right] \quad (9)$$

This probabilistic framework can be used for both non-proportional loadings and multiaxial loading. It also accounts for scatter in HCF fatigue data through the distribution of the slip system and the variability in the slip system activation level. Flaceliere and Morel [16] developed a probabilistic framework based on the endurance criterion proposed by Papadopoulos [17] which defined the equivalent stress as a function of the quadratic mean value of resolved shear stress T_a and the maximum hydrostatic pressure as:

$$\sigma_{eq} = M_\sigma + p \sum_{H, \max} \quad (10)$$

where M_σ is the quadratic mean value of resolved shear stress T_a , p is the coefficient reflecting the sensitivity to hydrostatic stress and $\Sigma_{H,\max}$ is the maximum hydrostatic pressure over a loading period. This equivalent stress is applicable to any complex stress states (in-phase or out of phase loading). The probability of failure is given as:

$$P_f = 1 - \exp \left[-\frac{1}{V_0} \int_v \frac{\sqrt{\langle T_a^2 \rangle} + p \sigma_{H,\max}}{\sigma_0} dV \right] \quad (11)$$

where V_0 is the reference volume and σ_0 is the damage threshold stress level. Flaceliere and Morel [16] also investigated the stress gradient and surface effects in probabilistic fatigue failure. Based on Papadopoulos proposal [17], they used an equivalent stress function dependent on the normalized gradient of the maximum hydrostatic stress given as:

$$\sigma_{eq,S} = M_\sigma + p \left(1 - \beta \left\langle \frac{G}{\Sigma_{H,\max}} \right\rangle^n \right) \Sigma_{H,\max} \quad (12)$$

with

$$G = \sqrt{\left(\frac{\partial \Sigma_{H,\max}}{\partial x} \right)^2 + \left(\frac{\partial \Sigma_{H,\max}}{\partial y} \right)^2 + \left(\frac{\partial \Sigma_{H,\max}}{\partial z} \right)^2} \quad (13)$$

where n is a constant assumed to be 1 while β is a normalized hydrostatic stress intensity factor. The surface stress Weibull function is then defined as:

$$P_f(\sigma_{eq,S}) = 1 - \exp \left[-\frac{1}{S_0} \int_s \frac{\sigma_{eq,S}(\sigma, G(\sigma_{H,\max}))}{\sigma_0} dS \right] \quad (14)$$

The results demonstrated a good correlation between the surface model approach and the experimentally determined failure probability for GS52 nodular cast iron and C36 mild steel. However, wide discrepancies were noted between the surface and volume approaches when applied to the nodular cast iron due to the presence of pores ranging in size from 50-1000 μm [16].

Delahay and Palin-Luc [18] developed a probabilistic approach for high cycle multiaxial fatigue by the combination of a three-parameter Weibull distribution with the deterministic energy-based and volumetric high-cycle multiaxial fatigue

criterion proposed by Banvillet et al. [19-20]. To account for the multiaxiality of the stresses, the Weibull stress is replaced by the strain work density per loading cycle. The resulting failure probability is given as:

$$P_f(V, \sigma) = 1 - \exp \left[-\frac{1}{V_0} \int_V \left(\frac{\langle W_g - W_g^* \rangle}{W_u} \right)^m dV \right] \quad (15)$$

Where W_g is the strain work density given to the material per loading period, W_g^* is the threshold value of W_g , W_u is a scale parameter and m is the Weibull slope. The predictions by the probability framework are in good agreement with experimental probability distribution when applied to five materials investigated: the 30NiCrMo16 and 35CrMo4 quenched and tempered steels, the C20 annealed steel, the EN-GJS800-2 nodular cast iron and the Ti-6Al-4V titanium alloy. Delahay and Palin-Luc [18] also investigated the size-effect which is usually linked to stress-strain gradient in HCF as shown by Papadopoulos [17] and they gave the probability of failure in fully reversed tension for a smooth component as:

$$P_f(V, \sigma_a) = 1 - \exp \left[-\frac{V}{\phi_u} \left\langle \frac{(\sigma_a)^2}{E} - W_g^* \right\rangle^m \right] \quad (16)$$

where V is the component volume, σ_a is the normal stress amplitude, E is the young modulus, and

$$\phi_u = V_0 W_u^m \quad (17)$$

In addition to materials defects which can be accounted for using some of the probabilistic framework, most engineering components have structural geometric discontinuities. These discontinuities can be in the form of keyways, weld fillets, holes for bolts, and rivets. For nickel base superalloy used in turbine engine, the turbine engine operates at a very high temperature and thus the blades have tiny holes for cooling purposes. The coolants are forced through the holes at high pressure for cooling of the system [21]. These holes serve as areas of stress concentration and are typical locations for localized micro-plasticity thus reducing the fatigue strength of the material when subjected to cyclic loading. The holes also serve as favorable zones for crack initiation leading to early retirement of the turbine blade and engine as shown in Figure 1. Notches and inclusions therefore form part of the major factors that dictate the fatigue strength of the components. Hence, a robust fatigue assessment model which includes effects of both material

and geometric discontinuities on the fatigue strength of the components would be of great importance in predicting the fatigue life and in the process of developing optimized, safe, and reliable structural components.

Fig. 1: Crack Initiation at cooling hole of turbine blade [22]

The geometric discontinuities are usually modeled as notches with a certain depth and notch root radius to investigate their effects on the fatigue life of components subjected to cyclic loading [23-24]. The resulting notch effect is characterized using a fatigue strength reduction factor also known as the fatigue notch factor, k_f . Based on different assumptions, several models have been developed for k_f in the past. The Neuber [25], the Kuhn et al. [26], the Peterson [27], the Heywood [28-29], the Buch [30-31], and the Siebel et al. [32] equations are based on an average stress assumption. The average stress assumption stipulates that fatigue failure will occur given that the average stress over a length scale in the vicinity of the notch root is equal to the smooth specimen fatigue limit. Other existing equations for k_f include: Ting et al. [33], and Yu et al. [34] that are based on fracture mechanics models and the Sheppard [35] model that is based on stress field intensity models.

It is important to study the interactions between both material and geometric defects in predicting the fatigue damage of components having a combination of these defects. At present, however, there is no simulation-based methodology for modeling the interactive effects of stress/strain field gradients at the notch-root and microstructure-scale behavior in predicting notch-root fatigue failure in service loads where performance outweighs other considerations. In this paper, the concept of fatigue notch factor and its associated notch sensitivity is effectively extended to incorporate microstructure sensitivity for notched components using

an approach that combines computational crystal plasticity with probabilistic mesomechanics. The framework involves computational crystal plasticity modeling of the notched components with and without non-metallic inclusions to obtain three dimensional perspectives of stress distributions in the notch root and inclusions regions. The stress distributions around these discontinuities are then used in the new probabilistic micromechanics-based model that accounts for the effects of nonlocal notch root plasticity, loading microstructural variability, and extrinsic defects on local cyclic plasticity at the microstructure-scale level to predict the fatigue notch factor and the probability of formation of microstructurally small cracks. This approach can reduce the amount of testing required to make design decisions on material or component reliability by systematically estimating the scatter of fatigue life associated with microstructure variations through the use of simulations.

2. Crystal Plasticity Models

The crystal plasticity constitutive model developed by Mahesh [36] is used in this work. Rate dependent method is employed for the model because as the temperature increases, strain rate effects become increasingly important. Physically-based hardening models are employed on the basis of dislocation-precipitate interactions under strengthening caused by dislocation interactions. The shearing rate on each slip system is expressed as [36]:

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_1 \left\langle \frac{|\tau^{\alpha} - \chi^{\alpha}| - \kappa^{\alpha}}{D^{\alpha}} \right\rangle^{n_1} + \dot{\gamma}_2 \left\langle \frac{|\tau^{\alpha} - \chi^{\alpha}|}{D^{\alpha}} \right\rangle^{n_2} \text{sgn}(\tau^{\alpha} - \chi^{\alpha}) \quad (18)$$

where $\dot{\gamma}_1$ and $\dot{\gamma}_2$ are constants, the flow exponents are represented as n_1 and n_2 , κ^{α} is the slip resistance on each slip system and it is called the mechanical threshold [37], D^{α} is the average drag resistance, χ^{α} is the back stress on each slip system. The back stress, unlike for pure single crystal, are very important component for two phase materials such as nickel base superalloys and thus cannot be neglected [38]. It is also important to note that the back stress is subtracted from the applied shear stress to reflect the net force responsible for driving the dislocation. The threshold stress accounts for the anomalous yield behavior of the $\gamma-\gamma'$ nickel base superalloy, i.e, the increase in yield stress resulting from increase in temperature in the intermediate temperature range.

The first part of Eq. (18) accounts for the dominant cyclic behavior where the threshold stress plays the role of the yield stress. Conversely, the second part of Eq. (18) accounts for the effect of creep thermally activated at lower stresses. When the first term is not active, especially at lower stresses, matrix faulting and

dissociation of heterogeneous plastic dislocation control the dominant flow mechanism. Complex cyclic stress-strain history like that of nickel base superalloy is best modeled by the two term flow rule presented in Eq. (18). A total of 18 slip systems are used to model dislocation motion within the matrix of the nickel base superalloy; 12 octahedral slip systems and 6 cube slip systems. A list of the slip systems is provided in Table 1.

Table 1: Slip systems in nickel base superalloy [36]

Slip System α	Octahedral Slip Slip Plane	Slip Direction	Cube Slip Slip Plane	Slip Direction
1	$\{111\}$	$\langle 01\bar{1} \rangle$	$\{100\}$	$\langle 011 \rangle$
2	$\{111\}$	$\langle \bar{1}01 \rangle$	$\{100\}$	$\langle 01\bar{1} \rangle$
3	$\{111\}$	$\langle 1\bar{1}0 \rangle$	$\{010\}$	$\langle 101 \rangle$
4	$\{1\bar{1}\bar{1}\}$	$\langle 0\bar{1}1 \rangle$	$\{010\}$	$\langle 10\bar{1} \rangle$
5	$\{1\bar{1}\bar{1}\}$	$\langle \bar{1}0\bar{1} \rangle$	$\{001\}$	$\langle 110 \rangle$
6	$\{1\bar{1}\bar{1}\}$	$\langle 110 \rangle$	$\{001\}$	$\langle \bar{1}10 \rangle$
7	$\{\bar{1}1\bar{1}\}$	$\langle 011 \rangle$		
8	$\{\bar{1}1\bar{1}\}$	$\langle 10\bar{1} \rangle$		
9	$\{\bar{1}1\bar{1}\}$	$\langle \bar{1}\bar{1}0 \rangle$		
10	$\{\bar{1}\bar{1}1\}$	$\langle 0\bar{1}\bar{1} \rangle$		
11	$\{\bar{1}\bar{1}1\}$	$\langle 101 \rangle$		
12	$\{\bar{1}\bar{1}1\}$	$\langle \bar{1}10 \rangle$		

The 12 octahedral slip systems are active at low temperatures within the γ matrix which is typical of a FCC lattice structure. However, at high temperatures and high resolved shear stresses, the 6 cube slip systems are activated in the γ' phase though their role is not yet well understood and characterized. Taylor relation is assumed for the hardening of the threshold stress on each of the slip system and it is expressed as [36]:

$$\kappa^\alpha = \kappa_0^\alpha + \alpha_i \tilde{\mu} b \sqrt{\rho^\alpha} \quad (19)$$

where each slip system dislocation density is represented as ρ^α (for both cube and octahedral slip systems), $\tilde{\mu}$ is the shear modulus, b is the effective burgers vector,

and α is a coefficient that accounts for the statistical arrangement of the dislocation population.

The shear modulus in Eq. (19) is governed by the rule of mixtures and expressed as:

$$\tilde{\mu} = (f_{p1} + f_{p2} + f_{p3})\mu_{\gamma'} + f_m\mu_m \quad (20)$$

where f_{p1}, f_{p2}, f_{p3} are the volume fractions of the three γ' matrix phases respectively i.e., primary, secondary and tertiary while f_m is the volume fraction of the matrix phase. Also the effective burgers vector is expressed as:

$$\tilde{b} = (f_{p1} + f_{p2} + f_{p3})b_{\gamma'} + f_mb_m \quad (21)$$

where $b_{\gamma'}$ is the burger vector of the γ' precipitates and b_m is the burger vector of the matrix.

The initial critical resolved shear stress $\kappa_{0,\lambda}^\alpha$ given by Heilmaier et. al. [39] and Reppich et al. [40] is expressed as:

$$\begin{aligned} \kappa_{0,oct}^\alpha &= \left[\left(\tau_{0,oct}^\alpha \right)^{n_\kappa} + \Psi_{oct} \left(f_{p1}, d_2, f_{p2}, d_3, f_{p3} \right)^{n_\kappa} \right]^{1/n_\kappa} + (f_{p1} + f_{p2})\tau_{ns}^\alpha \\ \kappa_{0,cub}^\alpha &= \left[\left(\tau_{0,cub}^\alpha \right)^{n_\kappa} + \Psi_{cub} \left(f_{p1}, d_2, f_{p2}, d_3, f_{p3} \right)^{n_\kappa} \right]^{1/n_\kappa} \end{aligned} \quad (22)$$

where,

$$\Psi_{oct} = \Psi_{cub} = \left[c_{p1} \sqrt{\zeta \frac{f_{p1}'}{d_1}} + c_{p2} \sqrt{\zeta \frac{f_{p2}'}{d_2}} + c_{p3} \sqrt{\zeta f_{p3}' d_3} + \frac{c_{gr}}{\sqrt{d_{gr}}} \right] \quad (23)$$

In Eq. (23), $\zeta = \frac{\Gamma_{APB}}{\Gamma_{APB,ref}}$, where Γ_{APB} is the anti-phase boundary energy. The primary, secondary and tertiary gamma prime precipitate sizes are represented by d_1, d_2 and d_3 respectively while the grain size is denoted as d_{gr} . f_{p1}', f_{p2}' and f_{p3}' are the normalized precipitate volume fractions. The value of exponent n_κ ranges from

1 to 1.2 and the values of c_{p1} , c_{p2} , c_{p3} and c_{gr} are determined by curve fitting the initial yield strength to the experimentally determined values.

Based on the work of Qin et al. [41-42] and Shenoy et al. [43], the non-schmid stress, τ_{ns}^α , dependence of the octahedral slip systems is expressed as:

$$\tau_{ns}^\alpha = h_{pe} \tau_{pe}^\alpha + h_{cb} |\tau_{cb}^\alpha| + h_{se} \tau_{se}^\alpha \quad (24)$$

Here the resolved shear stress on the primary, secondary and cube slip systems are denoted by τ_{pe}^α , τ_{se}^α and τ_{cb}^α respectively while h_{pe} , h_{cb} , h_{se} are constants.

Feaugas and Haddou [44] have identified a direct proportionality between the rate of dislocation recovery and the dislocation density. Thus, the evolution of the dislocation density is expressed as [45]:

$$\dot{\rho}_\lambda^\alpha = h_0 \left\{ Z_0 + k_1 \sqrt{\rho_\lambda^\alpha} - k_2 \rho_\lambda^\alpha \right\} |\dot{\gamma}^\alpha| \quad (25)$$

and

$$Z_0 = \frac{k_\delta}{\tilde{b} d_{\delta eff}}, \quad d_{\delta eff} \approx \left(\frac{2}{d_{2\delta}} \right)^{-1} \quad (26)$$

where $k_1 \sqrt{\rho_\lambda^\alpha}$ is the dislocation storage and $k_2 \rho_\lambda^\alpha$ is the dynamic recovery. k_1, k_2 and k_δ are constants, $d_{2\delta}$ is the secondary precipitate spacing and $d_{\delta eff}$ is the equivalent precipitate spacing. The hardening coefficient h_0 for cube and octahedral slip systems are 2.4 and 4.8 respectively.

The back stress is used to capture the effects of Bauschinger effect and it is expressed as [45]:

$$\dot{\chi}_\lambda^\alpha = C_\chi \left\{ \eta \tilde{\mu} \tilde{b} \sqrt{\rho_\lambda^\alpha} \operatorname{sgn}(\tau^\alpha - \chi_\lambda^\alpha) - \chi_\lambda^\alpha \right\} |\dot{\gamma}^\alpha| \quad (27)$$

and

$$\eta = \frac{\eta_o Z_o}{Z_o + k_1 \sqrt{\rho_\lambda^\alpha}} \quad (28)$$

where C_χ is a fitting parameter and η reflects the relative proportion of geometrically necessary dislocations to total dislocation density.

3. Microstructure-Characterization

The alloy used in this study is the polycrystalline nickel base superalloy, IN 100, which is used extensively for intermediate temperature ($\sim 650^\circ\text{C}$) applications such as turbine engine. Nickel base superalloys are strengthened through solid solution strengthening of the γ matrix and precipitation strengthening using ordered FCC γ' precipitate in the austenitic γ matrix. Non-metallic inclusions and pores are also present as minor phases depending on the alloy chemistry and heat treatment. The strength of IN100 is highly dependent on a number of interrelated microstructure features including the inclusion size distribution, the grain sizes of the γ matrix and the γ' precipitate phases. IN100 has been well characterized in the work of Wusatowska-Sarnet et al. [46] and Jha et al. [47]. Figure 2 shows typical microstructural features of IN 100. The distribution of the non-metallic inclusions in the IN100 is shown in Fig. 3a. Figure 3a shows that some inclusions are located at the grain boundaries while others lie predominantly within the grains. The size distributions of the non-metallic inclusions are shown in Fig. 3 b. These data will serve as inputs in the construction of the microstructures for the finite element analysis in Section 4.

Fig. 2: (a) the γ and the primary γ' structure, (b) the secondary γ' morphology, and (c) the γ grain size distribution [47].

Fig. 3: (a) SEM image showing the spatial distribution of carbide inclusions (the white dots) [46], b) size distribution of the non-metallic inclusions/particles (NMP) [47].

4. 3D Finite Element Modelling of Notched Component

The crystal plasticity model for nickel base superalloy presented in Section 2 is coded into ABAQUS 2006 UMAT. The notched geometry modeled in this work is a v-notched cylindrical component shown in Fig., 4. Different test cases are modeled which include: nickel base superalloy specimen without inclusion and nickel base superalloy specimen with inclusions at various orientations based on the distribution in Fig 3b. The material parameters for the nickel base superalloy in the crystal plasticity codes obtained from Musinski [48] and Przybyla et al. [49] are as presented in Table 1.

Table 1: Material parameters for crystal plasticity models [48-49]

$\tau_{o,oct}^{\alpha}$ (MPa)	$\tau_{o,cub}^{\alpha}$ (MPa)	c_{p1}	c_{p2}	c_{p3}	c_{gr} (MPa $\sqrt{\text{mm}}$)	n_k
85.1	170.2	1.351	1.351	$1.22 \cdot 10^{22}$	9.432	1
$b_{\gamma'}(\text{nm})$	$b_{\gamma}(\text{nm})$	$\mu_{\gamma'}(\text{MPa})$	$\mu_{\gamma}(\text{MPa})$	$k_1(\text{mm}^{-1})$	k_2	$\rho_{\lambda,o}^{\alpha}(\text{mm}^{-2})$
0.25	0.41	81.515	130.150	$2.6 \cdot 10^5$	8.2	10^5
h_o	h_{pc}	h_{cb}	h_{sc}	Γ_{APB}	η_o	k_{δ}
4.8 or 2.4	0.8	0	-0.4	$1.64 \cdot 10^{-3}$	2.82	$2.5 \cdot 10^{-3}$
$C_{11,\gamma'}$ (MPa)	$C_{12,\gamma'}$ (MPa)	$C_{44,\gamma'}$ (MPa)	$C_{11,\gamma}$ (MPa)	$C_{12,\gamma}$ (MPa)	$C_{12,\gamma}$ (MPa)	n_1

135,000	59,210	81,515	158,860	73,910	130,150	15
n_2	$\dot{\gamma}_1(s^{-1})$	$\dot{\gamma}_1(s^{-1})$	D^a (MPa)			
9	8.7	$3.9 \cdot 10^{-11}$	150(oct)	180(cub)

Fig. 4: cylindrical specimen with a circumferential V-notch

For the notched component without non-metallic inclusions, due to symmetry in geometry and loading, only one-quarter of the notched cylindrical geometry is modeled. Three different notch root radii and acuities are modeled to investigate the effect of notch root radius on the fatigue notch factor of the notched specimens. The dimensions of the three test cases modeled are as given in Table 2.

Table 2: Dimensions of the notched specimens

Test Case	D (mm)	Notch radius, ρ (mm)	Notch depth, h (mm)	R-ratio
1	5	0.150	0.142	0.1
2	5	0.213	0.267	0.1
3	5	0.284	0.714	0.1

To determine the optimum element size to use for meshing the 3D model, mesh refinement study was conducted using a cube specimen subjected to 568 MPa which is one of the loads applied to the specimens according to the experimental data obtained from Weiju et al. [50]. The von-Mises stress converged at an element size of 64 μm and thus element size of 64 μm is used in meshing all the nickel base superalloy specimens modeled. It is noted that the 64 μm falls within the range of grain size for nickel base superalloy which normally vary from 30 μm to 70 μm [51]. The model is meshed using 3D stress four-node linear tetrahedron

element type (C3D4). The bottom of the model is encastre and symmetry boundary conditions are applied on the planes of symmetry of the geometry.

For the notched components with non-metallic inclusions, the lognormal distribution of the inclusions in the nickel base superalloys shown in Fig. 3b is taken into consideration. It is assumed that the shape of the inclusions is elliptical with different aspect ratios. The MC inclusions are assigned linear elastic material properties with Young's modulus 405 GPa and a Poisson's ratio of 0.14 [36]. Here, the full geometry is modelled because there is no symmetry in the geometry due to presence of inclusions though symmetry is still maintained in the load application. The model is meshed using 3D stress four-node linear tetrahedron element type (C3D4) of size 64 μm as early established by the mesh refinement study. The inclusions are randomly distributed with different orientations as illustrated in Fig. 5.

Fig. 5: Different orientation of inclusions in the matrix.

5. Fatigue Damage Process Zone

Attempts have been made by different researchers to succinctly define the fatigue damage process zone [52-54]. In general, the fatigue damage process zone is a volume comprising of pre-fracture zones in the vicinity of the notch, inclusion or any other stress raisers identified in the material. The pre-fracture zone is normally due to the detrimental effects of the stress raisers. To accurately predict life in HCF, it is of paramount importance to be able to define the fatigue damage process zone with some level of precision. According to Ostash et al. [53], the fatigue

damage process zone is defined as some volume in the bulk material in which macro- and micro-plastic strains take place which also serve as source of initial damage of the material microstructure. Some of the factors that affect the size of the fatigue damage process zone include material properties, loading amplitude, and environment.

The fatigue damage process zone used in this work is an extension of the fatigue damage process zone as defined by Owolabi et al. [55]. The fatigue damage process zone is defined based on the distribution of stress within the material. The statistical distribution of stress around the notch root and inclusions is used as a new criterion in defining the fatigue damage process zone. It is based on the assumption that the fatigue damage process zone is a region around the notch and inclusions having grains with stress values equal to or greater than a specified microscopic threshold value as shown in Fig. 6. Here, the yield stress of the material is specified as the microscopic threshold value.

Fig. 6: Schematic of fatigue damage process zone.

6. Probabilistic Framework for Fatigue Notch Factor

The probabilistic models in Section 1 can be used to predict scatter of fatigue data and the dependence of fatigue limits on fatigue damage process zone. The predictive capabilities of these models can be enhanced by incorporating information regarding the origin of the scatter such as due the presence of defects and micro-scale plastic deformation using the crystal plasticity framework presented in Section 2. Using the stress distribution obtained from the crystal plasticity model, a weakest-link probabilistic framework is presented here to obtain the fatigue notch factor and the probability of formation of small crack following the framework presented in [56] with a few modifications based on the physical mechanisms of fatigue crack formation and growth for aero-engine materials with

inclusions. As stated earlier, IN 100 contains nonmetallic inclusions and pores that play a critical role in the component's failure. Fatigue is manifested by extremal microstructure attributes that promote slip intensification and hence does not conform to homogenization. Thus, a probabilistic formulation to determine the failure potency in heterogeneous materials should include a consideration for these defects. This study combined the framework in [56] with other existing probabilistic formulations that consider the size distribution and proximity of defects and different competing damage mechanisms for IN 100.

For a smooth specimen with defects having a fatigue damage process zone of volume V , the whole volume is divided into small volume elements, dV with probability of failure of a sufficiently small volume element given as:

$$dP = \lambda dV \quad (30)$$

Where here, λ is the critical defect density defined as the expected number of defects per unit volume of the smooth specimen. Using weakest link theory, the probability of survival of the entire volume is obtained from the probability of survival of all “ j ” number of sub-volumes i.e.:

$$P_s = \prod_{i=1}^j (1 - dP_i) = \prod_{i=1}^j (1 - \lambda dV) \quad (31)$$

This equations assumes that the defects are randomly distributed within the volume and thus do not interact, which is only reasonable when considering the formation of a fatigue crack(s) HCF and very high cycle fatigue (VHCF) regimes. As the volume of each small element tends to zero, equation (31) can be transformed into:

$$P_s = \exp \left(- \int_{V_d} \lambda dV \right) \quad (32)$$

Using the generalized extreme value distribution function, the distribution of defects, a , that are above the threshold, a_{th} , is modeled by a power law of the form

$$\lambda = \frac{1}{V_0} \left(1 + \xi \left(\frac{a - a_{th}}{a_0} \right) \right)^{-1/\varepsilon} \quad (33)$$

Where a_0 and ξ are the scale and shape parameters respectively. Substituting (33) into (32) yields:

$$P_s = \exp \left\{ -\frac{1}{V_0} \int_{V_d} \left(1 + \xi \left(\frac{a - a_{th}}{a_0} \right) \right)^{-1/\varepsilon} dV \right\} \quad (34)$$

If $a_{th} = a_0^* \xi$, re-arranging equation (34) yields,

$$P_s = \exp \left\{ -\frac{1}{V_0} \int \left(\frac{a}{a_0^*} \right)^{-1/\varepsilon} dV \right\} \quad (35)$$

where a_0^* is regarded here as the mean defect size. Equation (35) is valid only if $\xi \neq 0$. The critical defect size is related to the microscopic stress (taking here as a random variable) through a power law relationship of the form:

$$\sigma_a = \frac{A}{\sqrt[z]{a}} \quad (36)$$

Where A and z are materials constants. Similarly, the stress amplitude, σ_0 corresponding to the mean defect size a_0^* can be taken as the fatigue limit of the reference volume V_0 for 50% failure probability. The two parameters can also be related by a power law of the form:

$$\sigma_0 = \frac{A}{\sqrt[z]{a_0^*}} \quad (37)$$

Combining Eqs. (36) and (37) we have:

$$\frac{a}{a_0^*} = \left(\frac{\sigma_0}{\sigma_a} \right)^z \quad (38)$$

Substituting Eq. (38) into Eq. (35) yields:

$$P_s = \exp \left\{ -\frac{1}{V_0} \int \left(\frac{\sigma_a}{\sigma_0} \right)^b dV \right\} \quad (39)$$

where $b=z/\xi$. If $\sigma_a = \sigma - \sigma_{th}$, Eq. (39) becomes:

$$P_s = \exp \left[-\frac{1}{V_0} \int_{V_d} \left(\frac{\sigma - \sigma_{th}}{\sigma_0} \right)^b dv \right] \quad (40)$$

For $\xi > 0$, b , σ_{th} and σ_0 represents a 3-parameter Weibull shape, location and scale parameters. The cumulative probability of HCF failure of the component, specifically defined can be obtained from Eq. (40) as:

$$P_f = 1 - \exp \left[-\frac{1}{V_0} \int_{V_d} \left(\frac{\sigma - \sigma_{th}}{\sigma_0} \right)^b dv \right] \quad (41)$$

To facilitate development of the expression for fatigue notch factor from Eq. (41), the concept of stress homogeneity factors is used. Thus Equation (41) can be re-written as:

$$P_f = 1 - \exp \left[-\frac{kV_d}{V_0} \left(\frac{\sigma_{\max}}{\sigma_0} \right)^b \right] \quad (42)$$

where

$$k = \frac{1}{V_d} \int_{V_d} \left(\frac{\sigma - \sigma_{th}}{\sigma_{\max}} \right)^b dv \quad (43)$$

is regarded as the stress homogeneity factor. Conventionally, the fatigue notch factor is the ratio of smooth to notched fatigue strength at the same probability of failure (usually 50%). Using Eq. (42), the probability of failure of smooth specimen and a notched specimen will be the same when:

$$\exp \left\{ -\frac{k_s V_s}{V_o} \left(\frac{\sigma_{\max,s}}{\sigma_0} \right)^b \right\} = \exp \left\{ -\frac{k_n V_n}{V_o} \left(\frac{\sigma_{\max,n}}{\sigma_0} \right)^b \right\} \quad (44)$$

where the subscripts n and s represent the respective value of the variable for notched and smooth specimens. The ratio of the smooth to notch fatigue driving force parameters (i.e., the stress amplitude) is used to define a new fatigue notch factor given as:

$$k_f = \frac{\sigma_{\max,s}}{\sigma_{\max,n}} = \left(\frac{k_n}{k_s} \right)^{1/b} \left(\frac{V_n}{V_s} \right)^{1/b} \quad (46)$$

For smooth specimen that is loaded at a very low stress or strain amplitude in the HCF regime, the number of critically stressed grains (or elements) is very small. Thus for the life limiting case in which only one grain or element is critically stressed above the threshold, $V_s = V_{et}$ (i.e. volume of element or grain) and $k_s = 1$; thus Equation (46) becomes:

$$k_f = \frac{\sigma_{\max,s}}{\sigma_{\max,n}} = (k_n)^{1/b} \left(\frac{V_n}{V_e} \right)^{1/b} \quad (47)$$

$$k_f = \left[\frac{1}{V_d} \int_{V_d} \left(\frac{\sigma - \sigma_{th}}{\sigma_{\max,n}} \right)^b dv \right]^{1/b} \left(\frac{V_n}{V_e} \right)^{1/b} \quad (48)$$

It is important to state that if the materials contain some pores or inclusions as the case of nickel base superalloy , Eq. 46 must be used.

In Eq. 41 there are three unknown parameters namely the shape, location and scale parameter. The location parameter otherwise called the threshold stress is taken as the yield strength of the material leaving two unknown parameters. The remaining two unknown parameters are estimated using the modified moment estimation (MME) technique [57]. Here, the first two sample moments are used i.e., the mean $\bar{\sigma}_m$ and the variance $\bar{\sigma}_m^2$ of the stress distribution σ . With modification of the expression obtained from Cohen and Whitten [57] to account for notch size effect, the mean and variance are given as:

$$\bar{\sigma}_m = \sigma_{th} + \sigma_0 \left(\frac{V_0}{V_d} \right)^b \zeta_1 \quad (49)$$

$$\bar{\sigma}_m^2 = \sigma_0^2 \left(\frac{V_0}{V_d} \right)^{2b} (\zeta_2 - \zeta_1^2) \quad (50)$$

In Equations 49 and 50,

$$\zeta_k = \zeta(1 + kb), \quad k = 1, 2 \quad (51)$$

And $\zeta(\cdot)$ is the gamma function defined by the integral:

$$\zeta(s) = \int_0^{\infty} t^{s-1} e^{-t} dt \quad (52)$$

By solving Equations (49) and (50) simultaneously, the two parameters σ_0 and b are determined. The yield stress of the nickel base superalloy is 1045 MPa. From Equations (49) and (50), b is determined to be 15.6 while the scale parameter σ_0 is determined to be 2826.07 MPa. From the geometry of the specimens, the reference volume V_0 is calculated to be 11.152 mm³.

7. Results and Discussion

Three different notch root radii and acuties simulated in ABAQUS are assigned ten different random realizations of grain orientations for each of the notch root radius. The stress distribution from the simulation of the notched nickel based super alloy is extracted around the notch root and inclusion regions and used in Eq. 41 to determine the probability of failure for each notch root radius and the results are as plotted in Fig. 7. The fatigue notch factor is determined using Eq. (46) and the associated notch sensitivity index q for each case is also computed. Figure 7, shows the combined effect of notch root radius and the grain orientation of nickel base superalloy on its probability of failure. It is observed that the probability of failure rapidly increases with increasing notch root radius. Also, it can be seen that the orientation of the nickel base superalloy grains plays a significant role in determining the probability of failure and susceptibility of the bulk material to fatigue failure. It is observed that the probability of failure for each notch root radius varies with grain orientations. For example, for nickel base superalloy with notch root of 0.284 mm, the probability of failure ranges from 0.52 to 0.64. Thus, notches with favorably oriented grains in the vicinity of the notch and inclusions exhibit higher probability of failure.

Fig. 7: Probability of failure vs notch root radius for notched nickel base superalloy specimens without inclusion.

Using Eq. (46), the associated microstructure dependent fatigue notch factors for the estimated probability of failures are computed and the average fatigue notch factor for each notch root radius is plotted as shown in Fig. 8 and compared with experimentally obtained fatigue notch factor from Wei et al. [50] for nickel base superalloy. Figure 8 shows that the numerically obtained fatigue notch factors follow the same trend as the experimentally obtained values. The result also shows that the fatigue notch factor increases with increasing notch root radius. It can be inferred from the result that larger notch root radii are detrimental to fatigue failure of notched nickel base superalloy. The notch sensitivity index for both the experimentally determined k_f and the k_f determined using the newly developed probabilistic framework are computed and plotted as given in Fig. 9 for comparison purpose. Figure 9 shows that the notch sensitivity index follows the same trend as that of the experimentally determined value and increases with increasing notch root radius.

Fig. 8: Comparison of experimentally determined k_f with the determine k_f using the developed probabilistic framework.

Fig. 9: Comparison of notch sensitivity index obtained from experiment and that obtained from developed model.

The fatigue notch factor obtained using the probabilistic framework and closed form solution are plotted against the fatigue notch factor determined using existing conventional empirical methods such as the Neuber (Eq. 53), the Peterson [Eq. 54], and the Heywood [Eq. 55] models given respectively as:

$$k_f = 1 + \frac{k_t - 1}{1 + \sqrt{\frac{a_n}{\rho}}} \quad (53)$$

$$k_f = 1 + \frac{k_t - 1}{1 + \frac{a}{\rho}} \quad (54)$$

$$k_f = 1 + \frac{k_t}{1 + 2\sqrt{\frac{a}{\rho}}} \quad (55)$$

where k_t is the stress concentration factor and a is a material constant. The results obtained using the various methods are shown in Fig. 10. The percentage variance/deviation of each method from the experimental value is presented in Table 3. The material constants for the empirical formulas in Eq. [53] to Eq. [55] were obtained from [50].

Table 3: Percentage variance of k_f from experimental value for different methods

ρ	Experiment	Weibull		Neuber		Peterson		Heywood		Closed form sol.	
	K_f	K_f	% Var	K_f	% Var	K_f	% Var	K_f	% Var	K_f	% Var
0.150	1.56	1.54	1.28	1.61	-3.21	1.54	1.28	2.56	64.10	1.58	-1.28
0.213	1.73	1.70	1.73	1.69	2.31	1.69	2.31	2.68	54.91	1.75	-1.16
0.284	1.73	1.74	-0.58	1.74	-0.58	1.80	-4.05	2.77	60.12	1.78	-2.89

Figure 10 and Table 3 shows that the probabilistic framework exhibits relatively lower percentage variance from experimental values compared to other existing conventional methods. Also, the closed form solution is also observed to give relatively accurate prediction compared to the existing classical methods as it has lower percentage variance from experimental results. The probabilistic framework

and the closed form solution more accurately predict fatigue notch factor of notched nickel base superalloy compared to the existing conventional methods.

Fig. 10: Comparison of k_f determined by the new model with existing conventional methods

For nickel-base superalloy with non-metallic inclusions, the k_f is computed based on the stress distribution extracted from Abaqus for notch nickel base super alloy. Table 4 shows how the computed k_f compare with the k_f of notched nickel base superalloy without inclusions. Table 4 shows that the introduction of inclusions in the matrix of the notched nickel base superalloy increases the k_f . Thus component with inclusions of any kind will tend to have lower fatigue strength than components without inclusion. This is expected based on the fact that inclusions serve as favourable sites of premature plastic deformation due to high stress concentration in the vicinity of the inclusion curvature.

Table 4: Fatigue notch factor of nickel base superalloy with and without inclusion

ρ	k_f	
	Without Inclusion	With Inclusions
0.150	1.54	2.01
0.213	1.70	2.38
0.284	1.74	2.61

8. Conclusions

A new probabilistic mesomechanics-based model was developed to obtain the fatigue notch factor, the associated notch sensitivity index and probability of forming microstructurally small for notched nickel base superalloy materials with and without non-metallic inclusions. The result shows that the probability of failure, the fatigue notch factor and associated notch sensitivity index all increase with increasing notch root radius. Also it is noted that the grain orientation of the material plays an important role in determining or predicting the fatigue strength of the material; the probability of failure varies at the same notch root radius for different grain orientation. The presence of inclusions around the fatigue damage process zone increases the fatigue notch factor of the notched nickel base superalloy.

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The Editor-in-Chief
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Dear Sir:

Nomenclatures

I wanted to inform you that the Nomenclatures are embedded in the main texts.

Yours very truly;

Gbadebo Moses Owolabi, PhD, P.Eng.
(Assistant Professor)