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An experimental validation of unified mechanics theory for predicting stainless steel low and high cycle fatigue damage initiation.

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ABSTRACT

An experimental campaign of stainless-steel specimen tests has been completed. Three different types of tests have been performed: UTS (Ultimate Tensile Strength), LCF (Low Cycle Fatigue) and HCF (High Cycle Fatigue). This experimental campaign has been conceived and performed to validate the fatigue damage initiation prediction capabilities of UMT (Unified Mechanics Theory). Two different formulations have been used for LCF and HCF. For the latter, a modification to the existing approach is proposed in this paper. Good agreement has been found between UMT predictions and experimental results.

1. Introduction

Predicting damage initiation [1] of metallic structures subjected to cyclic load is of fundamental importance in many industries, such like aerospace [2], automotive [3], railways [4] and many others. It is an industrial practice to test either the component itself, a sub-component, or a specimen of the material to have a database of fatigue damage initiation to be able to guarantee a safe life in service. In other words, the design against fatigue is heavily reliant on testing [5]. Testing in fatigue has high financial costs [5]. For this reason, it would be a fundamental asset and a competitive advantage for industries to have reliable formulations able to predict metal fatigue initiation by knowing only the material properties and the loading conditions, in such a way to reduce or even avoid testing. Work has been done in this direction in the attempt to reach this goal. Cristal Plasticity has been successfully used in predict damage initiation of metallic [6–9] structures. AI (Artificial Intelligence) and machine learning tools have also been created by interpolating existing test data [10–13]. Focus of this work is however to test the prediction capabilities of a novel thermo-dynamic approach to predict fatigue damage initiation: Unified Mechanics Theory [14–18]. Unified Mechanics Theory (UMT) attempts to merge Newton's law of motion with the second law of thermodynamics. This novel approach makes use of an additional axis called Thermodynamic State Index (TSI), which can have values between zero and one: zero corresponding to no accumulated damage, one corresponding to fatigue damage initiation. Evolution along the TSI axis, and therefore path towards crack initiation, is ruled by Boltzmann's entropy formulation [14] and the thermodynamic fundamental equation of the material [14]. As a result, governing differential equations of any structural system subjected to cyclic loading include energy dissipation, and degradation evolution. In other words, by simply knowing the thermo-dynamic and mechanic (elastic and inelastic) parameters of the material, and by knowing its loading condition, it is possible to make accurate predictions in terms of fatigue damage initiation. A similar approach, especially in the industrial design, would be beneficial financially and in terms of accuracy. UMT could, in fact, help reducing the fatigue testing required, which is time consuming and financially onerous.

An experimental campaign has been completed to validate the UMT predictions. Three types of tests have been performed: UTS (Ultimate Tensile Test) [19], LCF (Low Cycle Fatigue) test [20] and HCF (High Cycle Fatigue) test [21]. In this manuscript, LCF is meant as a cyclic load involving inelastic behaviour of the material. HCF is meant a cyclic load with failure at relatively high number of cycles with purely elastic material behaviour in the macro-scale. The Ultimate Tensile Test has been replicated with an explicit Finite Element (FE) built and analysed in Abaqus CAE [22] and solved in Abaqus 6.14 [22]. LCF test results predictions have been performed with the formulation proposed by Noushad Bin Jamal et al. [23]. The HCF test results predictions have

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been performed the formulation proposed by Hsiao Wei Lee [24]. The material is stainless steel whose properties are given in Section 2.

2. Material data

Stainless steel (SS) used for this experimental campaign has a high Chromium content (22%), a moderate Nickel content (5.5%) and 3% Molybdenum. The main advantage this stainless steel is the combination of properties given by both the austenitic and ferritic steels. The material properties used for predicting LCF and HCF damage initiation and for predicting the ultimate tensile test are given in Table 1. All the properties are at 20 °C as all tests have been performed at ambient temperature.

The material is considered as isotropic and defect free, although no inspection (CT-scan, X-rays) has been directly performed by the authors to demonstrate it but it has been guaranteed by the material's vendor.

3. Specimen geometry

A specific geometry has been conceived for both the UTS and Fatigue tests. The specimen 2D sketch and actual geometry are shown in Fig. 1.

Specimens have been produced by forging. The manufacturing tolerance for each dimension reported in Fig. 1 is ±0.05 mm. The surface finish has been measured directly as a part of this work and an average value of 1.5 μm has been found.

4. Experiment set-up

Instron Test Machines have been used for UTS, LCF and HCF Tests. The size of the specimen is important when characterising the material behaviour of a material [25]. Given that this project was conceived for industrial application, a relatively big specimen size has been chosen. A bigger volume of material, in fact, may tend to include a larger number of weaknesses and it may be more prone to damage initiation [25]. The UTS test has been performed in displacement control. The speed of the test has been 0.05 mm/s. This relatively slow speed has been chosen to minimise the strain rate effects [19,20]. Quasi-static condition has been therefore guaranteed. Both fatigue tests have been performed in load control. The HCF Tests have been performed at $R = -1$, where R is the ratio between the minimum and maximum stress at the smallest cross section of the specimen ($R = \frac{\sigma_{min}}{\sigma_{max}}$). The LCF Test has been performed with $R = 0.1$

The failure was visible (specimen rupture) in case of the UTS test. In more formal terms, no more load could be carried by the specimen when failed and a sudden drop in the load-displacement curve of the test machine was observed. In case of fatigue tests, the failure criterion was taken as 10% drop of the load carrying capability [20]. This is a limitation of the experimental campaign as the exact fatigue initiation (micro-damage) was not recorded. The recorded damage was already macroscopic but not such to cause the specimen to burst (sudden failure). However, the author's opinion is that is approach is very relevant for practical industrial applications.

Table 1
Material properties of SS used for UTS, LCF and HCF predictions.

Material Property	Symbol	Numerical Value
Density [Mg/mm3]	ρ	7.78e-9
Young Modulus [MPa]	E	203,040
Ramberg-Osgood Stiffness [MPa]	K	630
Ramberg-Osgood exponent	n	0.26
Molar Mass [g/mole]	ms	55.85
Poisson's ratio	ν	0.3
Yield Stress [MPa]	σ_0	550
Strain to failure	ε_f	0.27

5. UTS and fatigue UMT predictions

The main goal of this paper is to propose a new validation of UMT for the produced set of fatigue experimental data. Given that three different kind of tests have been performed, three different set of correspondent predictions have been made. For what concerns the UTS, a model has been built with Abaqus Explicit [22], i.e., the simulation was time dependant. The modelling technique is well established, and no technical or scientific claim is here made. The failure was modelled with a simple strain to failure value of the material, reported in Table 1. The experimental results themselves are however quite relevant for the technical community. The LCF test has been also modelled with Abaqus Explicit as the damage model used is time dependant and coded in an Abaqus VMAT to tackle a variety of structural problems. Only one LCF cycle has been modelled via simulation. The plastic hysteresis of this material is, in fact, stable after only few cycles (2 or 3, negligible compared to the LCF life) and modelling one cycle instead of the full low cycle fatigue life allows a computational time saving for engineering analyses purposes. The contribution to the total damage accumulated after each cycle is considered identical and this assumption is correct given that a stabilised plastic hysteresis has been considered and given as an input. The thermo-dynamic degradation proposed by Noushad Bin Jamal [23] has been implemented in a Fortran VMAT [22] to calculate the damage at each cycle. The inverse of such a damage is the total amount of cycles to damage initiation. In other words, if φ_1 is the LCF damage after one fatigue cycle (or TSI in terms of Unified Mechanics Theory; coded as SDV2 in the Abaqus VMAT), the number of cycles to damage imitation N_i is given simply by:

$$N_i = \frac{1}{\varphi_1} \tag{1}$$

In other words, the damage corresponding to one fatigue cycle is read from Abaqus (via the SDV2 shown in Fig. 2. SDV2 is the damage to initiation, i.e. TSI in the UMT). This numerical value is inverted to calculate how many cycles are needed to the damage to reach its critical value of 1.

The HCF test has been modelled with the specific HCF implementation proposed by Hsiao Wei Lee [24]. A Matlab M-File [26] has been written and used to make the predictions.

5.1. Finite elements modelling

The FE model has been built with 17,920 HEX8 elements. One end of the specimen is fixed, i.e., the displacements are restrained in all the other directions (Fig. 3). The other end of the specimen is free to move only in the direction of the load/displacement (x-direction in Fig. 3). The UTS test is displacement controlled. For this reason, a time dependant axial displacement has been applied to the end of the specimen until failure was observed in Abaqus Explicit. Mass scaling and numerical damping have been used.

5.2. UTS predictions

Abaqus explicit has been used to model the UTS test. Beside the material properties and the strain to failure value reported in Table 1, inelastic data reported in Table 2 has been added.

The model can re-produce the stress-strain behaviour of the material measured during the Test. Also, the final failure is proceeded by the necking at the critical (minimum area) cross section. A model screenshot of the necking is shown in Fig. 4.

Experimental and analysis curves are shown in Fig. 5.

Some post-processing of experimental data is required to produce the results given in Fig. 5. The raw experimental data are in fact the axial load as a function of the axial displacement of the actuator. This data needs to be converted in true strain and true stresses [21] before being able to match the result of the Abaqus simulation.

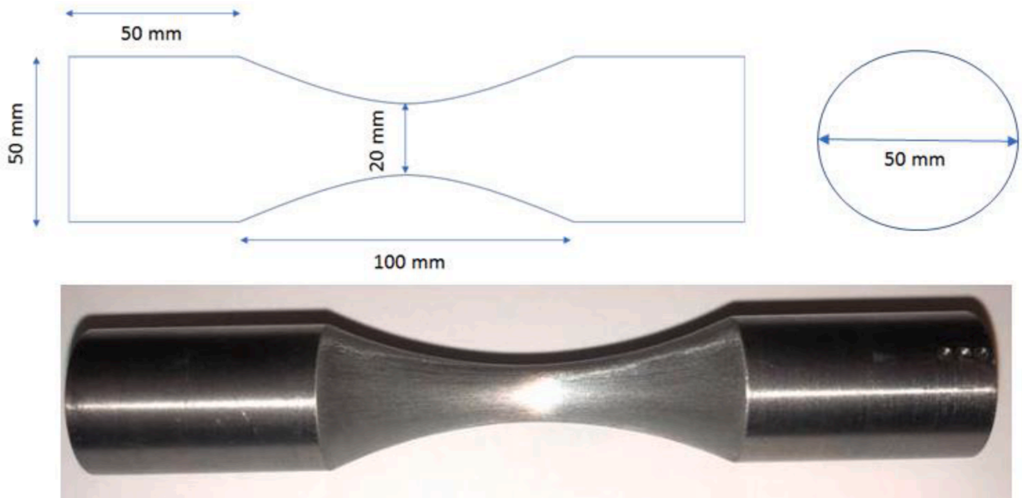

Fig. 1. a sketch of the mid plane cross section of the specimen with its dimensions together with an image of the specimen itself.

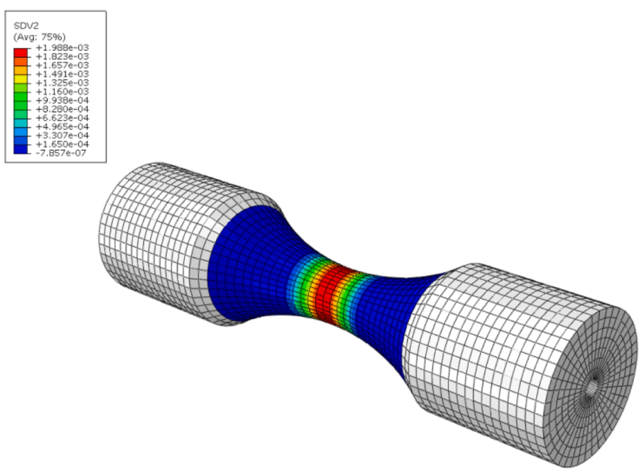

Fig. 2. Example of damage at the end of one LCF cycle. This damage (TSI in UMT) is critical when the unit is reached (Fatigue damage initiation condition).

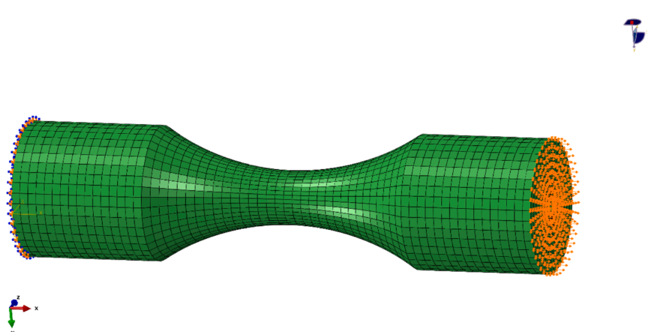

Fig. 3. Boundary Conditions and loads of the UTS/LCF model.

5.3. LCF predictions

The LCF Formulation of Noushad Bin Jamal [17] has been used to make prediction. The Unified Mechanics Theory is based on the simple but powerful concept that fatigue damage initiation is consequence of the entropic degradation of the material. In other words, a TSI (Thermodynamic State Index) parameter is defined and denoted with the symbol φ. This parameter has a value in the interval [0,1], 0 meaning no

Table 2
Inelastic properties in the Abaqus UTS analysis.

True Stress [MPa]	Plastic strain
550	0
630	0.0475
715	0.0975
782	0.1475
840	0.1975
880	0.2275
500	0.26
0	0.27

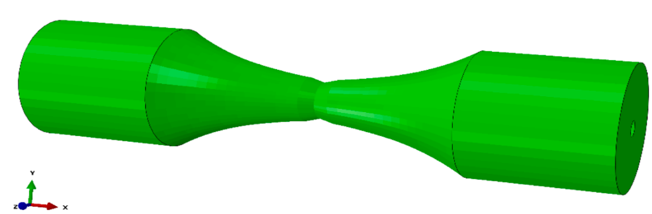

Fig. 4. Necking of the minimum area cross section of the specimen before final failure.

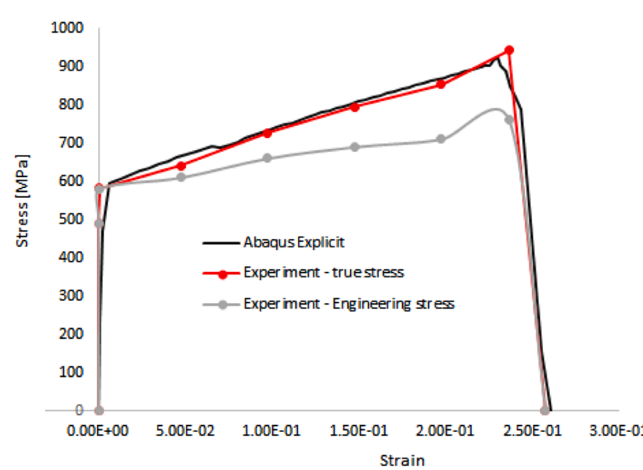

Fig. 5. Test data compared to simulation results - UTS Test.

damage, 1 meaning damage initiation. The mathematical expression of TSI is given in Eq. (2):

$$\varphi = \varphi_c\left(1 - \exp\left(-\Delta s\frac{m_s}{R}\right)\right) \quad (2)$$

where:

- φ is the TSI (Thermodynamic State Index)
- φ_c is a fitting parameter defined for the specific problem
- m_s is the molar mass of the metal
- R is the gas constant
- Δs is the total change in entropy.

In the LCF cycle, the increase in entropy is calculated with Eq. (3).

$$\Delta s = \frac{1}{\rho T}\int_{t1}^{t2} \sigma * d\varepsilon^p \quad (3)$$

where

- ρ is the material density
- T is the material temperature
- t_1 is the time at the beginning of the fatigue cycle
- t_2 is the time at the end of the fatigue cycle
- ε^p is the plastic strain

The plastic strain ε^p is found as per Eq. (4).

$$\varepsilon^p = \varepsilon^{tot} - \frac{\sigma_0}{E} \quad (4)$$

where

- ε^p is the total strain (elastic and inelastic)
- σ_0 is the yield stress.

The full algorithm for entropy calculation in a 3D structure is provided in Reference 17. It has been translated into an Abaqus VMAT (Abaqus explicit user material modelling). A full fatigue cycle has been modelled and the TSI (φ) calculated at the end of it (the TSI output can be plotted in the SDV2 variable shown in Fig. 2). The number of cycles to damage initiation is given by the inverse of the TSI calculated after 1 cycle. The comparison between UMT prediction and experimental results is shown in Fig. 6.

Numerical values are reported in Table 3.

Abaqus explicit has been used to define a fatigue loading cycle. The

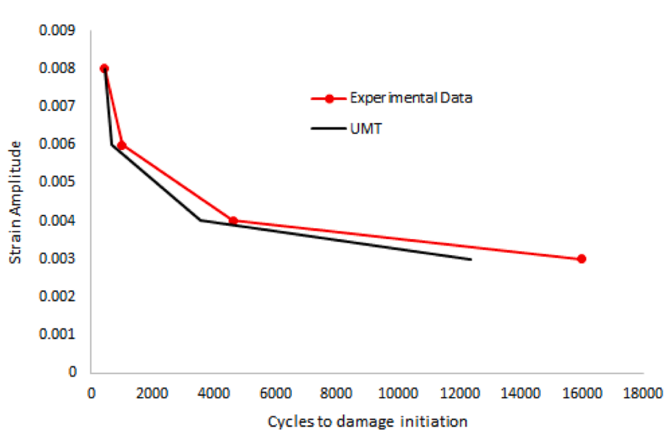

Fig. 6. LCF Predictions against experimental results.

Table 3
LCF Data: Predictions and actual experiment.

Strain Amplitude	Test Results [cycles]	Simulation cycles (Abaqus UMT)
0.003	15,985	12,345
0.004	4611	3538
0.006	1010	649
0.008	425	438

entropy damage degradation has been calculated with a Fortran VMAT for 1 cycle. The inverse of this calculated damage gives the number of cycles needed before a damage equal to unity is reached. It is important to remark that a power law hypothesis has been made for the isotropic hardening. The plastic hysteresis is stable after the first fatigue cycle, therefore extrapolating the damage of one single fatigue cycle to calculate the number of cycles to initiation is a valid approach given the all the cycles are identical.

5.4. HCF predictions

The formulation of Hsiao Wei Lee [18] has been used to make HCF predictions. The TSI definition is obviously the same expressed in Eq. (1). The entropy generation mechanism, however, is not directly related to inelastic strain. During HCF, the material remains elastic. According to the HCF formulation used, the main contribution to the entropy generation the micro-plasticity, i.e. the plasticity generated at microscopic level. The entropy generation is expressed as follows [Eq. (5)].

$$\Delta s = \int_{t1}^{t2} \varphi f_v \frac{\sigma^\mu \dot{\varepsilon}^\mu}{T} dt \quad (5)$$

where

- σ^μ is the microscopic stress. Its local value is a fuction of the macroscopic stress (the stress calculated with an analytical approach or a FE model. Details are given in Reference 18.
- ε^μ is the microscopic strain rate. Its local value is a fuction of the macroscopic strain (the strain calculated with an analytical approach or a FE model. Details are given in Reference 18.
- f_v is a fundamental parameter of this formulation. It is, in fact, conceived as a constant numerical value establishing a relation between stresses and strains at macro and micro level. It is the ratio of the micro-defects volume with respect to the volume of elastic material [18]. From a different perspective, f_v is the maximum percentage of dislocation planes that can be activated. It is assumed, in this work, that such a percentage follows the evolution of TSI. It is indeed a point of novelty proposed in this manuscript. There is, to the best of authors knowledge, no evidence or even a hypothesis of considering f_v as a function of the applied stress. In Reference 18, f_v has been used as a constant. In our work instead, f_v has been considered such like a fitting parameter. In other words, the original formulation proposed by Hsiao Wei Lee to consider f_v as a constant value has been modified. The authors of this manuscript suggest considering fv as a linear function of the applied stress amplitude (the microplasticity volume increases as the applied stress approaches the yield capability of the material). This proposed modified HCF UMT is described in Section 5.4.1.

It is important to remark the additional following assumptions on the micro-plasticity behaviour of the HCF UMT used:

- The hardening of the metal is modelled with a bi-linear kinematic hardening curve. The hardening modulus is defined as the slope between the ultimate stress and the yield stress.

- The hysteresis loop is stabilised. When the TSI goes from 0 to 1 microplasticity is induced in more and more portions of the material volume.
- The energy dissipation (and consequent temperature increase) at the micro-plasticity sites is small enough to be neglected [22].

5.4.1. A modified HCF UMT

The UMT HCF formulation has been applied to a problem of fully reverse (tension-compression) fatigue cycle. The original UMT HCF formulation [18] has been modified in one detail: the calculation of f_v [Eq. (5)]. Instead of taking a single value to predict a HCF S/N curve, the following hypothesis has been made:

- f_v is 0 when the peak applied stress (half of the stress range in a fully reverse cycle) is below the fatigue threshold of the metal (stress below which the fatigue life is greater than 10^7 cycles).
- f_v is equal to 1 when the peak applied stress reaches the value of yield stress at the test temperature.
- f_v increases linearly in the interval [0,1] as a function of the applied stress. In other words, its value is ruled by Eq. (6).

$$f_v = \frac{\sigma_{va} - \sigma_{th}}{\sigma_0 - \sigma_{th}}$$

$$\text{with } \sigma_{th} \leq \sigma_{va} \leq \sigma_0 \quad (6)$$

where

- σ_0 is the yield stress
- σ_{th} is the fatigue threshold stress, conventionally taken as the value of stress below which the number of HCF cycles in greater than 10^7 cycles.
- σ_{va} is the HCF vibration amplitude (half of the HCF stress range).

Before using this proposed modified HCF UMT with the experimental campaign presented in this work, the approach has been validated with some data already available in the open literature. The results obtained with INCO718 [23] are shown in Fig. 7.

Results shown in Fig. 7 are considered as a good validation in terms of fatigue prediction. If a constant value $f_v = 0.2$ had been chosen for this validation case instead of the hypothesis proposed in this work, the prediction would have been quite far from the actual experimental data, as shown in Fig. 8.

A similar validation has been performed on Aluminium 2024 HCF fatigue data available in the open literature [24], with results shown in Fig. 9.

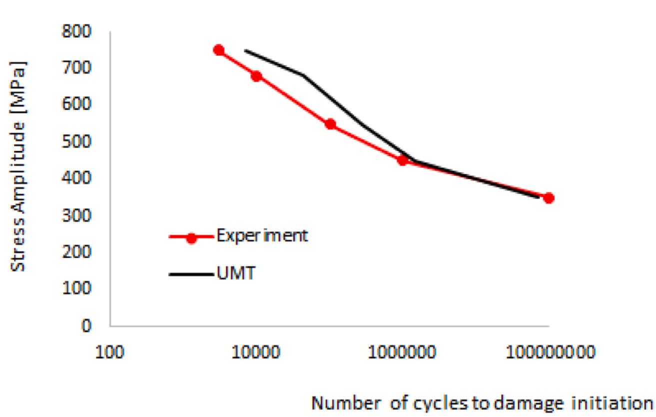

Fig. 7. Replicating the INCO718 test results of Reference 23 with the modified UMT HCF.

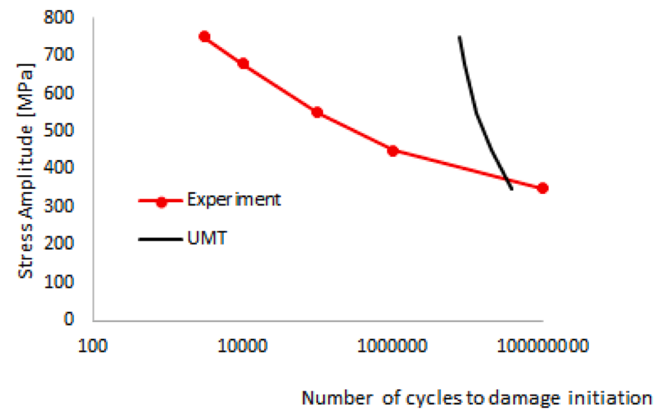

Fig. 8. Replicating the test results of Reference 23 with the original UMT HCF [17] and $f_v = 0.2$.

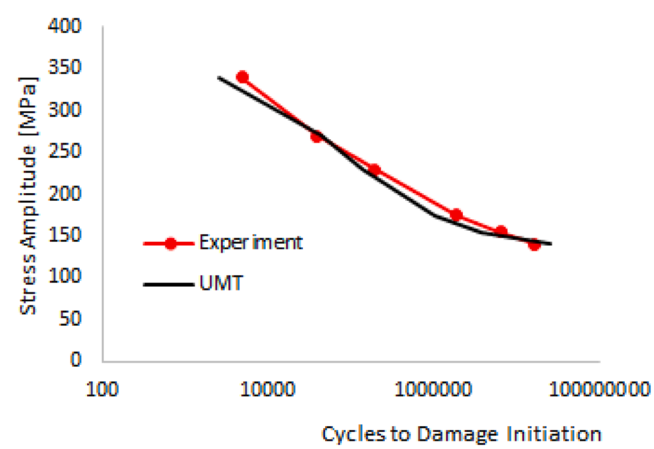

Fig. 9. Replicating the test results of Reference 24 (Aluminium 2024) with the modified UMT HCF.

Very good agreement between predictions and experimental results has been found also for this validation case.

The new approach proposed in the evaluation of the parameter f_v is giving better HCF predictions compared to test results (Figs. 7, 8, 9). The main advantage of the new proposed approach is, in author's view, the hypothesis of considering micro-plasticity as a monotonically increasing function of the applied stress rather than a constant value not-dependant on the load applied.

5.4.2. Stainless steel results

Once the validation with two test cases (Fig. 7 and Fig. 9) has been completed, the proposed modified HCF UMT has been applied to the test results produced as a part of the work described in this manuscript. The comparison is shown in Fig. 10.

A good agreement between theory and experimental results has been found.

6. Discussion

UTS tensile test predictions are matching with good accuracy with the experimental results. The simulation performed with Abaqus Explicit can follow the time evolution of stresses and strains. This is "per se" not a point of novelty. However, the experimental results are now published and available to a wider technical and scientific community.

UMT is a powerful tool to predict damage initiation. Both LCF and HCF predictions are close to the actual test results. The LCF formulation presented in Reference 17 has been used as it is, without modifications.

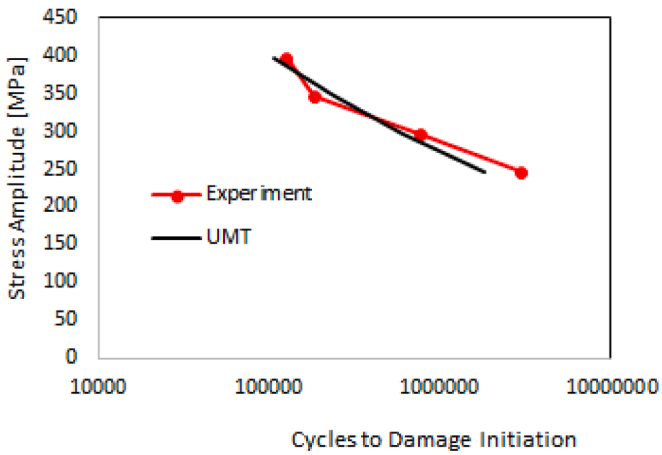

Fig. 10. Stainless Steel HCF test results compared with modified UMT HCF predictions.

The simulation values slightly underpredict the fatigue data points. In author's opinion this is mainly driven by the fact the UMT predicts microscopic damage initiation whilst the experiment was catching a 10% drop in load, which clearly implies a macro-damage. The authors claim that this prediction is however quite accurate in terms of fatigue results, especially when considering practical industrial applications. Two are the main limitation of this work. The first one, is that more test data will be needed a part of future work to validate the UMT approach. The second one is that, in author's opinion, UMT does not consider the surface finish, a main damage initiation factor in metallic fatigue.

The HCF formulation proposed in Reference 18 has been modified to keep into account that the amount of micro-plasticity (the main entropy generation mechanism in HCF) is a function of the applied stress and not a constant value as per original formulation. It increases linearly as the applied stress approaches the yield strength of the material. UMT could be a potential game changer in the fatigue damage initiation prediction. However, fatigue damage initiation in HCF (as in LCF) is strongly influenced by the surface finish [25] as the damage initiation (in the form of macroscopic cracks or micro-cracks) tends to appear on the surface of metallic components [26]. It is important that, in the future, UMT could be capable of predicting damage initiation of same materials with different surface finish. As already remarked for the UTS test, in terms of LCF and HCF, the test results itself, the test procedures and predictions are available with this document to a wider technical and scientific community.

7. Conclusions

An experimental campaign of stainless-steel specimens has been completed. Three types of tests have been performed: UTS, LCF and HCF. For each test type, numerical predictions have been made. The tensile test has been modelled with Abaqus Explicit by embedding a strain to failure criterion of the finite element. Good time history agreement of stress and strains between the FE model and the experiment has been obtained. Unified Mechanics Theory has been, on the other hand, used to make fatigue damage initiation predictions. UMT is a formulation that, if further proved effective, could potentially reduce the amount of fatigue tests needed for certification of industrial products, with massive financial benefits. Good agreement between test results and UMT predictions has been found. The LCF UMT theory formulation has been used as it is and already proposed in the open literature. A modification on the micro-plasticity of the HCF UMT has however been proposed to obtain better accuracy. UMT can become a game changer in fatigue initiation predictions, as it may allow the amount of fatigue testing to be reduced. However, the ability of UMT to capture the influence of surface finish on fatigue damage initiation of metals should be object of further studies and efforts.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

No data was used for the research described in the article.

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