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An iterative framework for crack nucleation and propagation in high cycle fatigue

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ABSTRACT

The objective of numerical frameworks properly devoted to fatigue life estimation is becoming of great interest in the mechanical field. Indeed, these approaches allow for the investigation of both crack nucleation and propagation stages, reducing the amount of cost and time resources that are necessary in classical experimental approaches. Unfortunately, current solutions necessitate either the crack nucleation definition or multiple mesh refinements that require specific hardware equipment for the simulation process. This work presents a numerical framework for predicting the fatigue life and fracture behaviour of specimens under High Cycle Fatigue (HCF) conditions. An iterative Python-based algorithm was developed and integrated with the open-source Finite Element Method (FEM) solver Code_Aster for simulating both the crack nucleation and propagation stages. The nucleation stage was investigated using the multiaxial critical plane formulation proposed by Smith-Watson-Topper, while the propagation stage was modelled by means of the eXtended Finite Element Method (XFEM) combined with the Paris law. Then, the proposed numerical framework was validated through experimental activities conducted on two different materials, i.e., C45 and 20MnCr5 steels. A detailed material characterization in terms of hardness, roughness, static and fatigue properties was performed with the specific purpose of calibrating the developed numerical framework. A proposal of an innovative curve for nucleation prediction was also presented for a complete fracture behaviour analysis based directly on S–N curves. Thus, experimental and numerical results were compared in terms of crack analysis and number of fatigue cycles, allowing for the validation of the presented work.

1. Introduction

In the field of fatigue assessment of mechanical components, the prediction of failure mechanisms such as crack initiation and propagation becomes crucial for guaranteeing the integrity of the component itself. Experimental methods provide valuable insights into failure mechanisms, even though they are often limited by cost, time, and resolution constraints, as is well known in the literature [1]. Over the years, numerical simulations have become a valuable tool for predicting these mechanisms and offering numerous advantages [2]. As a matter of fact, accurate modelling of crack nucleation and propagation is crucial for a complete understanding of both durability and integrity aspects of materials subjected to cyclic loading, specifically under High Cycle Fatigue (HCF) conditions.

The Fatigue Crack Growth (FCG) phenomenon is generally investigated in two main parts: the nucleation and propagation stages.

Moreover, as demonstrated in Ref. [3], the connection between propagation and nucleation stages is strongly unbalanced toward the latter under HCF conditions. For this reason, engineers have assessed and predicted the crack initiation stage by means of methods that consider classic stress-life (S–N) curves based on empirical testing or more sophisticated models for local material response and damage accumulation [4–6].

Over the years, modern fatigue design approaches have been developed employing multiaxial critical plane criteria in HCF analysis [7–9]. This approach generally permits the assessment of both nucleation and the orientation of the early crack propagation plane. Regarding the modelling possibilities of the investigated phenomena, various approaches have been proposed in the literature depending on the type of stress or the physical conditions involved in the crack initiation process. These include, for example, the Findley criterion [10], the Crossland criterion [11], the Fatemi Socie criterion [12], and the Smith Watson Topper (SWT) criterion [13,14].

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Nomenclature			
Symbols		σ'_f	Fatigue strength coefficient [MPa]
a	Semi-length of the initial crack [mm]	$\sigma_{n,\max}$	Maximum normal stress on the critical plane [MPa]
b	Fatigue strength exponent []	ΔK	Stress intensity factor range [$\text{MPa}\sqrt{\text{m}}$]
c	Fatigue ductility exponent []	$\Delta \varepsilon_{n,\max}$	Maximum normal strain range on the critical plane []
C	Paris law coefficient [$\text{MPa}\sqrt{\text{m}}$]	ε'_f	Fatigue ductility coefficient []
$da_{\max}$	Maximum advancement per cycle [mm]	$\frac{da}{dN}$	Crack growth rate [mm/cycle]
E	Young's modulus [MPa]	Acronyms	
$h_{\max}$	Maximum element size in refined mesh [mm]	FEM	Finite Element Method
m	Paris law exponent []	XFEM	eXtended Finite Element Method
n	Number of iterations []	HCF	High Cycle Fatigue
N	Number of cycles []	FCG	Fatigue Crack Growth
R	Load ratio ($F_{\min}/F_{\max}$) []	SWT	Smith-Watson-Topper
σ_a	Stress amplitude [MPa]	S–N	Stress-Number of cycles
σ_m	Mean stress [MPa]	CCZM	Cyclic Cohesive Zone Modeling
σ_{UTS}	Ultimate tensile strength [MPa]	CDM	Continuous Damage Mechanics
σ_y	Yield strength [MPa]	CZM	Cohesive Zone Modeling

The application of such criteria has been significantly facilitated by the advancement of numerical simulation techniques. In fact, critical plane approaches require knowledge of the time-dependent stress tensors at each evaluation point, and this information is efficiently provided by numerical methods such as Finite Element Method (FEM)-based analyses. Several studies proposed in the literature have applied these criteria in various contexts. As an example, in Ref. [15], the Fatemi Socie criterion was employed in the case of aluminium components for aerospace applications with the aim of evaluating the influence of the material microstructure on the crack process. In Ref. [16], the same criterion was used to analyse the effects of inclusions and grain orientation on Hertzian contact fatigue life in bearing steels. Focusing attention on the SWT criterion, the critical plane is defined as the one experiencing the maximum strain, since the target planes are those subjected to the highest normal strain. On the basis of these considerations, the SWT criterion is more effective for materials that typically fail in tension under fatigue conditions dominated by significant tensile loading [17]. In addition, the identification of the location and orientation of the initial crack provides theoretical insight into the number of cycles required for the crack nucleation stage. In Ref. [9], the Findley and Wang & Brown criteria were adopted to investigate crack initiation in welded joints subjected to multiaxial random loading. Other examples are reported in Ref. [18], where the SWT criterion was used to assess crack initiation in notched structural steel for bridge applications, and in Ref. [19], where the criterion was used to assess crack initiation under biaxial conditions. In the specific case of gears, as illustrated in Refs. [20–22], several criteria were investigated for the assessment of early crack propagation in components subjected to HCF testing. These studies demonstrate that such criteria can be applied across a wide range of contexts, ranging from the investigation of the influence of microstructure on fatigue life to the analysis of mechanical components under real operating conditions. As a matter of fact, the entire process of crack nucleation and propagation can be studied using various numerical techniques. On the basis of these considerations, one of the most common approaches involves the adoption of FEM analyses in combination with crack growth laws, with the aim of assessing the fatigue life of the material or component under study. By extracting stress and strain information over a single loading cycle, it is possible to apply the Paris law, or alternative formulations, to estimate crack growth for each fatigue cycle, as detailed, for example, in Refs. [8,23,24]. Over the years, the application of these methodologies has moved toward more advanced approaches rather than classical analyses. For example, in Ref. [25], Cyclic Cohesive Zone Modelling (CCZM) was employed to study crack growth in notched specimens subjected to multiaxial cyclic

loading. Although this technique allows for the definition of a user-defined cohesive law, the proposed approach was limited because the crack path was typically predefined. The adoption of this solution may be advantageous when the crack trajectory is known a priori, but it becomes less suitable for more complex geometries and unpredictable loading conditions. Other examples are reported in Refs. [5,26–30], where FEM-based approaches were adopted with a focus on the Continuous Damage Mechanics (CDM) method. This method accounts for the accumulation of damage on a cycle-by-cycle basis by progressively updating a material-specific parameter as the crack propagates. Although CDM is a powerful tool, its implementation often requires advanced programming knowledge and, in some cases, it is unavailable through user-defined subroutines in commercial software packages. Among advanced numerical techniques, the eXtended Finite Element Method (XFEM) has also been commonly employed to study crack propagation paths or fatigue life estimation [31,32]. Introduced in the late 1990s, XFEM is based on the partition of unity framework, which enables the augmentation of classical FEM approximations with specialized functions that capture crack-tip singularities and displacement discontinuities across crack surfaces [33]. It can be coupled with other techniques, such as the virtual crack closure technique [34] or Cohesive Zone Modelling (CZM) [35]. In standard FEM, accurately resolving discontinuities typically requires the mesh to be conformed to the geometry of the evolving defect, which often involves complex and computationally expensive remeshing. It is clear that XFEM is an effective method for simulating crack growth under a variety of loading scenarios. Unlike conventional FEM, it can model discontinuities such as cracks without requiring mesh updates during propagation. This is made possible through the introduction of additional degrees of freedom at nodes near the crack front and the use of enrichment functions, which enable the crack to evolve independently of the mesh structure. As a result, XFEM is particularly advantageous when dealing with complex geometries and variable loading conditions, where traditional FEM would otherwise necessitate frequent remeshing [36]. It is clear that numerical frameworks devoted to fatigue life estimation are becoming of great interest in the mechanical field. As a matter of fact, these approaches allow for the investigation of both crack nucleation and propagation stages, reducing costs and time requirements compared to classical experimental approaches. Unfortunately, current solutions require the definition of crack nucleation or multiple mesh refinements, which in turn require specific hardware for the simulation process. In addition, no studies have been found in the literature addressing work performed with open-source software in HCF; instead, only studies using commercial software with integrated routines, such as Abaqus or

ANSYS, are available.

This work presents a numerical framework for HCF life prediction, integrating an iterative Python algorithm with Code_Aster. The crack nucleation stage was modelled using the SWT parameter, while the propagation stage was described through XFEM and the Paris law. The model was experimentally validated for C45 and 20MnCr5 steels. In more detail, a full material characterization was carried out with the aim of calibrating the proposed numerical framework. Then, a comparison was performed in terms of the number of nucleation cycles and crack length evolution between numerical and experimental results. An innovative curve for nucleation prediction based on S–N data was also introduced.

2. Material and methods

2.1. Samples

In this study, the focus was on the investigation of two distinct materials: C45 and 20MnCr5 steels. A complete characterization of the samples was performed, examining several aspects. Firstly, the chemical analysis of the steels was conducted with the objective of assessing the composition of the bars from which all samples were fabricated. Subsequently, hardness and roughness analyses were conducted for each sample in order to verify the uniformity of the manufacturing process. Static and fatigue tests were performed for both materials (C45 and 20MnCr5 steels).

Fig. 1 presents the technical drawing of the tested samples. The sample geometries (Fig. 1) were the same for both materials (C45 and 20MnCr5 steels) and were produced by turning operations. Specifically, the sample geometry depicted in Fig. 1 (a) was used for the static tests. The static characterization was conducted using cylindrical samples with dimensions specified in the Standard [37]. One sample of each material (C45 and 20MnCr5 steels) was manufactured for the evaluation of the static mechanical properties. The sample geometry used for the fatigue tests is illustrated in Fig. 1 (b). A total of 15 samples were manufactured from the material bars of each material (C45 and 20MnCr5 steels) for fatigue characterisation. This type of geometry was selected to assess the effectiveness of the proposed framework in identifying the exact crack nucleation point. The use of “classic” notched specimens would have made this aspect secondary, as the crack would generally nucleate at the notch.

Hardness and roughness characterizations were performed for each tested sample and for each material (C45 and 20MnCr5 steels) prior to the experimental testing campaign (static and fatigue characterization). Fig. 2 provides a detailed description of the measurement process. In particular, hardness measurements were conducted using a hardness tester in accordance with the Vickers method. The measurements were carried out on the planar surface at the external tip of the samples (see n. 1 in Fig. 2), allowing for a non-destructive evaluation. The analysis was performed over three distinct zones to detect hardness variations across the entire external surface of the sample. On the other hand, roughness measurements were performed using a roughness meter, evaluating the

roughness profile along the central part of the sample (see n. 2 in Fig. 2). Also in this case, three measurements were conducted along the central region with the objective of evaluating the surface roughness variability across three distinct zones along the central diameter.

The static characterization was performed with the aim of estimating mechanical properties in terms of yield stress (σ_y) and ultimate stress (σ_{UTS}). The experimental tests were conducted in accordance with the ISO 6892-1:2019 Standard [37]. The objective of the fatigue characterisation was to investigate the fatigue limit of the material under consideration. The Staircase method [38] was adopted to determine the fatigue limit, and the runout condition was fixed at 2 million cycles. Subsequently, the material behaviour in the finite life region was analysed using fatigue samples that had not been previously tested. However, due to the limited number of available samples, the experimental trend was compared with analytical ones, which were defined based on formulations derived from the estimated fatigue limit and the corresponding static mechanical properties. In particular, one analytical formulation was characterized by the implementation of the Basquin equation (Formulation 1), whereby the definition of the stress amplitude at 10^3 cycles was established as 0.9 times the σ_{UTS} . The second analytical formulation (Formulation 2) was proposed by Ref. [39], in which the stress amplitude corresponding to 10^3 cycles was evaluated by correcting the σ_{UTS} with a specific factor (f) that is dependent on the σ_{UTS} itself.

The fractured samples obtained from both fatigue limit and finite life region analysis were then employed to validate the numerical model concerning crack nucleation and crack length. For this purpose, an optical microscope was employed for the analysis.

2.2. Nucleation: SWT criterion

The SWT criterion defines the critical plane as the one experiencing the maximum range of normal strain ($\Delta\epsilon_{n,max}$) throughout the fatigue loading history. On this plane, the accumulated damage from cyclic loading is evaluated and correlated with fatigue life using Eq. (1):

$$\frac{\Delta\epsilon_{n,max}}{2} \cdot \sigma_{n,max} = \frac{\sigma_f^2}{E} \cdot (2N_f)^{2b} + \sigma_f' \epsilon_f' \cdot (2N_f)^{b+c} \quad (1)$$

here, E is the elastic modulus, σ_f is the fatigue strength coefficient, b is the fatigue strength

exponent, ϵ_f' is the fatigue ductility coefficient and c is the fatigue ductility exponent. The left-hand side of the equation represents the Fatigue Indicator Parameter (FIP) defined by the SWT criterion.

Since the SWT model focuses on the plane experiencing the maximum normal strain range, it is particularly suited for materials prone to tensile failure and for loading conditions dominated by high tensile stresses. Due to its combined stress strain formulation, analogous to the Fatemi Socie criterion, the SWT approach is applicable to both HCF and Low-Cycle Fatigue (LCF) analyses [17].

2.3. Propagation: XFEM

The XFEM is an advanced computational approach that extends

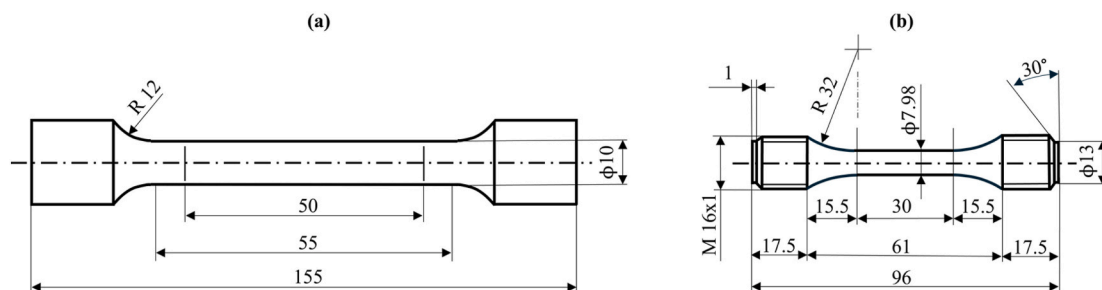
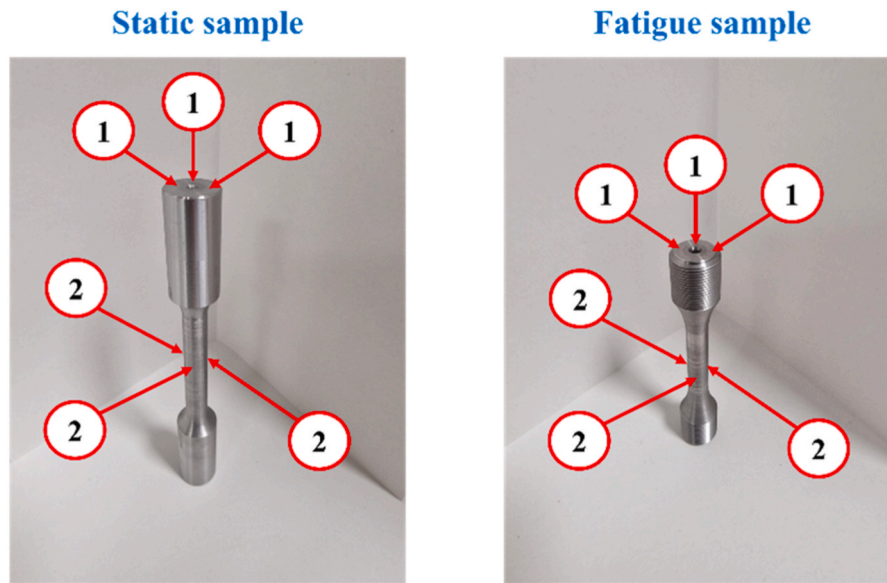


Fig. 1. Samples geometry: (a) static tests, (b) fatigue tests.



1. Hardness analysis 2. Roughness analysis

Fig. 2. Hardness and roughness measurements.

traditional FEM by integrating discontinuous enrichment functions, allowing the modelling of cracks, material interfaces and other discontinuities without the need for global and manual mesh refinement or strict adherence to the geometry of such features [40]. XFEM addresses this challenge by embedding enrichment functions into the finite element formulation. These functions are specifically designed to replicate the local mechanical behaviour near discontinuities, such as the sharp displacement variations across cracks, allowing the use of a fixed mesh throughout the analysis. Two main types of enrichment functions are employed in XFEM: Heaviside functions and asymptotic functions. The first function represents displacement jumps across crack faces [41], while the second function typology allows for the description of singular stress and strain fields near crack tips [42]. Through the inclusion of these functions XFEM can accurately simulate advanced fracture mechanics phenomena, including crack initiation and growth, material failure and phase boundary evolution, while maintaining computational efficiency. Additionally, XFEM has been coupled with other numerical techniques, such as the level set method, to effectively track the evolution of discontinuities over time. This integration enhances its capabilities in applications like topology optimization and problems involving dynamic boundaries [43]. Nonetheless, successful implementation of XFEM demands careful treatment of enriched elements and appropriate numerical integration schemes to ensure solution stability and accuracy. Current research continues to improve these aspects, broadening the method's applicability to increasingly complex and time-dependent problems in engineering and the applied sciences.

To handle propagation, the XFEM method relies on the Paris law, presented in Equation (2):

$$\frac{da}{dN} = C \cdot \sqrt{\Delta K}^m \quad (2)$$

with $\frac{da}{dN}$ the propagation rate, ΔK the effective stress at crack tip, and C and m material constants. The Paris law describes the stable crack growth regime under cyclic loading conditions, relating the crack growth rate to the applied stress intensity factor range. Within the proposed iterative framework, this formulation is used to determine the number of cycles associated with each crack increment. At each propagation step, the stress intensity factor is evaluated at the crack front, and the corresponding crack growth rate is used to compute the cycle

increment required to reach the prescribed crack advance.

3. Numerical model on crack nucleation and propagation

For the purpose of performing the FCG analysis a 3D model of the fatigue specimen was properly developed. To replicate the HCF tests conducted during the experimental campaign (fatigue tests), Fig. 3 reports the boundary conditions applied to the model. Specifically, the entire bottom face was fully constrained ($DX = DY = DZ = 0$) (see red line in Fig. 3) and a cyclic force was applied to the top surface (see green arrow in Fig. 3).

The applied force was selected based on the loading conditions used in the experimental tests. A nonlinear static analysis was carried out to improve convergence. The mesh consisted exclusively of tetrahedral elements, with a total of around 50000 elements, determined after a sensitivity analysis based on von Mises stress distribution. No further mesh refinement was applied at this stage, given the associated computational cost and the additional local refinement steps that will be required once the crack is introduced.

The FCG analysis follows the work now proposed in Algorithm 1. The process begins with a FEM simulation necessary for the application of the SWT criterion, aimed at identifying both the crack initiation point and its initial orientation. In this first analysis, a cyclic load is applied ($R = 0.1$) and the time-dependent stress and strain tensors are extracted. The loads chosen for the analysis are derived from a previous testing campaign conducted to estimate the fatigue limit of the two materials. A dedicated Python script is then used to apply the SWT criterion and determine the critical plane and location for crack nucleation. The material parameters adopted for the SWT criterion were selected thanks to the previous material characterization performed and according to the method proposed by Ref. [44]. Values are presented in Table 1.

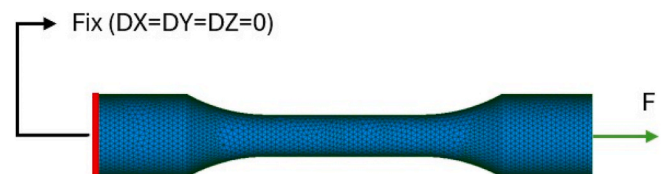


Fig. 3. BC and mesh of the specimen.

Table 1

Material parameters used for SWT criterion and Paris law.

Material	C[MPa $\sqrt{m}$]	<i>m</i>	σ'_f [MPa]	ϵ'_f [mm/ mm]	<i>b</i>	<i>c</i>
C45	1×10^{-12}	3	1393.75	0.4258	−0.09	−0.5829
20MnCr5	5.1×10^{-13}	3.2	1194	0.4642	−0.0725	−0.57

Subsequently, a crack was automatically inserted at the previously identified point with the corresponding orientation. A generic elliptical surface crack with a length of $a = 0.05$ mm was chosen. Before starting the first propagation cycle, a local mesh refinement was performed around the crack to improve the accuracy of the analysis. The refinement was automatically defined based on key parameters related to the defect's dimensions. A maximum element size was chosen equal to $1/10$ of a surrounding area of $2 \cdot da_{max}$, where da_{max} is the maximum crack increment per cycle. The entire procedure was automated through an iterative loop that checks the local element sizes. Once the required mesh density was reached, the first propagation step was performed. The step was governed by the predefined increment da_{max} , and the output was the number of cycles required to reach this imposed crack advance. This value depends on the parameters of the adopted Paris law. In addition to the number of cycles, the software provides the updated crack orientation and propagation direction, resulting in the updated crack geometry.

Algorithm 1 Fatigue Crack Growth Analysis

```

1: Input: Cyclic load parameters ( $R = 0.1$ ), material properties, Paris law constants
2: Run initial FEM simulation under cyclic load
3: Extract time-dependent stress and strain tensors
4: Apply SWT criterion using Python script
5: Determine crack initiation point and orientation
6: De ne number of iterations = n
7: for i = 1, ..., n do
8:   Insert initial crack (elliptical surface,  $a = 0.05$  mm)
9:   Refine mesh locally:
     • Max element size:  $h_{max} = a/10$ 
     • Refinement area radius:  $2 \cdot da_{max}$ 
10:  while local mesh density not sufficient do
11:    Further local refinement
12:  end while
13:  Propagate crack by  $da_{max}$  using FEM simulation
14:  Compute number of cycles for increment via Paris law
15:  Update crack orientation and geometry
16:  while propagation not complete do
17:    Compute error eld near current crack front
18:    Re ne mesh in high-error zones
19:    Dere ne mesh in low-interest regions
20:    Propagate crack by  $da_{max}$ 
21:    Update cycle count and geometry
22:  end while
23: end for
24: Compute total nucleation cycles (from SWT)
25: Sum propagation cycles
26: Output: Total cycles to failure = nucleation + propagation

```

At this point, the code enters a new loop in which an error field (line 17 of Algorithm 1) is calculated around the updated geometry and progressively reduced through further local mesh refinement. This is achieved using the same approach described above. Simultaneously, a derefinement strategy is applied to areas no longer of interest, reducing the computational cost (lines 18–19 of Algorithm 1). This adaptive approach was adopted to avoid excessively long computation times during the full propagation simulation. The entire procedure is governed by an outer loop that controls the number of propagation steps to be performed. At the end of the simulation, the total number of cycles required for nucleation is obtained via the SWT criterion, and the number of cycles required for propagation is calculated by summing the

cycles corresponding to each propagation step. The sum of these two contributions is compared with the experimentally measured number of cycles to failure.

4. Results

This section is dedicated to the presentation of the results obtained from the proposed activity.

Firstly, the results obtained from the samples characterisation are presented.

The chemical compositions of the materials under investigation are reported in Table 2 (for C45 steel) and Table 3 (for 20MnCr5 steel). The tables present the chemical compositions of the bars from which the samples (for static or fatigue analysis) were manufactured. The chemical analysis was conducted directly by the manufacturer on a representative sample of the material bar, and the resulting values were found to be in accordance with the specified material standards [37,38,45]. Figs. 4 and 5 present the hardness and roughness measurements obtained from the sample characterisations conducted prior to experimental testing (static and fatigue analysis). The hardness characterisation (see Fig. 4) of the materials (C45 and 20MnCr5 steels) and sample typologies (static and fatigue samples) resulted in values ranging between 200 and 300 HV. The obtained values were then compared with the indications provided by the Standard [45]. The results were found to be in good agreement with the lower limits of the proposed ranges (185 HV for C45 steel and 150 HV for 20MnCr5 steel), while the upper limits were slightly exceeded (255 HV for both steels). In case of discrepancies in the hardness results, the tensile strength values are considered the decisive factor, as reported in the Standard [45]. Regarding the roughness characterisation (see Fig. 5), the analysis allowed the inspection of the finished surfaces required for both specimen typologies. The fatigue samples produced from the C45 bar exhibited a less uniform roughness trend compared to those produced from the 20MnCr5 bar. It can be concluded that the results presented in Figs. 4 and 5 indicate that the manufacturing process is generally uniform in terms of mechanical properties, as evidenced by the consistency of hardness and roughness measurements, except for the less uniform roughness observed in the case of C45 steel.

The results obtained from the static and fatigue tests are now presented.

The C45 steel shown a σ_y of 596 MPa and a σ_{UTS} of 760 MPa. On the other hand, the 20MnCr5 steel shown a σ_y of 1179 MPa and a σ_{UTS} of 1420 MPa. The obtained results were then compared, where possible, with the indications provided by the Standard [38] to validate the obtained values. The results obtained from the fatigue characterization are illustrated in Fig. 6, which shows the S–N curves for both C45 (Fig. 6 (a)) and 20MnCr5 (Fig. 6 (b)) steels. The analysis was conducted utilising mean stress values (σ_m) of 240 MPa for the C45 steel and 320 MPa for the 20MnCr5 steel, respectively. In particular, each graph presents data points that were necessary for the two-fatigue analysis (see 2.1). Firstly, the fatigue limit (σ_{lim}) analysis was carried out using both failure and run out results (Failure - Staircase and run outs - Staircase data points on Fig. 6), which were adopted to determine σ_{lim} according to the Staircase method [38] (fatigue limit on Fig. 6). Secondly, the finite life region analysis was based on both experimental results (Finite life curve on Fig. 6) and analytical trends (Formulation 1 and Formulation 2 curves on Fig. 6). However, two C45 fatigue samples failed within the grips of the testing machine, reducing the number of data points to 13. With regard to the σ_{lim} analysis, a total of 9 samples were utilised for the Staircase analysis of the C45 steel, whereas the analysis of the 20MnCr5 steel relied on the use of 11 samples for the Staircase analysis. The σ_{lim} evaluation in the corresponding testing conditions was performed according to the computations provided by Standard [38] and in terms of a 50% probability of failure for both the tested materials. The results obtained for C45 steel and 20MnCr5 steel were 211 MPa and 259 MPa, with a standard deviation of 5 MPa, respectively. The utilization of the

Table 2
C45 chemical compositions (mass fraction).

Bar	C [%]	Si [%]	Mn [%]	P [%]	S [%]	Cr [%]	Al [%]	Mo [%]	Ni [%]	Cu [%]
For static samples	0.439	0.248	0.677	0.0099	0.0040	0.077	-	0.0388	0.135	0.1864
For fatigue samples	0.490	0.237	0.601	0.0096	0.0040	0.063	0.0202	-	0.073	0.0802

Table 3
20MnCr5 chemical compositions (mass fraction).

Bar	C [%]	Si [%]	Mn [%]	P [%]	S [%]	Cr [%]	Al [%]	Mo [%]	Ni [%]	Cu [%]
For static samples	0.1939	0.2195	1.2050	0.0144	0.0223	1.2235	0.0225	0.0367	0.2036	0.2597
For fatigue samples	0.1850	0.2600	1.3100	0.0144	0.0243	1.2200	0.0243	0.0220	0.0800	0.1900

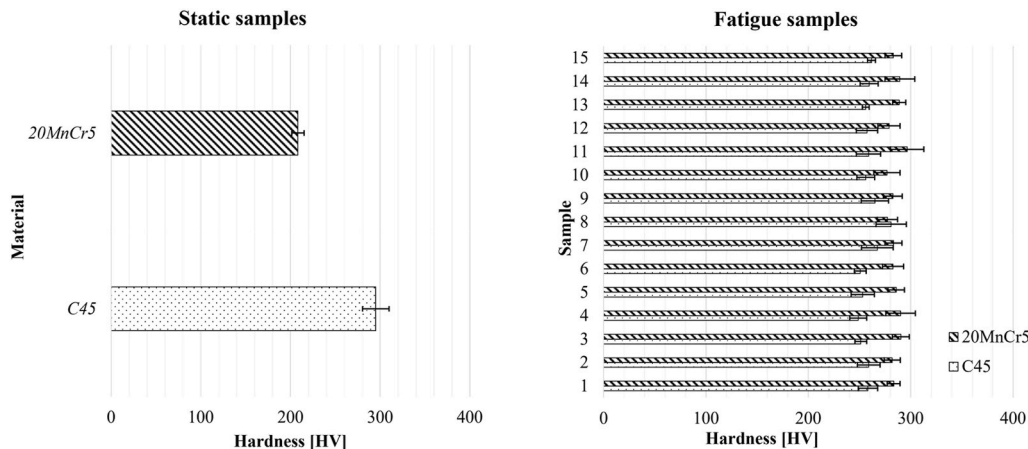


Fig. 4. Hardness characterization.

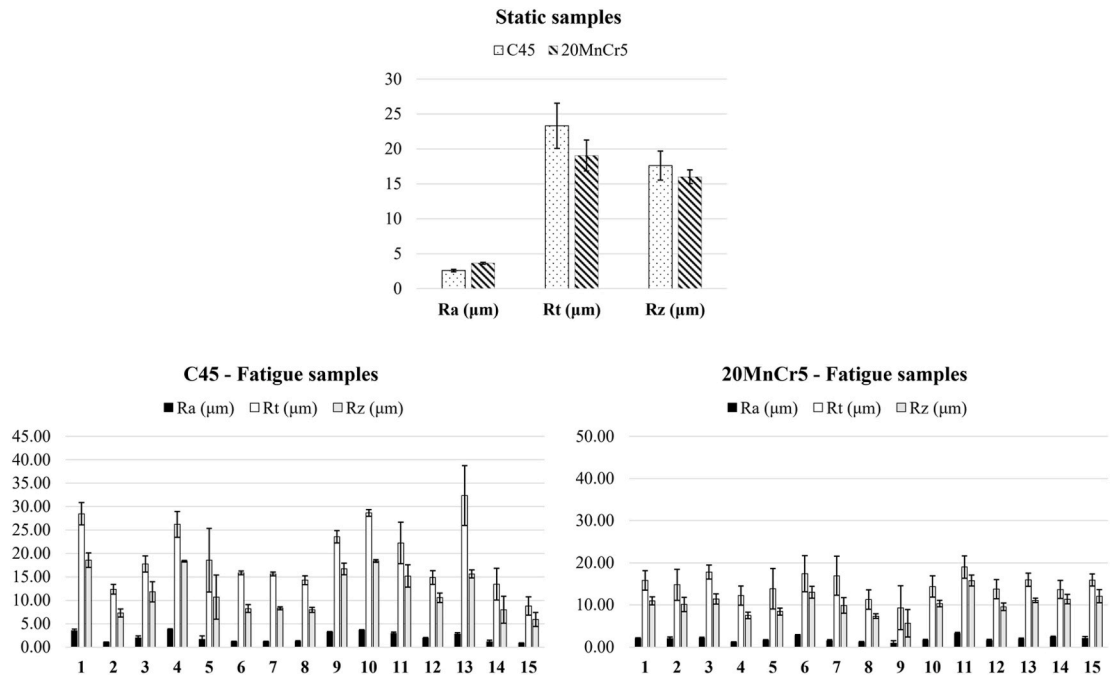


Fig. 5. Roughness characterization.

remaining available fatigue samples (for both C45 and 20MnCr5 steels) allowed for a simplified analysis of the finite life region. As a matter of fact, the samples were tested with stress amplitude (σ_a) values corresponding to alternate loads in the finite life region. The aim was to

provide an estimation of the experimental data regression curve of the finite life zone, as illustrated in Fig. 6. The finite life curve for C45 steel is proposed in Fig. 6 (a), and the finite life curve for 20MnCr5 steel is reported in Fig. 6 (b). The R^2 values obtained from the approximations of

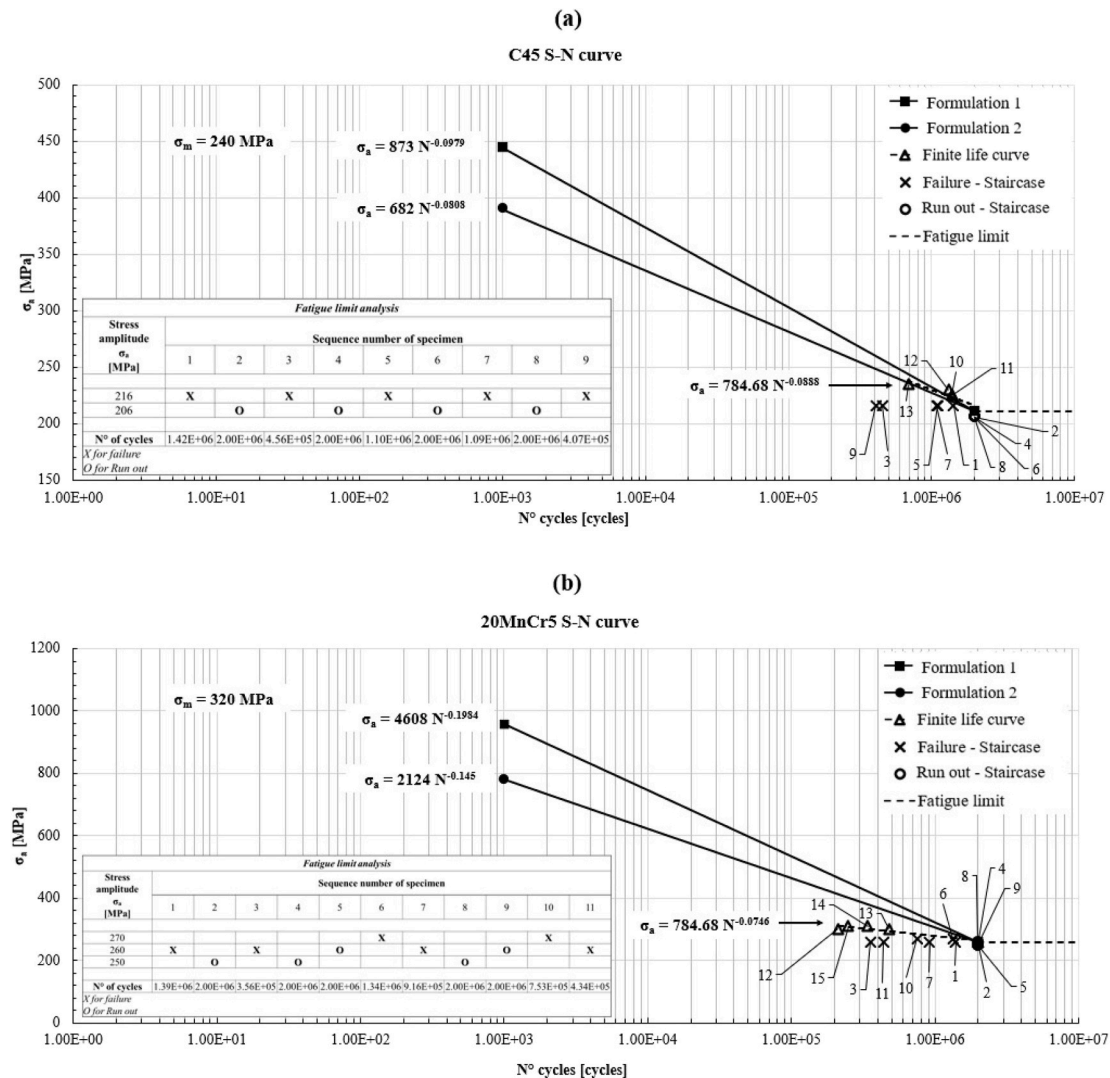


Fig. 6. Fatigue characterization: (a) C45, (b) 20MnCr5.

the experimental data points were of 0.78 for the C45 steel and of 0.83 for the 20MnCr5 steel. A comparison was made between the finite life curves obtained experimentally for both materials (Finite life curves in Fig. 6) and those evaluated using the analytical formulations which were based on the corresponding material properties and testing conditions (Formulation 1 and 2 in Fig. 6). In particular, Formulation 1 denoted the trend obtained with the adoption of the Basquin equation, while Formulation 2 described the results obtained adopting the approach proposed in Ref. [39] (see 2.1). The experimental trend exhibited a consistent pattern with those obtained analytically only in the case of C45 steel. A discrepancy in the results was observed in the case of 20MnCr5 steel. This deviation may be attributed to several factors. First, the adopted modelling approach relies on material parameters derived from standard correlations and literature data, which may introduce some approximation when applied to specific materials such as 20MnCr5. Second, the experimental S-N curve in the finite life region shows a certain level of scatter, which influences the interpolation of the reference fatigue behaviour. In addition, possible microstructural effects, surface roughness variations and local variability in the material response, not explicitly included in the current modelling framework, may contribute to the observed differences between numerical and experimental results.

In any case, a high level of accuracy in the finite life region definition requires more data points, which were impossible to obtain due to the

unavailability of samples. The results regarding the crack growth analysis from both experimental and numerical models are now illustrated. The first result is the morphological analysis. In Fig. 7, the difference in

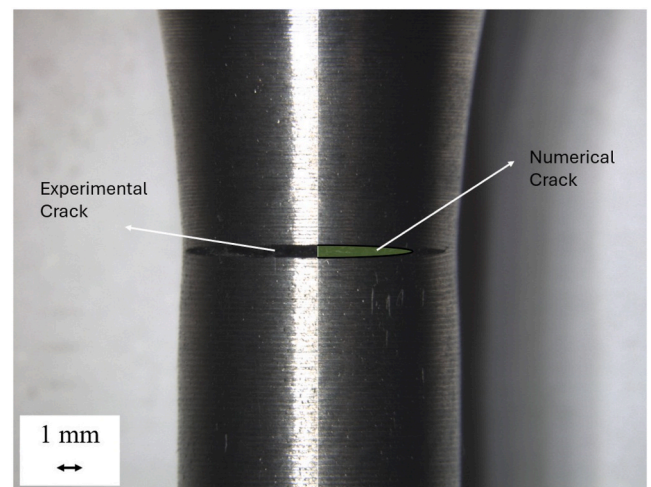


Fig. 7. Microscopic comparison: Numerical crack (green) vs Experimental crack (blue).

crack topology between the numerical model and the experimental test is shown. As can be observed from Fig. 7, there is a discrepancy between the two cases. The propagation direction is well captured, with the crack advancing perpendicularly to the loading direction. However, the final crack length slightly differs. This can be explained by the fact that, during the experimental tests, the testing machine stops only after detecting a significant drop in the material's resistance. In other words, the crack may continue to grow rapidly during the final unstable propagation phase. On the other hand, the numerical model terminates the simulation once the number of cycles required to propagate the crack falls below one. As presented in Fig. 8, in the numerical model, the crack initiation point was identified at 14.9 mm from the centre of the specimen along the vertical axis. Experimental observations indicated that crack initiation occurred within the same region of the specimen. Therefore, while an exact spatial correspondence cannot be claimed, the proposed approach is able to identify the preferential nucleation area in good agreement with the experiments.

The initial crack orientation predicted by the SWT criterion was perpendicular to the loading direction, in agreement with the fracture surface observed in the post-mortem analysis. The second result of the numerical analysis involves the crack nucleation and propagation phases for the two different materials, presented in Figs. 9 and 10, respectively. In Fig. 9 (C45 steel) and Fig. 10 (20MnCr5 steel), the proposed modifications to the S–N curves derived from numerical analyses are presented. In both figures, the black curve represents the nucleation phase, i.e., the number of cycles required for defect nucleation. For both materials, the red lines correspond to the S–N curves obtained from experimental tests, while the blue curve indicates the S–N curves derived from numerical simulations. In this analysis, two tests were discarded (tests n. 3 and n. 9), as they were considered invalid by the authors due to an experimental cycle count that was significantly lower compared to the corresponding results. All the curves were plotted by interpolating the individual data points and anchoring the initial point of the lines at σ_{lim} , obtained from the previously conducted Staircase method at 2×10^6 cycles.

As can be observed, a good level of approximation of the fatigue life has been achieved, with a slight underestimation of the total number of cycles, resulting in a maximum error of 20% for C45 steel and 12.7% for 20MnCr5 steel. Furthermore, the total simulation time ranged between 4 and 6 h for the different simulations performed. A load-level dependence was also observed in the ratio between crack nucleation and propagation. Numerical results indicate that, at higher load levels, the nucleation phase, defined as the number of cycles required to initiate a

crack, occupies a smaller portion of the total fatigue life. Conversely, at lower loads, a larger fraction of the total life is spent in the nucleation phase. Specifically, for the loads applied in this paper, an increment of 2% and 1.7% was observed for C45 and 20MnCr5 steels, respectively. This trend can be explained by the fact that, at higher load levels, the concentration of microdefects such as dislocations and microvoids is accelerated. Then, localized microplasticity may occur, promoting dislocation motion. Consequently, the damage threshold is reached more rapidly when the strain energy per cycle is higher.

5. Conclusion

A numerical framework for fatigue life prediction under HCF loading has been developed, integrating SWT for the crack nucleation stage and the Paris law for the crack propagation stage within an XFEM-based implementation in Code_Aster. The entire process is automated through a Python script that handles model setup, meshing, crack insertion, and iteration, with advantages in terms of reducing manual input and ensuring consistency across simulations. The framework was validated through experimental activities carried out on C45 and 20MnCr5 steels, which included material characterization, experimental tests (static and fatigue analysis), and microscopic investigations of fracture surfaces.

The SWT criterion successfully identified the crack nucleation location, showing good agreement with experimental observations and confirming the effectiveness of the critical-plane approach in HCF conditions. As expected in HCF, the majority of the fatigue life (over 90%) is consumed in the nucleation phase. The number of cycles required for nucleation decreased with increasing load, confirming trends observed in the literature.

For propagation, XFEM allowed for the simulation of crack growth without mesh regeneration, thanks to the use of enrichment functions. The Paris law governed crack growth per cycle, and a local remeshing strategy was implemented to refine the mesh around the crack front while derefining non-critical regions. This approach ensured both computational efficiency and high accuracy in representing crack evolution.

Slight discrepancies were noted between numerical and experimental final crack lengths. This can be attributed to differences in failure criteria: while the simulation ends when the cycles required for a crack increment drop below one, the test machine interrupts the experiment when a 50% reduction in load-carrying capacity is detected, often allowing the crack to grow unstably in the final cycles. Despite this,

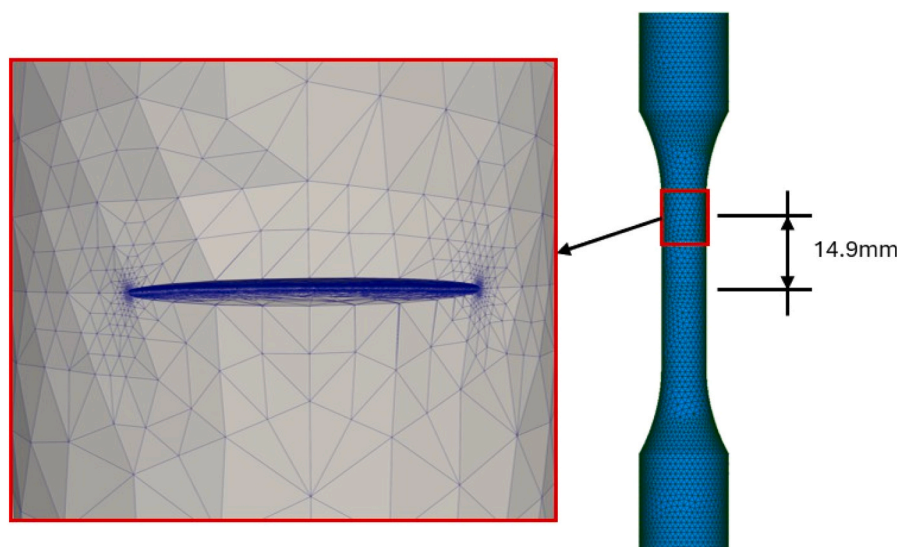


Fig. 8. Cracked specimen and crack nucleation position.

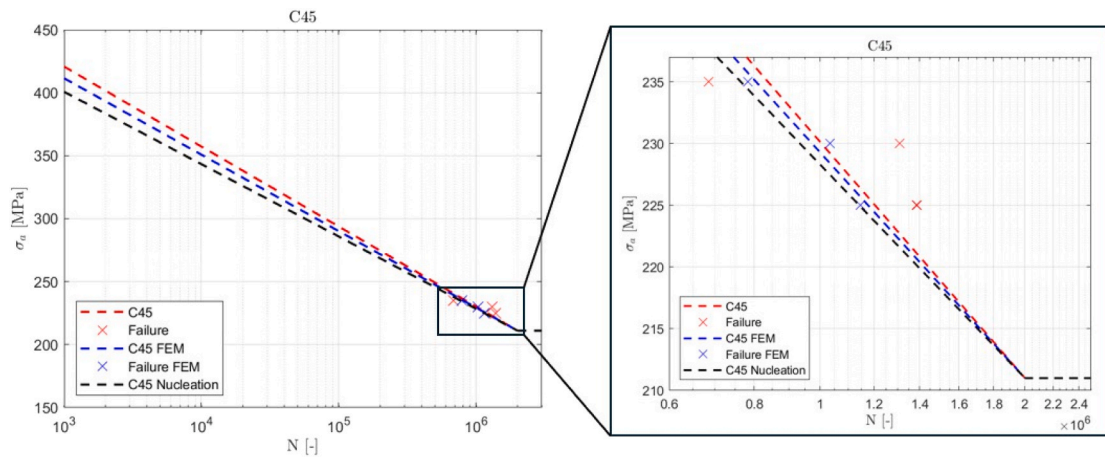


Fig. 9. Proposed numerical S-N curves for C45.

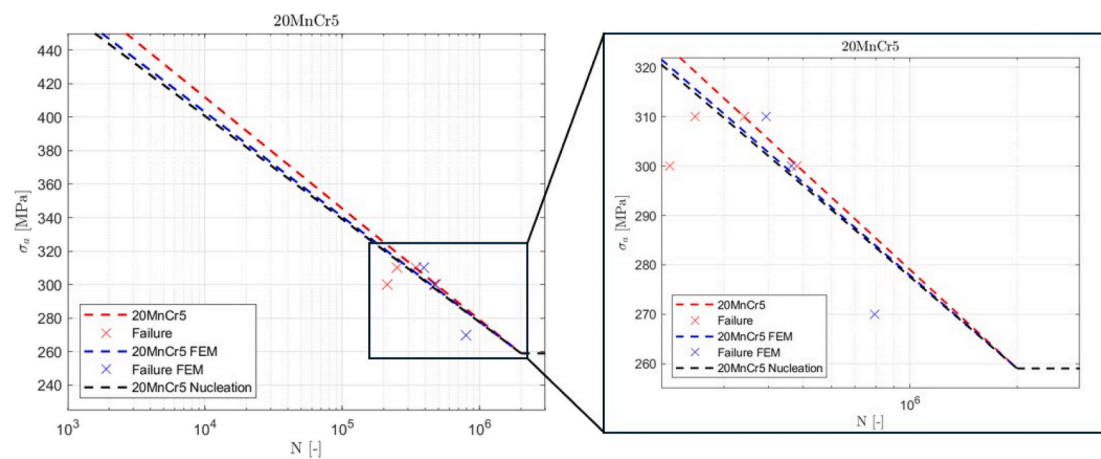


Fig. 10. Proposed numerical S-N curves for 20MnCr5.

fatigue life estimations remained within acceptable error bounds, as presented in the results section.

From a computational perspective, the adaptive meshing strategy was critical in keeping the runtime reasonable. The automation of the code allows for easy extension to other geometries or loading conditions. However, some limitations remain. The SWT model assumes that failure occurs on the plane of maximum normal strain, which may not hold under all multiaxial loading conditions.

The S-N curves derived from the numerical simulation were consistent with experimental trends. A slight underestimation of fatigue life was observed at higher load levels, possibly due to the deterministic nature of the Paris parameters used. Overall, the framework captured the fatigue behaviour well across both steels (C45 and 20MnCr5). The numerical algorithm proved robust, with a full simulation (nucleation + propagation) taking 4–6 h per case on 15 GFLOPS hardware. Moreover, a decrease in nucleation time was observed at higher load levels. This can be attributed to the fact that material damage accumulates more rapidly under higher loads, whereas at lower load levels, the damage progresses more slowly, resulting in a longer nucleation phase.

The experimental campaign enabled a detailed analysis of the tested samples, including microstructural analysis and the assessment of their mechanical properties (surface roughness, hardness, and both static and fatigue behaviour). While the C45 numerical S-N curve showed good agreement with experimental results, some deviations were noted for 20MnCr5 steel.

A new numerical S-N curve formulation was also introduced to describe the crack nucleation stage separately from propagation,

enabling a more detailed estimation of the fatigue life. These curves were anchored to the experimental σ_{lim} results and showed good agreement with experimental data points, particularly for C45 steel. Despite some discrepancies in the 20MnCr5 case, the proposed formulation proved effective in capturing material-dependent trends linked to early crack formation.

In summary, the proposed methodology provides an efficient and accurate tool for predicting crack initiation and propagation in metallic specimens under HCF, providing a valuable alternative to current approaches proposed in the literature. As a matter of fact, the ability to combine SWT, the Paris law, and XFEM within an automated FEM workflow makes it suitable for advanced numerical fatigue analysis and further methodological development.

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.

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