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Prediction of Mechanical Response of Nickel Based Superalloy Subjected to Creep Fatigue Interaction Loading Using Unified Mechanics Theory

Saurabh Mangal[#,*], Sri Krishna Sudhamsu Kambhammettu[$], Lakshmana Rao C.[#] and Perumal Chellapandi[!]

[#]*Department of Applied Mechanics, Indian Institute of Technology Madras, Tamil Nadu-600036*
[$]*Department of Mechanical Engineering, National Institute of Technology, Jamshedpur - 831 014*
[!]*Bharatiya Nabhikiya Vidyut Nigam Limited (BHAVINI), Kalpakkam - 603 102*
[*]*E-mail: smangal1308@gmail.com*

ABSTRACT

In order to simulate and predictmaterial's real-time responses for a component under complex mechanical and thermal loads, continuum damage mechanics (CDM) is employed. However, majority of the models found in the literature are phenomenological and primarily based on curve fitting, which offer limited understanding of the underlying physics of the problem. A few physics-based models have been developed that provide greater insights. Unified mechanics theory (UMT) is one such approach thatcaptures entropy generation due to various dissipative mechanism which aims to explainthe physics of the problem. During hold time in strain-controlled creep-fatigue interaction loading, stress relaxation is observed.This study attempts to capture stress relaxation response due to creep-fatigue interaction of nickel-based superalloys using UMT, which is regarded as a more scientific method than simply fitting curves. The evolution of creep strain energy with hold time is used to understand how material ages over time due to stress relaxation during creep-fatigue interaction loading.

Keywords: Creep fatigue interaction; Stress relaxation; High temperature; Unified mechanics theory; Entropy; Nickel based superalloy

NOMENCLATURE

R	: Universal gas constant
T	: Temperature
T	: Time
m_s	: Molar mass of the system
ρ	: Material density
E	: Elastic modulus of the material
σ	: Stress
σ_{start}	: Stress magnitude at the onset of relaxation
σ_{end}	: Stress magnitude at the end of relaxation
$\varepsilon_{elastic}$	: Elastic strain
$\varepsilon_{plastic}$	: Plastic strain
ε_{creep}	: Creep strain
ε_{total}	: Total strain at which the specimen is held
ε_0	: Absolute total strain
SE	: Dissipated strain energy
SE_{cum}	: Cumulative strain energy
Δs	: Entropy generation
∅)	: Thermodynamic state index (TSI)
$\emptyset)_c$	: Critical TSI
E_p, E_s, τ, c_1, c_2	: Parameters subject to optimization

1. INTRODUCTION

Nickel-based superalloys find significant applications in aerospace industries, land-based power plants, superchargers, and other related fields. In gas turbine engines, these alloys are predominantly used for high-pressure and low-pressure turbines. These high-temperature alloys are typically subjected to cyclic loading or fatigue loading due to the nature of their use. The combination of high temperature, prolonged mechanical stress caused by centrifugal forces in rotating turbines, and forces generated by a pressurized combustion mixture create conditions favourable for creep deformation. Nickel-based superalloys are high-temperature metallic alloys well-known for their exceptional mechanical properties when exposed to elevated temperatures. These alloys possess desirable characteristics such as low cohesive energy, excellent surface stability, high resistance to creep and oxidation, and greater fatigue life and toughness.The crystal structure of nickel-based superalloy is face-centred cubic (FCC).Literature[1-2] cells that nickel serves as the base element and matrix (γ) material in the composition of nickel-based superalloys. These alloys are strengthened through solid solution, precipitation, and grain boundary mechanisms.Within the γ phase (i.e., matrix) of the alloy, nickel and aluminium atoms are mixed and are capable of occupying any sites within the FCC crystal structure. Aluminium replaces the corner atoms of nickel in FCC crystal lattice and forms nickel aluminide (Ni_3Al), an ordered γ' phase. The γ'' phase is formed due to the presence of niobium and is found as Ni_3Nb. Fatigue failure is characterized by transgranular fracture, primarily caused by surface cracks. On the other hand, creep deformation in these alloys typically leads to intergranular fracture, which occurs due to the formation

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of voids at the grain boundaries. In practical conditions, both fatigue deformation and creep deformation interact with each other and exacerbate the deformation, causing the component to fail sooner than it would if only experiencing pure fatigue. Performing tests at elevated temperatures and varying mechanical inputs can be nonviable and costly. As a result, developingmodels based on fundamental physics can be beneficial in predicting the behaviour of structural components under complicated loading scenarios, such as varying mechanical stresses, strain ranges, and hold times (relaxation times) at high temperatures during their service life.

In the context of creep-fatigue interaction, there is a phenomenon called stress relaxation, which occurs during the hold time. This refers to the reduction of stress over time in a constant strain condition, leading to material relaxation. During the hold time in the stress relaxation process, the stress-time curve displays three distinct stages: an initial rapid softening stage, a transition period, and an eventual stabilization state (steady state of relaxation). Behaviour of stress relaxation has been extensively studied in the literature and is commonly modelled using the creep Eqn.[3-4]. Power law of creep can be modified and incorporated with some damage terms to capture stress relaxation[3], but this process involves curve fitting throughout the relaxation time. Viscoelastic materials are those whose relationship between stress and strain depends on time. Constitutive models are theoretical deformation models that can be used to calculate incremental stress for a given incremental strain. Constitutive models for viscoelastic materials are analogous to combination of mechanical systems, such as a spring and a dashpot. Standard linear solid model (Zener model) is a popular model for viscoelastic materials, which combinesMaxwell model in parallel with spring and can be used to simulate stress relaxation behaviour[5].

Most stress relaxation models[3,6-8] used in creep-fatigue interaction studies are based on empirical data and involve curve fitting, which highlights the need for a physics-based model.The objective is to simulate and predict the stress relaxation behaviour during strain-controlled creep-fatigue interaction loading using a one-dimensional damage model based on unified mechanics theory[9-10]. This approach captures the physical degradation of the material in order to make predictions close to reality. Section 2 presents an outline of the unified mechanics theory, which is a physics-based approach for comprehending material decay. Section 3 elaborates on the technique utilized for predicting material behaviour, succeeded by the findings and inferences.

2. UNIFIED MECHANICS THEORY-BASED LIFE PREDICTION

Within the framework of Newtonian mechanics, it is presumed that the object under examination is ageless, and the notion of energy dissipation or entropy production is not considered once the initial acceleration is given. This means that no deterioration in the material is considered. Traditional continuum mechanics involves performing a structural or stress analysis on a new system, assuming that the results will be applicable throughout the entire lifespan of the structure. However, as the system or structure ages, the accuracy and validity of the initial analysis diminishes. By integrating the current state of the material using the laws of physics, it would be possible to make more accurate predictions about its behaviour. Cemal Basaran and Yan developed the Unified Mechanics Theory (UMT)[9] in 1998, intending to address this issue. UMT is a theory that combines Newton's laws of motion and the second law of thermodynamics (as formulated by Boltzmann-Plank) into a single framework.In order to account for the internal state of a body, UMT incorporates the degradation/dissipation/ageing of the system/structure into the equilibrium differential Eqn. by using the concept of entropy. This eliminates the need for an empirical dissipation or degradation evolution function. In UMT, the derivative of any field variable with respect to entropy is not zero (in Newtonian mechanics, it is zero). By incorporating entropy change in the differential Eqn., we can more accurately predict how the system would behave when subjected to complicated loads, such as mechanical, electrical, thermal and, oxidation etc. The evaluation of Δs should be based on the dissipation mechanisms involved in the process. Any dissipation processes associated with failure will result in an increase in entropy. Equation (1) represents the entropy generation at a point due to plastic work, with mechanical dissipation being the dominant mechanism considered, depending on temperature (T), and material density (ρ):

$$\Delta s = \frac{\int \sigma \, d\varepsilon_{plastic}}{\rho \, T} \tag{1}$$

The assumption is made that the entropy produced by heat generation and other entropies associated with microstructural change are negligible compared to the entropy generated by creep work (energy dissipation). Thermodynamic state index(TSI) is a damage parameter that is calculated using the change in entropy. TSI axis represents the entire thermodynamic response of a material point. The system's damage is indicated by the TSI, which has a range of 0 to 1. TSI ($\emptyset$)is given by the following Eqn. (2):

$$\emptyset = \emptyset_c \left(1 - e^{\frac{-m_s \Delta s}{R}}\right) \tag{2}$$

Here, $\emptyset_c$ is a user-defined parameter, represents a pre-established failure criterion and can be taken as unity. m_s is the molar mass of the system (in kg/mol), and R is the universal gas constant, i.e., 8.315 J/(mol k). UMT utilizes an analytical approach to identify all entropy generation during loading, which is crucial for determining material degradation. In the context of strain-controlled creep-fatigue interaction loading, stress relaxation occurs when the specimen is maintained at a constant strain condition, resulting in a decrease in stress and some energy dissipation. The area of stress-creep strain plot projected on the creep strain axis is utilized to quantify creep work (energydissipation), which is then used to calculate entropy change. To calculate the successive damage parameter throughout the relaxation time, time-marching simulation is employed. The detailed steps for this simulation are explained in section 3.

3. PREDICTION OF MATERIAL RESPONSE

The research work[3] suggests that stress relaxation can be predicted by a combination of the strain hardening creep law,

i.e., a deformation model and creep damage accumulation, i.e., a damage model. However, this method needs a lot of data on uniaxial creep loading to curve fit many parameters. Existing literature documents efforts comparable to this[11]. Viscoelastic material models, such as the Standard linear solid (Zener model), i.e., a deformation model, can also describe the phenomenon of stress relaxation[5]. However, these models try to capture the behaviour using a combination of spring and damper but do not provide any information about the state of degradation within a material. Zener model is represented by the following Eqns.[3-6]

$$\sigma = \varepsilon_0 * \left(E_p + E_s * e^{-\frac{t}{\tau}}\right) \quad (3)$$

where, $\sigma_0 = \sigma_{start} = \varepsilon_0 * \left(E_p + E_s\right)$ (4)

$$\sigma_{end} = \varepsilon_0 * E_p \quad (5)$$

$$\tau = \frac{\mu}{E} \quad (6)$$

Where, variables used such as σ for stress, ε_0 for absolute total strain at which specimen is held, and t for time. Parameters such as E_p, E_s and τ can be obtained from Eqns. (4)-(6). The values of E_p, and E_s reflect the material's resistance to deformation. Subscript *start* indicates the start of relaxation, and subscript *end* denotes the end of relaxation. The chosen material for the work is DZ445, a nickel-based superalloy[12], whose chemical composition is as follows given in Table 1:

This section explains how to develop a UMT-based approach to model the stress relaxation that occurs during the hold time.

3.1 Input Strain-Time Cycle for Creep-Fatigue Interaction Loading

The strain-time cycle depicts two distinct types of loading: creep loading and fatigue loading, which occur separately. Creep loading occurs during a hold time, while fatigue loading refers to strain variation over time. During the experiment[12], the specimen undergoes strain-controlled creep-fatigue loading, where it is held at the maximum tensile strain for some time, as depicted in Fig. 1. The occurrence of creep loading during the hold time followed by a single fatigue cycle demonstrates that both loadings are independent of each other but have some inherent interaction that will affect the fatigue life of the alloy. The stress relaxation data for nickel-based superalloys has been documented in the literature[10] for different hold times. However, for the purpose of demonstration, a hold time of 3 min. has been selected.

3.2 Determination of Time Step for Simulation

The accuracy of any numerical calculation depends on the time step used, which is determined based on the gradient of the stress-time function. The time step is controlled by monitoring the rate of stress decrement in each step in relation to the total drop in stress. Careful judgment is essential in choosing the time step when implementing the proposed model. It must strike a balance to ensure accurate stress prediction during relaxation. Overly small time steps can lead to stress overprediction. Substantial time steps can result in stress underprediction. Using a time step of 10 sec. ensures that the stress does not decrease excessively and stays within the appropriate range.

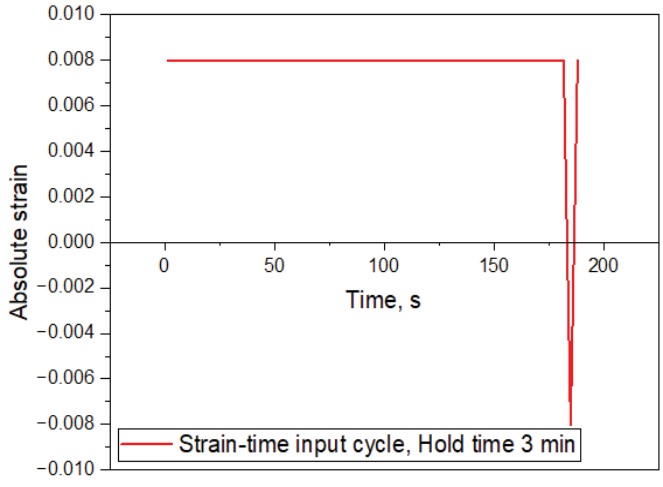

Figure 1. Input cycle of creep-fatigue interaction loading: Strain-time plot with 3 min hold time.

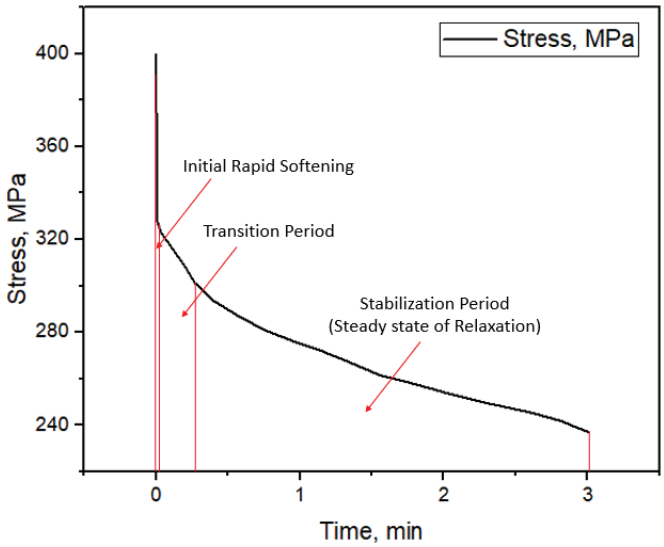

Figure 2. Stress relaxation experimental data[12] of DZ445 subjected to creep-fatigue interaction loading with 3 min hold time and 1.6 % strain range at 900 °C.

3.3 Modelling of Stress Relaxation

Degradation is a continuous process within a material, and the aim is to determine the entropy generation over time to understand the material's real-time response. During stress relaxation, there are two primary mechanisms[13] that occur: matrix damage and grain boundary damage. Figure 2

Table 1

Constituents	Cr	Co	Ta	W	Al	Ti	Mo	C	B	Ni
Weightage (%)	13.1	9.99	4.8	4.53	4.07	2.38	1.75	0.072	0.024	Bal.

depicts the stress relaxation behaviour for a 3 min. hold time. The data shows three distinct stress relaxation regions: an initial rapid softening, a transition period, and a stabilization period. The initial rapid softening of the material is a result of matrix damage, while the steady state of relaxation is due to grain boundary damage[13]. Due to the challenge of accurately capturing the initial rapid softening, it is typically excluded from the analysis. The model specifically focuses on the transition period and stabilization (steady state) of stress relaxation rather than the initial period of rapid softening.The UMT-based model is employed for prediction because it closely aligns to relate material damage with some physical quantity like entropy. The strength of the physics-based UMT model in relating material damage to physical quantities like entropy makes it the ideal choice for predicting material behaviour. The curvature of the stress relaxation data indicates a change in mechanism across the regions. Therefore, describing the material's behaviour in both the transition and stabilization period is challenging using a single expression. The stress relaxation simulation in this study utilizes a powerful model that cleverly merges two exponential decay functions with unique parameters. The first decay function takes the reins during the initial hold time, while the second decay function propels the model towards the end of the relaxation period with great force. Furthermore, it's been assumed that the exact same degradation process occurs throughout the steady-state stress relaxation time, with absolutely no variations in the underlying mechanism.Here is the time-marching based model representation (Eqns. (7)-(8)):

$$\sigma_{i+1} = f(\sigma_i, \emptyset_i) \tag{7}$$

$$\sigma_{i+1} = \sigma_i * \left(\left(1 - \frac{t_{i+1}}{t_{Holdtime}}\right) * e^{(c_1 + \emptyset_i)} + \left(\frac{t_{i+1}}{t_{Holdtime}}\right) * e^{(c_2 + \emptyset_i)}\right) \tag{8}$$

Where, t is time. Stress and TSI at the i^{th} time increment are denoted by σ_i and $\emptyset_i$, respectively. The stress at the $(i+1)^{th}$ time increment, denoted by σ_{i+1}, is a function of σ_i and $\emptyset_i$. During relaxation, the stress at any given point σ_{i+1} at time t_{i+1} depends on two variables: the stress at the previous point σ_i and the total damage accumulated up to that point $\emptyset_i$ in the simulation. This UMT-based model to predict stress relaxation combines two crucial factors, with the initial portion of the relaxation time being influenced primarily by the first factor and the latter being dominated by the second factor. The modified exponential function is employed to capture stress relaxation patterns, enabling the computation of the material's lifespan through a physics-based damage parameter. After taking the simplest assumption without any parameters, the model and experimental data did not match for a small time step.

To achieve a desired match with the depicted result in Fig. 3, the model was improved by the incorporation of two essential parameters, namely c_1 and c_2. These parameters were carefully optimized through the implementation of a sophisticated nonlinear least-square technique during the initial time step of 10 sec. Optimization Toolbox employs the Generalized Reduced Gradient (GRG) method, a non-linear least square approach. This method optimizes an objective function by adjusting the target variables c_1 and c_2, without being constrained by any limitations. The objective function is defined as the RSME for predictions of first time step in relation to experimental data.Once the optimal values of c_1 and c_2 were determined, they were utilized for the remaining relaxation time. The table below shows the optimized values of c_1 and c_2:

Table 2. Optimized values of parameters employed in the UMT-based model

Parameter	Value of parameter for time step 10 sec.
c_1	-0.052546069
c_2	0.011379696

The proposed model for stress relaxation is simple, making it easy to implement computationally. It doesn't require extensive computational resources, as it only needs a nonlinear least square optimization technique to fine-tune both parameters c_1 and c_2 in a single iteration.

The aim is to determine the energy dissipation that occurs within a given time increment and use that information to predict the stress values in the subsequent time increments leading up to the hold time. Entropy is generated due to energy dissipation during each time increment, contributing to damage accumulation over time. TSI value derived from entropy generation is updated through each iteration to predict the stress levels in the upcoming time increments.The developed model is based on observation, calibrated for atime step and allows a better understanding of the relaxation process. In order to utilize the model, it is required to input initial stress values for the first time step during the transition period.

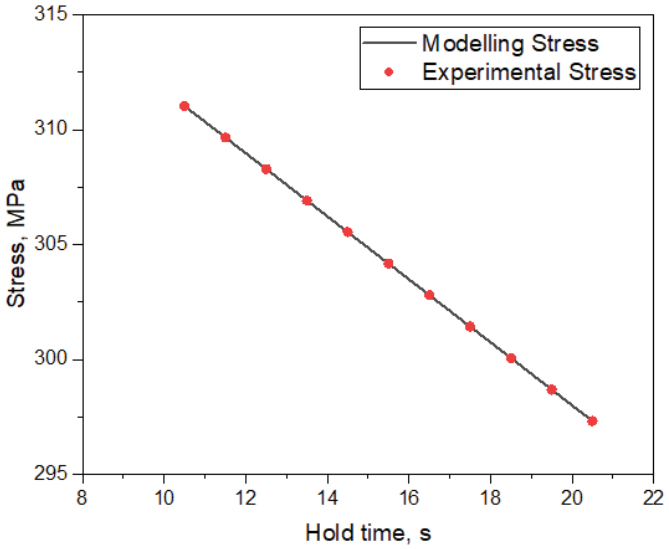

Figure 3. After optimization, an agreement between the proposed model and experimental values for an initial time interval of 10 sec.

3.4 Calculation of Change in Entropy and Damage Parameter TSI

While being held, the elastic strain transforms into creep strain (Eqn. (10)). The amount of creep deformation during each

time increment is calculated using Eqn. (12). Eqn. (13) is used to calculate the strain energy. The cumulative strain energy is derived to determine the change in entropy (Eqn. (15)) and the corresponding TSI value (Eqn. (16)). The assumption is made that the damage is uniform throughout the cross-sectional area of the dog bone sample. According to the UMT-based model, as shown in Eqn. (8), the stress value for each iteration can be determined by utilizing the stress and TSI values from the previous iteration.

$$\varepsilon_{total} = \varepsilon_{elastic} + \varepsilon_{plastic} + \varepsilon_{creep} \quad (9)$$

$$\varepsilon_{total} - \varepsilon_{plastic} = \varepsilon_{elastic} + \varepsilon_{creep} = constant \quad (10)$$

$$\varepsilon_{creep,i} = \varepsilon_{total} - \varepsilon_{plastic} - \varepsilon_{elastic,i} \quad (11)$$

$$\varepsilon_{creep,i} = \varepsilon_{total} - \varepsilon_{plastic} - \frac{\sigma_i}{E} \quad (12)$$

$$SE_i = \frac{1}{2} * (\sigma_i + \sigma_{i-1}) * (\varepsilon_{creep,i} - \varepsilon_{creep,i-1}) \quad (13)$$

$$SE_{cum,i} = \sum_{m=1}^{i} SE_m \quad (14)$$

Using Eqn. (1)

$$\Delta s_i = \frac{\int \sigma \, d\varepsilon_{plastic}}{\rho \, T} = \frac{SE_{cum,i}}{\rho \, T} \quad (15)$$

Using Eqn. (2)

$$\emptyset_i = 1 - e^{\frac{-m_s \Delta s_i}{R}} \quad (16)$$

Where, ε_{total} represents the value of constantstrain at which the specimen is held, which is taken as 0.8%[12]. It is assumed that the plastic strain, denoted as $\varepsilon_{plastic}$ remains constant throughout the relaxation time and taken as 0.3783 %. Elastic strain $\varepsilon_{elastic}$ is calculated using Hooke's law. *E* and ρ are Young's modulus and density of the material, respectively, assumed to be constant during relaxation at 900 °C. During hold time, elastic strain converts into creep strain ε_{creep}. Subscript *i* denotes the value of the variableat the end of i^{th} time step. SE_i denotes the value of dissipated strain energy (creep work) at the end of i^{th} time step while $SE_{cum,i}$ denotes the cumulative strain energy from start of relaxation to the end of i^{th} time step. Δ*s* denotes the difference in overall entropy change between the initial state and the simulated state. *T* represents temperature in Kelvin.

4. DISCUSSION AND RESULTS

Prediction of successive stressvalues starting from the transition period to the end of stress relaxation is achieved by computing the cumulative energy dissipation. As stress gradually decreases, this indicates that the incremental area is deteriorating with each uniform subsequent time step which is also observed in case of fatigue life simulation[14-15]. The outcomes achieved with the UMT-based model (Eqn. (8)) at a time interval of 10 sec. are presented in Fig. 4, and are compared to both the experimental results and the standard linear solid model (Zener model), a type of viscoelastic model (Eqn. (3)).

Figure 5. depicts the variation of absolute percentage error with hold time for UMT-based model and Zener model. According to this data, the most significant difference occurs during the middle section of the hold time. However, the outcomes from the UMT-based model (Eqn. (8)) and the experiments are in good agreement at the start and end of the relaxation period. For stress relaxation simulations using the UMT-based model, the maximum absolute percentage error is 9.1605 %, and the root mean square error (RMSE) is calculated to be 16.1879 MPa with 10 sec. time step. With respect to the decrement in experimental stress during the holding period, the modelling stress shows a maximum deviation of 25.6612 % compared to the corresponding experimental data.

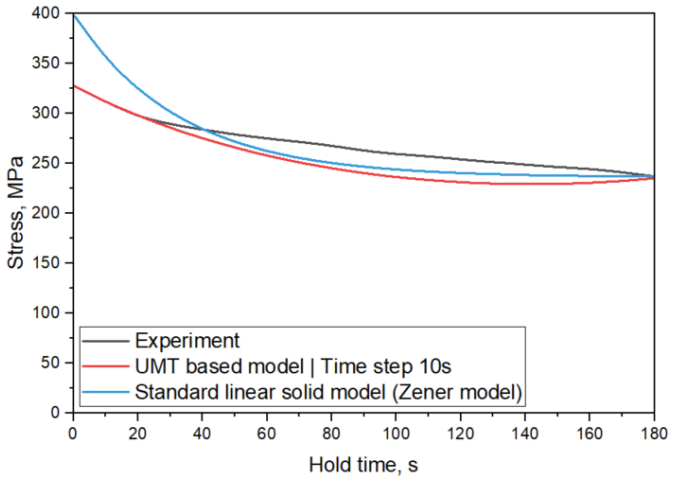

Figure 4. Comparison of the stress relaxation experimental data and predicted values for DZ445 material at 900 °C, 1.6 % strain range, and 3 minutes hold time with 10s time step size. UMT-based simulation captures thestress relaxation behaviour, which can be easily validated with experiments.

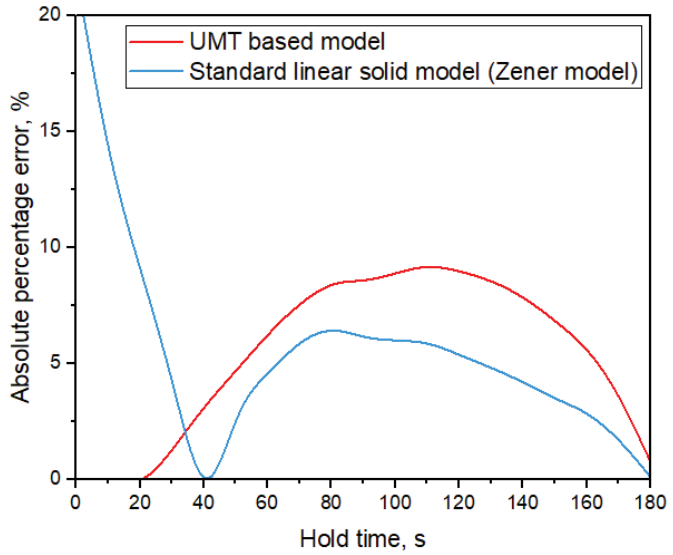

Figure 5. Absolute percentage error calculated during the hold time, which consistently remains less than 10 % for proposed UMT-based model.

Figure 6 shows the evolution of creep strain with the passage of time. Figure 7 displays a graph showing the inelastic strain rate as a function of time obtained by differentiating the creep strain-time response. The proposed UMT-based model effectively captures the early stress relaxation behaviour

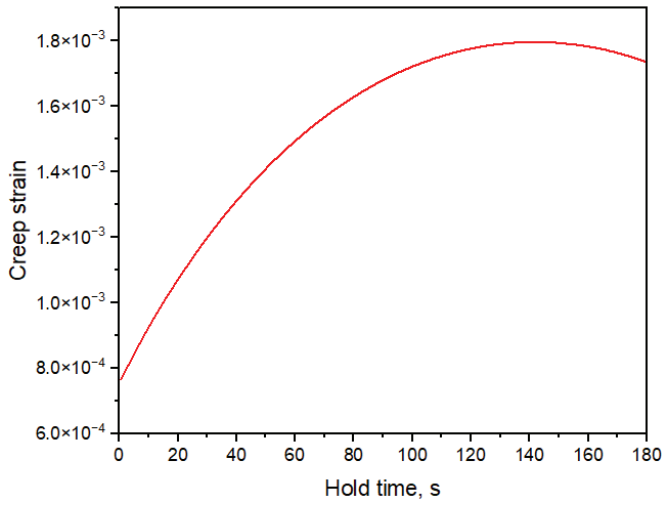

Figure 6. Variation of creep strain with hold timederived from UMT-based model for DZ445 material subjected to creep-fatigue interaction loading at 900 °C, 1.6 % strain range, and 3 min. hold time with 10s time step

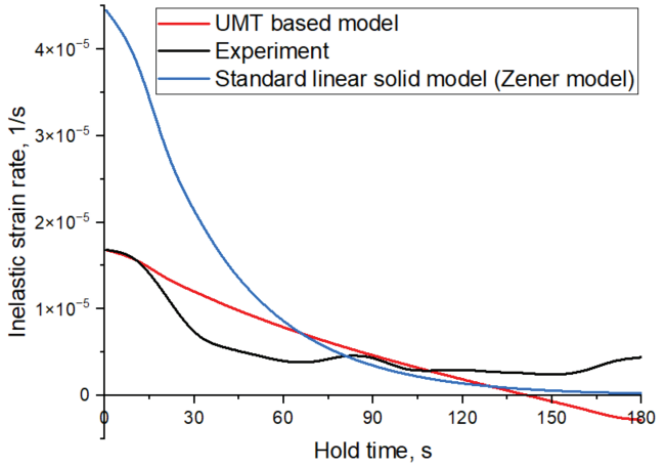

Figure 7. Comparison of modelling creep strain rate with experimental creep strain rate for DZ445 material subjected to creep-fatigue interaction loading at 900 °C, 1.6 % strain range, and 3 min. hold time with 10s time step.

within 140 seconds and outperforms the traditional linear solid Zener model. However, to model the saturation effect after that point, additional parameters need to be incorporated. The current version of the model does not account for saturation effects, likely because it only employs two parameters, which makes capturing saturation difficult. Further studies are being conducted to improve the UMT-based model by including additional parameter to better simulate the saturation effects. Figure 8 displays the variation in strain energy with respect to hold time. The energy dissipated in the material during the hold time increases monotonically and eventually reaches a saturation point towards the end of the hold time. This indicates that the energy dissipation in the material is nonlinear. The nonlinear pattern of TSI evolution is also observed in Fig. 9, although on a different scale.

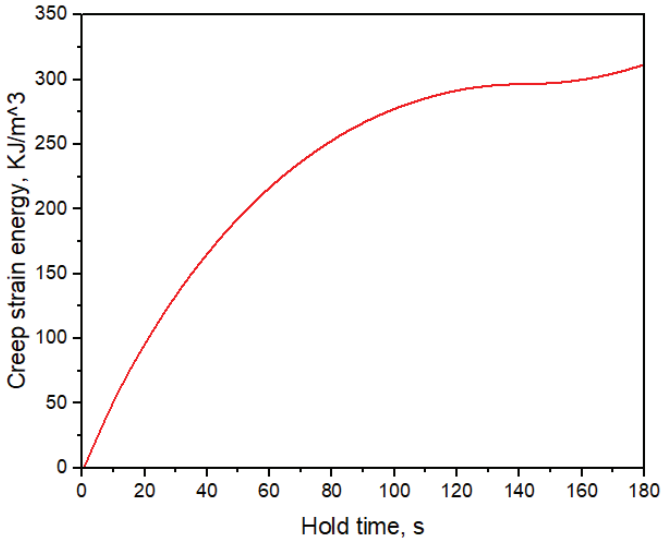

Figure 8. Variation of creep strain energy with hold time derived from UMT-based model for DZ445 material subjected to creep-fatigue interaction loading at 900 °C, 1.6 % strain range, and 3 min. hold time with 10s time step.

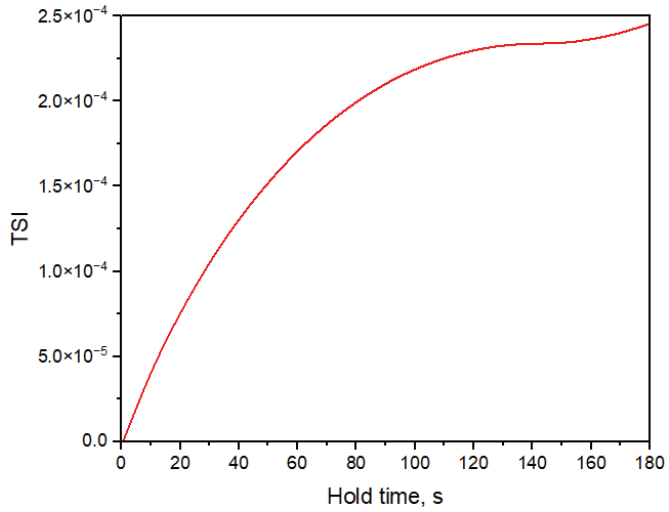

Figure 9. Development of TSI with hold time derived from UMT-based model for DZ445 material at 900 °C, 1.6 % strain range and 3 min. hold time with 10s time step size.

Our goal is to capture the time-dependent behaviour of materials during relaxation over time. Rapid softening is a time-independent, instantaneous behaviour that accounts for a small fraction, specifically 0.28 % (in the case study), of the total relaxation time, which is insignificant.

Unified mechanics theory assumes that energy dissipates through various micro-mechanisms as a material undergoes loading or use. Pinpointing the exact entropy contribution of each damage-causing mechanism can be an intricate and extensive process. However, once these contributions are established, calculating the dissipated energy and quantifying the overall damage using the thermodynamic state index (TSI) becomes straightforward. Understanding the energy dissipation in stress relaxation is crucial. Physics approaches

rely on pinpointing the micro-mechanism, primarily matrix damage and grain boundary damage. However, this requires continual observation of the material's intricate structure during experiments, which is expensive. Therefore, this research takes a practical approach. It assumes that both damage mechanisms contribute to a single, observable effect: the mechanical energy dissipated through creep strain, represented by the area under the stress-creep strain curve. This area, tracked over time through time marching, provides a comprehensive measure of overall damage reflected in thermodynamic state index (TSI). Essentially, this research bypasses the complex microscopic analysis and focuses on the readily measurable indicator – creep strain – to quantify the sequential effect of matrix damage and grain boundary damage on material health.

The simulation progresses by sequentially summing up entropy generation from stress relaxation and fatigue loading for each loop until it reaches the predefined TSI value, indicating the material's ultimate fracture[16]. The simulation concludes by stopping at the specified TSI value, determining the number of hysteresis loops as the material's life under creep-fatigue interaction loading.

5. CONCLUSIONS

UMT-based model, which is a non-phenomenological and physics-based model, offers a simple and different approach for predicting stress relaxation behaviour during creep-fatigue interaction. It is important to note that physics-based models are superior to curve-fitting models since they provide an explanation for the physical aspects of the problem. TSI depends entirely on entropy generation due to loading and material properties, wherein entropy arises from various dissipative micro-mechanisms during loading. Following a single simulation of stress relaxation, at the conclusion of a 180 sec. hold time, the obtained results include quantified values of creep strain, creep strain energy, generated entropy, and TSI. During the holding period, when the experimental stress decreases, the model's prediction of stress deviates from the actual data by up to 25.66 %. The accuracy of the assumptions used to formulate an analytical model determines the validity of the model. The predicted stress values do not match the experimental data for certain time intervals, which could be due to the assumption that the mechanisms remain the same throughout the steady state relaxation time, which might not be accurate. If there is more deviation, increasing the number of parameters can always enable us to match the experimental data. Nonetheless, physically capturing damage in the material has the potential to enable more accurate predictions of the material's behaviour. Further examination of the stress relaxation mechanism and its usage in the creation of the model will be a part of future research.

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CONTRIBUTORS

Mr Saurabh Mangal is an MS Research Scholar at the Department of Applied Mechanics, IIT Madras. His areas of research include: Material modelling, finite element analysis, numerical simulations, creep, fatigue, creep-fatigue interaction, etc. For the current study, he contributed to conceptualization, analytical formulations, investigation, methodology, validation, data curation, formal analysis, software, writing-original draft preparation and writing-review & editing.

Dr Sri Krishna Sudhamsu Kambhammettu is an Assistant Professor at National Institute of Technology Jamshedpur. He works in the general area of solid mechanics with a focus on engineering applications pertaining to specific areas such as damage mechanics, impact mechanics and sealing technology. In the current study, he contributed to conceptualization, methodology, formal analysis, and writing-review & editing and supervision.

Dr Lakshmana Rao C. is a Professor at the Department of Applied Mechanics, IIT Madras. He obtained his Master's degrees from the Department of Civil Engineering at IIT Madras and DS in mechanics of materials from Massachusetts Institute of Technology. His areas of specialization include: Solid mechanics in general and damage mechanics, impact mechanics, fracture Mechanics and finite element analysis in particular.
For this work, he contributed to analytical investigation, resources, writing-review & editing and supervision.

Dr Perumal Chellapandi is a Distinguished alumnus of IIT Madras with PhD in Applied Mechanics. He got his DS from AMET University, Chennai. Currently, he is an INAE Distinguished Professor at IIT-Madras Chennai. His areas of specializations are Fast reactor design & technology in general and high-temperature design and fast transient fluid-structure interaction dynamic in particular.
For the current study, he contributed to analytical investigation, resources, writing-review & editing and supervision.