

Interaction of stress corrosion cracks in single crystals Ni-Base superalloys

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ABSTRACT

Stress corrosion cracking (SCC) can be detrimental to nickel-based superalloy components exposed to harsh environments in aero-gas turbines. During flight, engines consume contaminants deposited on the surface of a blade, often leading to degradation. Cracking can initiate within minutes and rapidly propagate, depending on the temperature, contaminants, and applied stress.

This study investigated the interaction between cracks in single-crystal turbine blades at intermediate temperatures by integrating experimental and computational methods. We performed C-Ring tests to quantify the time required for cracking, along with microscopic characterisation of the damage. In parallel, we developed a finite-element simulation for C-Ring tests using a phase field model calibrated to match the location of the cracks. The results demonstrated that the crack's characteristic spacing and length determine the likelihood of shielding or coalescing mechanisms.

1. Introduction

The interaction between multiple cracks and their effect on the crack growth rate (CGR) is a well-known phenomenon that is difficult to assess [1]. Depending on the configuration, crack interactions affect the response ahead of crack tips [2] and can accelerate or decelerate CGR. For example, Qiao [3] observed an increase in the stress intensity factor owing to the coalescence of multiple small cracks. On the other hand, long cracks may shield neighbouring cracks, often resulting in stress relaxation, slowing down, or even arresting further propagation [4].

Crack interaction is particularly important for components exposed to corrosive environments because of the large number of cracks simultaneously initiating [5]. Aero gas turbine components operating in high-temperature corrosive environments exhibit widespread stress corrosion cracking (SCC). In addition, the surface deposition of contaminants and high stresses further promote cracking owing to the hot corrosion mechanisms [6]. Even at moderate temperatures (450–650 °C), corrosion has detrimental effects on the underplatform regions of the turbine blades. These harsh environments often result in a high density of crack initiations on the surface, whose interaction determines the service lives of the turbine components [7].

Phase field modelling has been used in the past to investigate crack interactions in several materials and environments. Specifically, Xu et al. [8] assessed crack growth and interactions in sandstone and concluded that three modes of crack coalescence occurred. Zhao

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et al. [9] investigated the interactions between double cracks in Zircaloy-4, a cladding material, and found that there was a critical distance below which the hoop stresses of the material reached minimum values. Carlsson and Isaksson [10] used phase field modelling to investigate the role of porosity on crack dynamics and shielding and found that as the porosity increased, the chances of shielding also increased. However, the novelty of this work lies in the integration of the phase field model with experiments to understand crack interactions in single crystals in high-temperature corrosive environments. Aero gas turbines are often associated with high operational temperatures, but the intermediate temperature ranges (450–700 °C) found in the lower shank region of turbine blades are often neglected. Despite the lower temperatures, catastrophic cracking was still recorded, making this research extremely relevant.

This study explores the interaction and propagation of corrosion-induced cracks in single crystal nickel-based superalloys at 550 °C. A phase field model was used in the Abaqus finite element software to quantify corrosion-driven crack interactions using the distribution of cracks from the experiments. The models were parameterised with experimental data from the C-Ring tests to match the time and stress required to induce cracking. These results explain the origin of the crack spacing and the likelihood of cracks coalescing or arresting. Moreover, the parameterisation supports the potential role of sulphur in cracking [11] or at least acts as a proxy for a species with a diffusion coefficient like that of sulphur in nickel [12]. As such, this study further demonstrates the value of integrating modelling and experimental approaches to perform crack prognosis and design crack-resistant components.

2. Experimental assessment of SCC

The evaluation of SCC for turbine components requires samples to undergo high stresses and temperatures under damaging environments. C-Ring testing [13,14] is a convenient experimental methodology for evaluating stress-controlled cracking [15] and consists of an incomplete circular section tightened with a bolt (Fig. 1). We consider C-Rings machined from CMSX-4 single crystals [16] with the composition in Table 1 and aligned such that the [0 0 1] direction is approximately parallel to the geometric axis of the cylinder. The C-Ring has two holes in which bolts, nuts, and washers are used to compress the specimen and apply calibrated tensile stress along the apex. The position and value of the peak stress depend on the exact crystal orientation, which was experimentally measured using X-ray diffraction.

Samples were pre-strained by displacing the bolt 0.44 mm using a laser C-Ring tensioner to introduce a peak stress of approximately 700 MPa (as shown later), which is highly dependent on the highly anisotropic nature of CMSX-4. Next, a contaminant layer of NaCl salt was deposited on the C-Ring surface at a flux of 1.2 $\mu\text{g}/\text{cm}^2/\text{h}$ [17]. The samples were exposed to air containing 50 ppm of SO_2 , at 550 °C for periods between 10 min and 400 h (600 to 1440000 s). Periodic inspection demonstrated that cracking appeared as little as 15 min (900 s) after starting the experiment.

Fig. 2: Optical image which captures the anisotropic dependent nature of cracking in this material and the distance from the apex beyond which further crack initiation was not observed, illustrates the anisotropic-dependent nature of this corrosion cracking mechanism for these types of materials, in which cracks do not nucleate beyond a certain distance from the C-Ring apex. This results in asymmetric crack propagation behaviour, which is further investigated in this study. Fig. 3 presents an SEM image of dozens of cracks initiated in the sample. This image is representative of a regular pattern observed, in which cracks are parallel to the C-Ring axis, which aligns approximately with the [0 0 1] crystallographic orientation. Furthermore, the cracks had consistent lengths and spacings, ranging from 100 μm to 200 μm . Further details regarding the experimental results can be found in Ref [18].

X-ray microscopy (XRM) data were also obtained from a C-Ring test with an exposure time of 400 h and digitalised (following the methodology in refs [19,20]). From these data, three cracks were selected, highlighting the potential for both crack shielding and coalescence. A plasticity-based model was implemented to assess the stress variation in areas surrounding the crack tip. As shown in

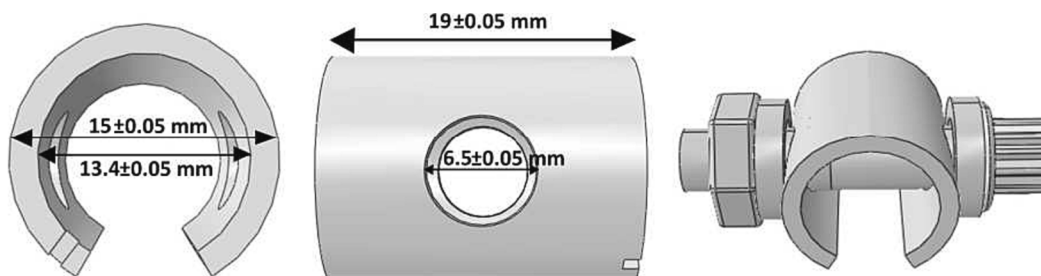


Fig. 1. C-ring geometry without and with the compressing bolt and accompanying dimensions. The apex of the C-ring section developed calibrated tensile stresses that induced cracking.

Table 1
Composition of CMSX-4 (wt. %).

Ni	Cr	Al	Co	Ta	W	Mo	Ti	Re	Hf
Balance	6.5	5.6	9.0	6.5	6.0	0.6	1.0	3.0	0.1

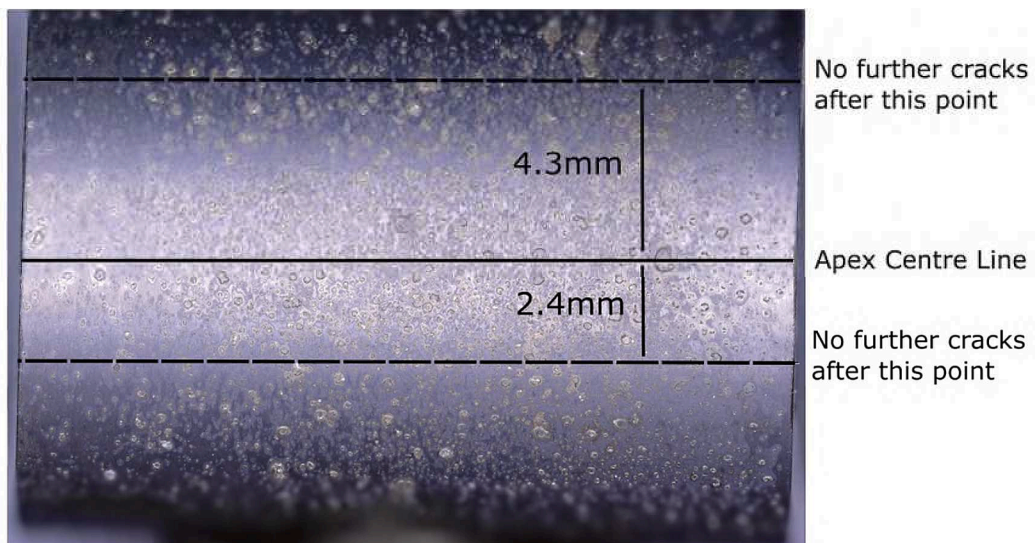


Fig. 2. Optical image which captures the anisotropic dependent nature of cracking in this material and the distance from the apex beyond which further crack initiation was not observed.



Fig. 3. SEM image of a sample exposed for 15 min illustrates the general pattern of crack embryos, noting that all cracks were initiated under salt particles.

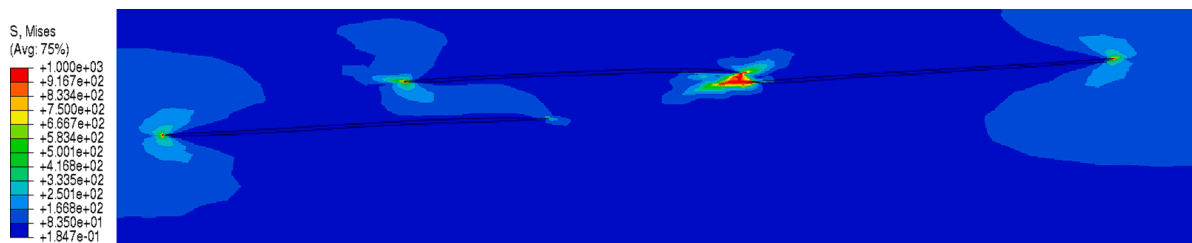


Fig. 4. Results from an elastic model that was ran on digitalised XRM cracks to highlight potential stress intensification and relaxation using real cracks.

Fig. 4, owing to the critical spacing and positioning, there was stress intensification between the two right cracks and a clear stress relaxation between the two left cracks.

3. Phase field modelling

Phase field models [21–23] represent a sharp interface using a smooth characteristic transition and employ a field parameter, Φ , to represent undamaged ($\Phi = 0$) or fully damaged ($\Phi = 1$) material [24]. Following the implementation by Martínez-Pañeda [25], which was initially applied to represent hydrogen-induced degradation, the phase field parameter is calculated as [26],

$$\Phi(x) = e^{-\frac{|x|}{l}} \quad (1)$$

where l denotes the length scale parameter responsible for controlling the width of the smear crack and x is the distance from the stationary predefined crack. The length scale effect is highlighted in Fig. 5a for the traditional sharp crack interface and Fig. 5b for a diffused interface. For this study l has been given a value of eight times the mesh size used along the expected crack propagation path in order to guarantee an adequate number of elements are considered in the process zone. However, it is believed that a more physical meaning can replace this numerical approach that is used in many cases through the literature and will be discussed in a later section.

Parameter Φ is used to calculate the crack functional variable $\Gamma_l(\Phi)$ which informs Eq. (3) to compute the fracture energy needed to form new surfaces and hence crack the material [26]. In this case, $G_c(\theta)$ refers to the reduced critical energy release rate based on diffused species.

$$\Gamma_l(\Phi) = \int_{\Omega} \left(\frac{\Phi^2}{2l} + \frac{l}{2} |\nabla \Phi|^2 \right) dV \quad (2)$$

$$\int_{\Gamma} G_c(\theta) ds = \int_{\Omega} G_c(\theta) \left(\frac{\Phi^2}{2l} + \frac{l}{2} |\nabla \Phi|^2 \right) dV \quad (3)$$

Eq. (4) introduces a degradation function that accounts for the reduction in the stiffness of the material. As this study is only concerned with the linear elastic response of the material, the elastic strain energy density formulation, $\Psi_0(\epsilon)$, is given the formulation in Eq. (5). ϵ and C_0 represent the strain and stiffness tensors of the undamaged material, respectively. It should be noted that a history variable, ψ_H , is introduced in Eq. (6) to ensure that there is no regression in the simulation, where ψ_T is the calculated value from the previous time increment, meaning that it cannot drop below this value.

$$D_g = (1 - \Phi)^2 \quad (4)$$

$$\psi_0(\epsilon) = \frac{1}{2} \epsilon^T : C_0 : \epsilon \quad (5)$$

$$\psi_H = \begin{cases} \psi_0(\epsilon), & \text{if } \psi_0(\epsilon) > \psi_H \\ \psi_T, & \text{otherwise} \end{cases} \quad (6)$$

Eqs. (4) and (6) can be combined with Eq. (3) and integrated over the volume of the body to obtain the total potential energy function in Eq. (7).

$$\psi = \int_{\Omega} (D_g \psi_H + G_c(\theta)) \left(\frac{\Phi^2}{2l} + \frac{l}{2} |\nabla \Phi|^2 \right) dV \quad (7)$$

When this is considered with respect to $\delta \Phi$, the weak form of the phase field formulation is achieved in the following,

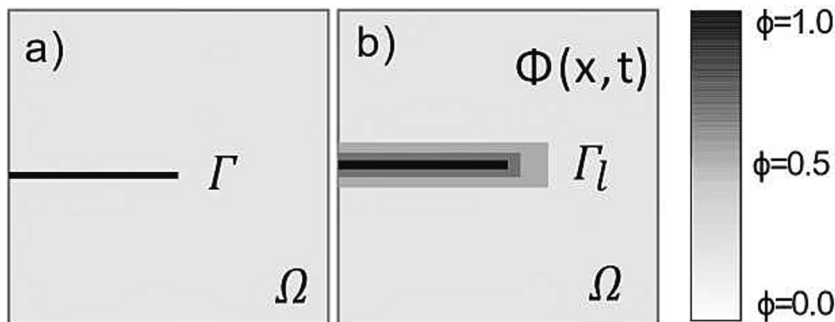


Fig. 5. Cracked material in a body, Ω , for both a) sharp interface and b) diffusive crack.

$$\int_{\Omega} (-2(1 - \Phi)\psi_H \delta\Phi + G_c(\theta) \left(\frac{1}{l} \Phi \delta\Phi + l \nabla \Phi \bullet \nabla \delta\Phi \right)) dV = 0 \quad (8)$$

As such the final phase field equation in the solid body Ω becomes,

$$G_c(\theta) \left(\frac{1}{l} - l \Delta \Phi \right) - 2(1 - \Phi)\psi_H = 0 \quad (9)$$

This study follows the work of Griffith [27], whereby a defined crack propagates when the calculated critical energy release rate is degraded below a critical point. The material's critical energy release rate is degraded owing to the diffusion of contaminants, and this process is driven by θ , the surface coverage (otherwise known as the Langmuir Isotherm [28]). This effect is represented by Eq. (10), where Δg_b^0 is the Gibbs free energy difference, c is the concentration, R is the molar gas constant, T is the temperature, and finally 'a' is a scaling parameter that controls the rate of θ .

$$\theta = \frac{c^* a}{(c^* a) + \exp\left(\frac{-\Delta g_b^0}{RT}\right)} \quad (10)$$

Eq. (10) is linked with Eq. (11) to calculate the new and degraded G_c values, where $G_c(\theta)$ is the critical energy release rate with the coverage of the corrosive impurity, $G_c(0)$ is the critical energy release rate of the raw material, and χ is a damage coefficient that accounts for the role of impurities in reducing the material fracture energy.

$$G_c(\theta) = G_c(0)(1 - \chi\theta) \quad (11)$$

Justifications of the values used in Eqs. (10) and (11) are presented in the next section.

An extension of Fick's law of diffusion [29] was used to solve for the diffusion of potentially embrittling species. This is highlighted by Eq. (12) which comprises the diffusion coefficient, contaminant concentration, molar gas constant, temperature, and chemical potential gradient $\nabla\mu$, that drive the diffusion process. Eq. (13) equates the chemical potential (in a stressed state) and μ_0 is the chemical potential at a given concentration (C_0), partial molar volume of impurity x ($\bar{V}_x$), and hydrostatic stress (σ_H). The predicted values for hydrostatic stress gradients in turn influences the diffusion matrix and as such are calculated using the nodal displacements (as per the integration points), which are multiplied by the spatial derivatives of the shape functions. Eq. (14) was obtained when 12 and 13 were combined to summarise the stress-driven diffusion process.

$$J = -\frac{Dc}{RT} \nabla\mu \quad (12)$$

$$\mu = \mu_0 + RT \ln\left(\frac{C}{C_0}\right) - \bar{V}_x \sigma_H \quad (13)$$

$$J = -D \nabla c + \frac{Dc}{RT} \bar{V}_x \nabla \sigma_H \quad (14)$$

The predicted crack propagation, under a weakly coupled impurity diffusion and mechanically driven phase field fracture, was solved using a 'User ELeMent' subroutine (i.e., UEL) implemented in the Abaqus 2019 finite element software [30]. The UEL is used to compute the material stiffness matrix and the accompanying right hand side nodal force vectors which are then returned to Abaqus. The resolution of the PF is based upon a staggered scheme.

4. Finite element modelling

4.1. Model parameterisation

The bolt tightening of the C-Ring was replicated by using a pinned boundary condition ($U_X = U_Y = U_Z = 0$) to one end and displacing the other end to achieve a displacement of 0.44 mm, as in the experiments, as shown in Fig. 6. We employ an anisotropic elastic model with cubic symmetry defined by Eqs. 15, 16, and 17.

$$C_{11} = \frac{E(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \quad (15)$$

$$C_{12} = C_{11} \frac{\nu}{1 - \nu} \quad (16)$$

$$C_{44} = G \quad (17)$$

along with the elastic constants provided to us by Rolls-Royce (at intermediate temperatures of approximately 540 °C, which differs by 10 °C from the experimental conditions but will have a minimum effect on the results), in Table 2 [18]. The crystal orientation is represented using three angles δ , γ , and κ , which correspond to rotations around the X-, Y-, and Z-axes, respectively. Thus, the crystal

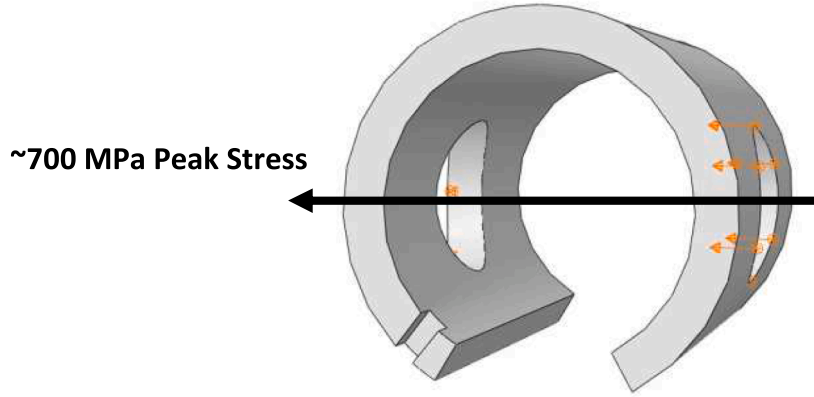


Fig. 6. Boundary conditions applied to the C-Ring geometry to replicate the 0.44 mm displacement experienced during experimental loading.

Table 2
Model parameters used for phase field modelling.

Young's Modulus (GPa)	110.0
Poisson's Ratio (ND)	0.3858
Shear Modulus (GPa)	115.0
Initial Sulphur Concentration (wppm)	0.5
Environmental Sulphur concentration (wppm)	50.0
Diffusion Coefficient (mm ² /s)	1.4x10 ⁻¹⁰
$G_C(0)$ (MPa mm)	44.0
Temperature (°C/K)	540/813
Molar Gas Constant (N mm/ (mol K))	8314.5
Δg_b^0 (kJ/mol)	-30
χ	0.998
Rate of θ , 'a'	1.25

orientation was computed by the subsequent rotation along these axes.

Since loading conditions are nominally below the yield, plastic strains will only be on a small scale and will have limited impact on the results. Indeed, a simulation using J2 plasticity was performed using the same boundary conditions and only saw a slight reduction in the stress; therefore, it does not justify the additional computational costs associated with the plasticity calculations. Creep can also be neglected because the temperatures are below the creep regime range, as per Ref. 31, which shows that inelastic creep deformation to be insignificant around 500 °C.

The critical energy release rate equation by Griffith [27] was adapted to include Irwin's contribution [32], resulting in Eq. (18) [33], to estimate the material's fracture toughness value,

$$G_C(0) = \frac{K_{IC}^2}{E'} \quad (18)$$

Where,

$$E' = \begin{cases} E & \text{planestress} \\ \frac{E}{1 - \nu^2} & \text{plane strain} \end{cases} \quad (19)$$

K_{IC} was estimated to be 2400 MPa $\sqrt{\text{mm}}$ [34].

The diffusion coefficient, activation energy (Δg_b^0), and degradation (χ) depend on the particular species that damage the metal substrate. Owing to the complexity of the issue being assessed, it is still not known which species (or combinations of species) are responsible for crack propagation. As such, a simple 1D Fick's law simulation was performed for five different species of Ni (at 600 °C), the results for which are shown in Fig. 7. The length scales considered (i.e., 10 μm for 900 s (15 min) and 1 s) were used as they matched the typical crack lengths seen from the SEM images of these sectioned 15-minute samples. It was found that oxygen and hydrogen diffused too quickly, whereas tungsten and aluminium diffused too slowly. Sulphur was the only species that matched the length scales described below. To simplify the analysis, the diffusion of the named species was considered in pure Ni with the assumption that it is a good first-order approximation for Ni superalloys.

The thermodynamic database software FactSage [35] was used to estimate the values of Δg_b^0 for the simple reaction described below. Because of the abundance of hydrogen in the atmosphere, it was assumed that H_2 is present in the reaction. For an environmental temperature of 550 °C (823 K), a value of -30 kJ/mol was predicted.

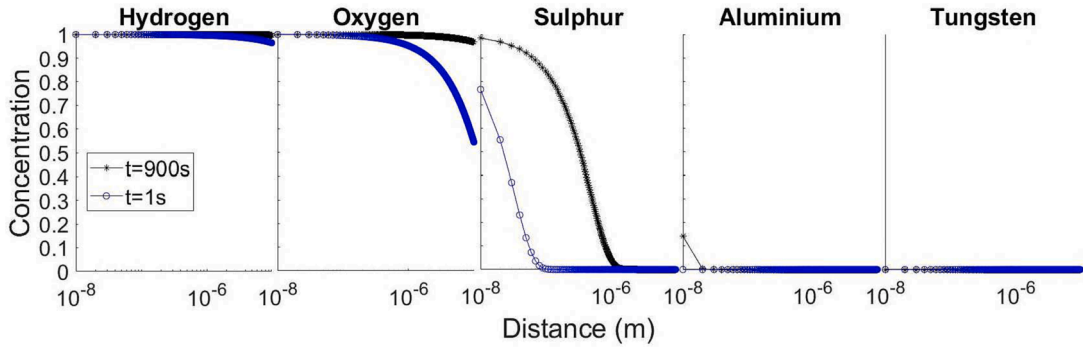
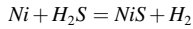


Fig. 7. Results from a 1D Fick's law simulation which looks at the diffusion of the above species in Ni at 600 degrees.



(20)

This value is further corroborated by the work of Jo et al. [36] who also estimated a value of approximately -30 kJ/mol. The parameters χ and a (which controls the rate of θ) were adjusted to match the crack growth experiments and agreed with the values of Yamaguchi et al. [37].

In C-Ring experiments, cracks initiate under salt deposition sites because of the surface reactions occurring between the materials, salt deposition, and the environment. As such a predefined crack is associated with a salt deposition site and therefore a species concentration is given to the crack (in this case 'sulphur', or something with similar diffusion kinetics). Thus, as the diffusion problem is solved, and sulphur travels ahead of the crack tips, a reduction in G_c occurs until it is sufficiently low for crack extension to occur. This is highlighted in Fig. 8 which shows both Φ and concentration maps at the start, middle, and end of the simulation.

First, we implemented an elastic model using five equivalent crack embryos ($80 \mu\text{m}$ in length and $40 \mu\text{m}$ in depth) at different locations away from the C-Ring apex (Fig. 9). The first crack was located at the apex, and the subsequent cracks were separated by $1500 \mu\text{m}$. The simulation matches the orientation of the crystal in the experiment, as measured by X-ray diffraction. The results in Fig. 9 depict the maximum principal stress before cracking and show that cracks A and B undergo a stress of just under 700 MPa (in the centre of the C-Ring surface), C is subjected to stresses of approximately 500 MPa, while cracks D and E fall into regions of significantly lower stresses between 350 and 50 MPa, respectively. The stress levels are asymmetric owing to the small deviation of the $[0\ 0\ 1]$ crystal direction from the C-Ring axis.

A C-Ring geometry with five parallel cracks was implemented for a phase field simulation spanning 300 s, and the results are shown in Fig. 10. Experiments [17] have shown that cracks form in the vicinity of the C-Ring apex, beyond which no cracks are observed because of the lower local stresses. Hence, we employed the experimental distance from the apex for a given exposure time, beyond which no crack embryos ($<80 \mu\text{m}$) were found, to estimate the phase field parameters in Table 2. As previously mentioned, the diffusion coefficient of sulphur in nickel was assumed. As expected, small variations in the crystal orientation also affected the exact location of the cracks and peak stress values.

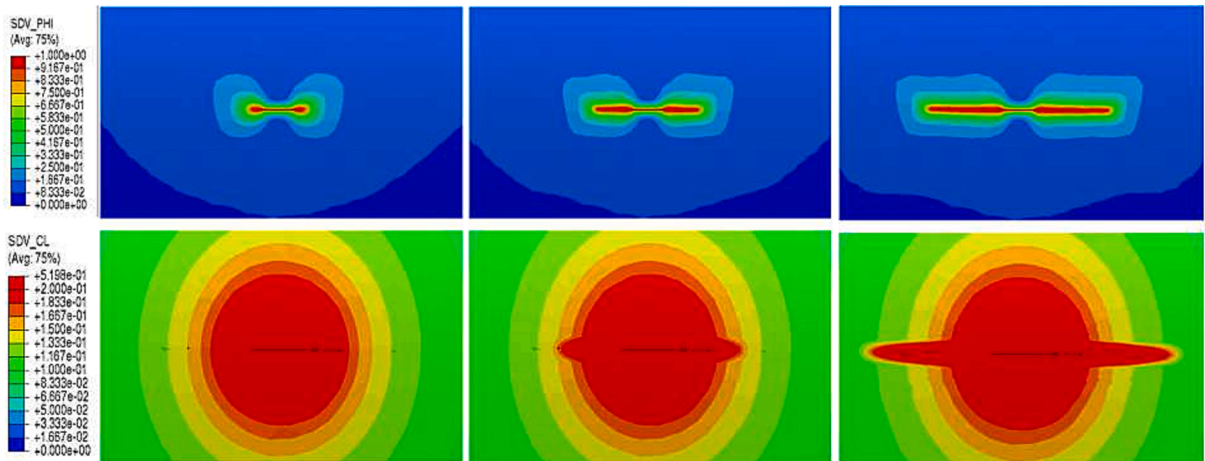


Fig. 8. Highlighting the concentration (top) and Phi (bottom) change taken from different stages of the simulation.

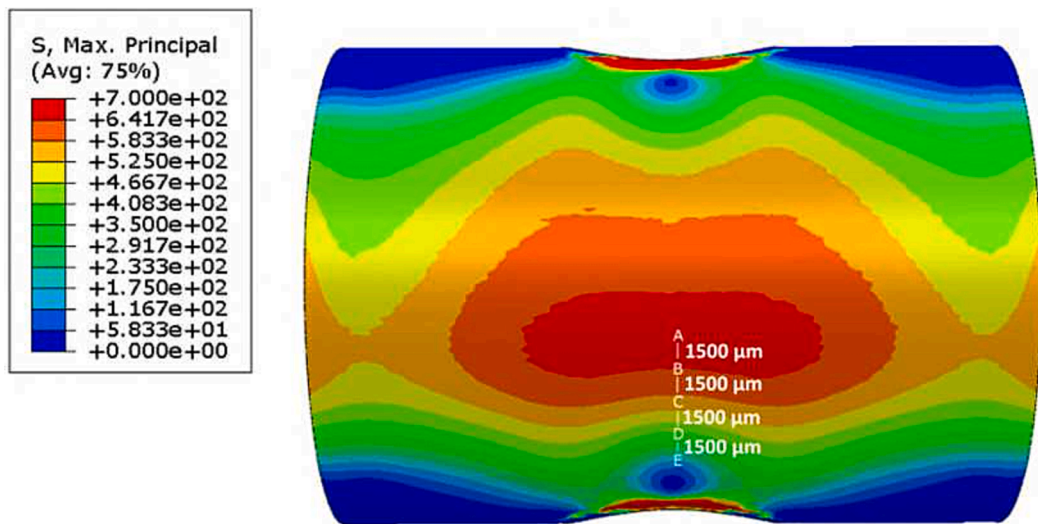


Fig. 9. Stress distribution for given secondary crystal orientations and crack positioning.

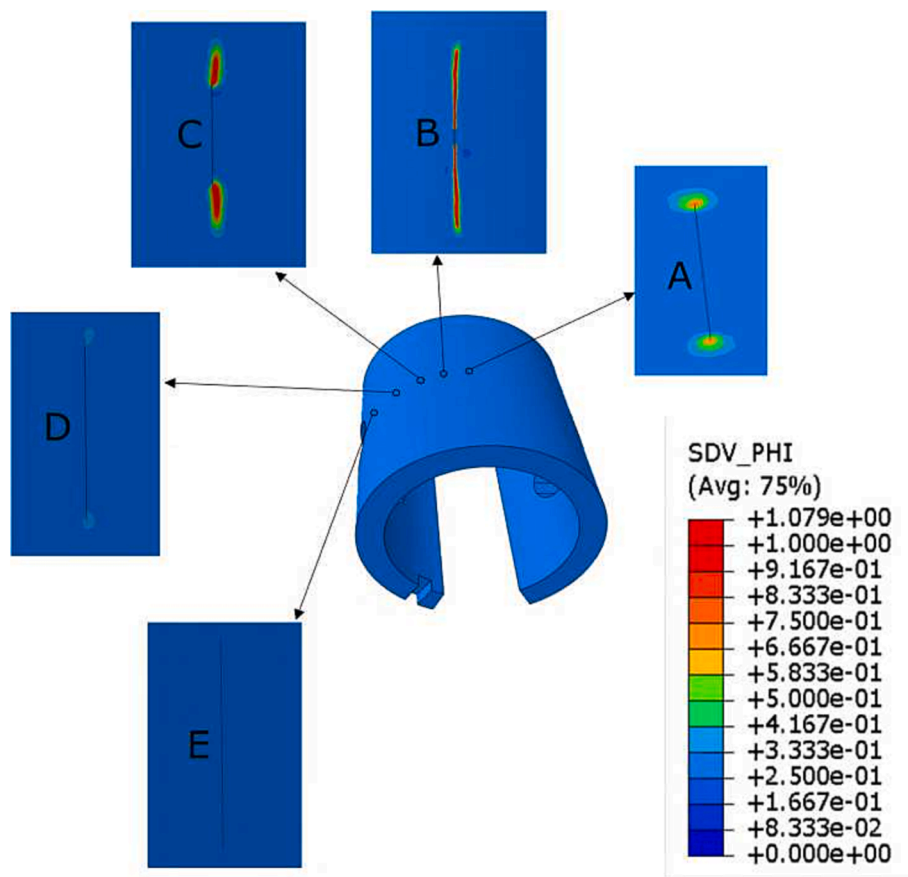


Fig. 10. Simulation results showing different crack lengths after 300 s for five parallel predefined cracks. The colour bar corresponds to the field parameter Φ .

Table 3
Crack Morphology Properties.

CRACK	TOTAL CRACK LENGTH (μm)	CRACK INITIATION LENGTH (μm)	CRACK PROPAGATION LENGTH (μm)
A	81	80	1
B	790	80	710
C	125	80	45
D	80	80	0
E	80	80	0

Overall, Crack B in Fig. 10 resulted in the largest crack length of 790 μm , followed by Crack C with a length of 125 μm . Crack A had a significantly lower crack length of 81 μm , whereas cracks D and E presented no crack growth in 15 min owing to their position on the lower stresses, hence reducing the driving forces needed for cracking. Note that the experiments have shown that cracks at position D can grow after a longer exposure time, which was verified by simulations. The crack lengths are summarised in Table 3 and shown in Fig. 10.

4.2. Mesh sensitivity and length scale parameter

Phase field modelling requires dense meshes to converge the solution to Φ . Several studies [25,38–40] have assumed that the length scale parameter (l) is a function of the mesh size, generally between two and ten times the mesh dimension. To quantify the role of l , a separate study was conducted by simulating a single-edge notched specimen, as shown in Fig. 11. The initial crack length was 25 % of the total length (i.e., $a/w = 1/4$) and it was loaded by displacing 0.005 mm perpendicular to the top surface while pinning the bottom nodes ($U_X = U_Y = U_Z = 0$). For this assessment, the same CMSX-4 properties at intermediate temperatures were applied for a simulation time of 100 s. The prediction of the crack extension was then assessed by assuming a threshold for cracked material corresponding to a value of $\Phi \geq 0.95$, to account for any uncertainties. Fig. 12 and Fig. 13 the threshold for cracking and point of the predefined crack, respectively.

For the first assessment, all aspects of the simulation were kept identical, except for the mesh sizes and l , which were varied (l equal to eight times the mesh size in all cases). Fig. 13 demonstrates that the simulations predicted propagation lengths ranging between 0.33 mm and 0.62 mm. Hence, these results suggest that making l dependent on the mesh size results in mesh-sensitive predictions.

A second assessment involved fixing the value of l to 0.0125 mm, but varying the mesh size, and all other aspects were identical. Fig. 13 shows far less variability in predicted propagation lengths compared to Fig. 12, and suggests that there is a physical meaning behind l in addition to the numerical interpretation used in [24,41–43]. Hence, we argue that the properties of the crack tip morphology, such as the constancy of the Crack Tip Opening Displacement (CTOD) or Crack Tip Opening Angle (CTOA) throughout propagation [44] can justify a fixed length scale parameter. This imposes an upper limit on the required mesh size. Microscopy data, such as that from X-ray microscopy (XRM) scans of both short and long cracks from experimental C-Rings, are a potential avenue to measure such parameters.

A further length scale parameter test was conducted on C-Rings and again found little change when ' l ' was fixed, and the mesh size was changed. These results can be viewed in Appendix A.

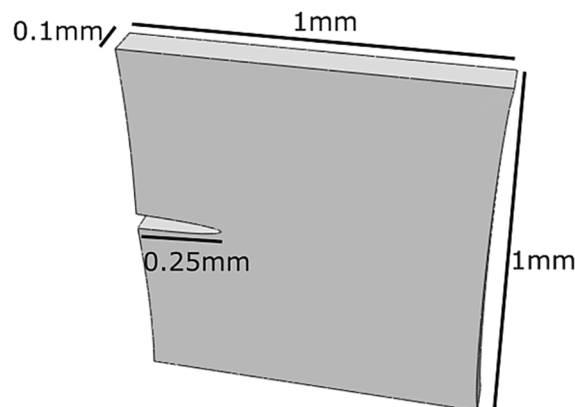


Fig. 11. Schematic of 1 $\times$ 1 mm geometry with a predefined edge crack used for the mesh and length-scale parameter sensitivity tests.

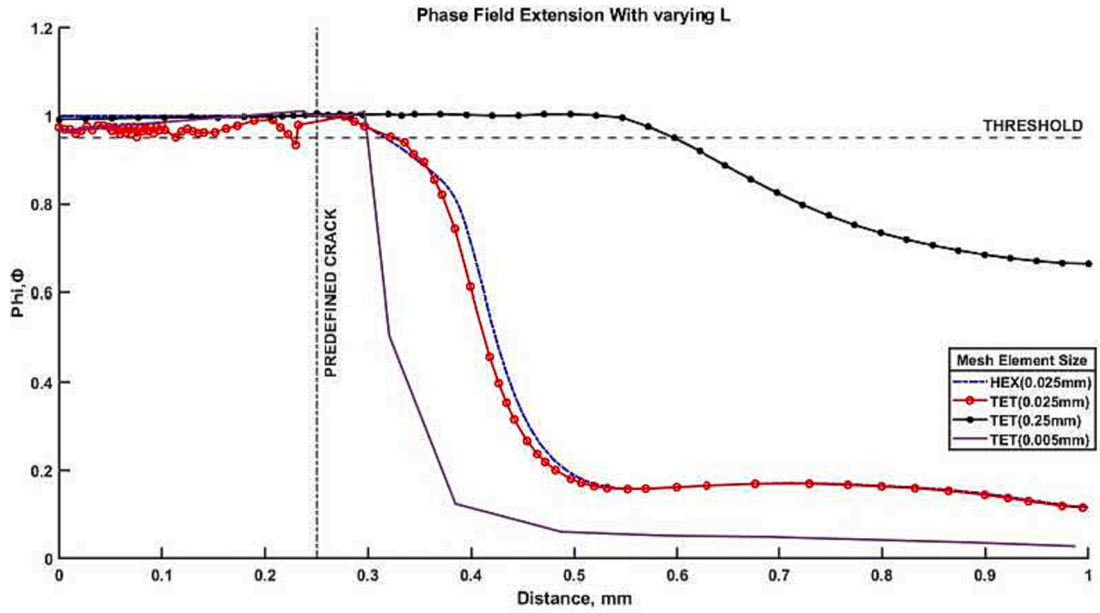


Fig. 12. Prediction of crack extension based on a variety of mesh sizes, each time having a length scale parameter 8 times that size.

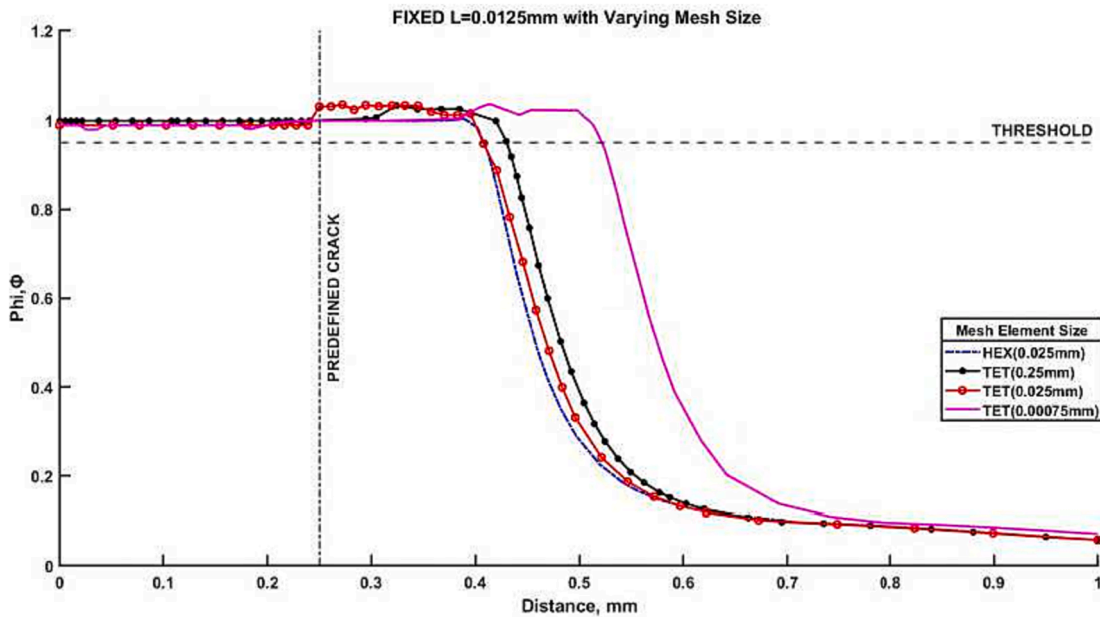


Fig. 13. Prediction of crack extension based on using a fixed-length scale parameter but varying mesh size.

4.3. Time dependence

The C-Ring tests showed that a longer exposure time resulted not only in longer cracks but also initiated cracks further away from the C-Ring apex, where the stresses were lower. To assess the model response under these conditions, we performed additional simulations matching the experimental crystal orientation, temperature, and loading for a total time of 7200 s (2 h). Again, a crack embryo (40 μm in length and 20 μm in depth) was initiated 4.5 mm from the apex of the C-Ring (as seen in Fig. 15), corresponding to a stress level of approximately 450–550 MPa. Again, these predefined cracks were associated with the sulphur concentration through a specific boundary condition. Accounting for the 600 s required to initiate cracks, the simulation was run with an experimental time of

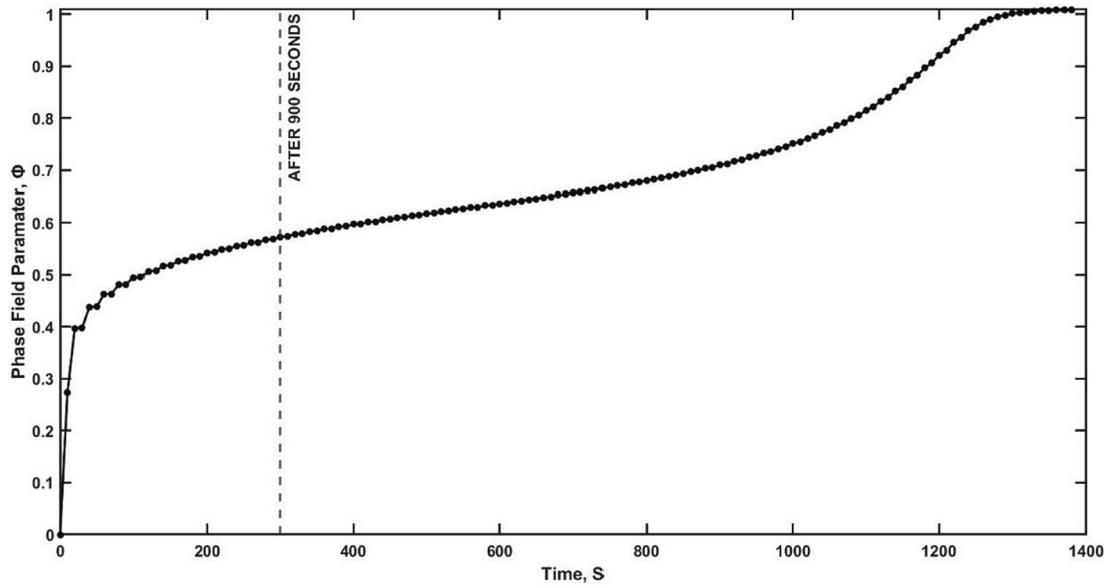


Fig. 14. Assessment of the time-dependent nature of crack extension for 300 and 7200 s at lower bulk stresses.

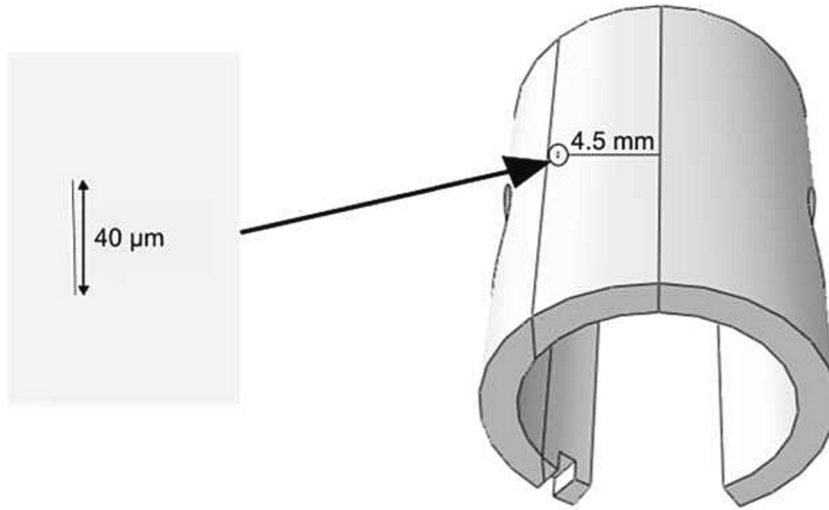


Fig. 15. Simulation with a predefined crack shifted by 4.5 mm from the apex of the C-Ring to run in a region of lower bulk stresses.

6600 s (1 h and 50 min) to predict the propagation. After 300 s, the results showed that the phase field parameter increased monotonically at the crack tip, but without fully cracking ($\Phi < 1$), as shown in Fig. 14. In contrast, Fig. 14 demonstrates that given sufficient time, the crack propagates, and the crack tip phase field parameter reaches a value of 1, approximately 650 s, or almost 11 min after the propagation starts (this would be 21 min in total if the 10 min initiation period is considered). This simulation is a prime example of a time-dependent mechanism that plays a significant role in allowing propagation as cracks initiate further from the apex. .

4.4. Modelling crack spacing interaction

The results in Fig. 10 show that parallel cracks with a normal spacing of 1500 μm propagated without any noticeable interference. Thus, we further evaluated the shielding or coalescence effects with simulations in which two parallel cracks ($80 \times 40 \mu\text{m}$ and $40 \times 20 \mu\text{m}$) were separated by a distance L of 50, 100, 150, and 200 μm , as shown in Fig. 16a. These configurations and crystal orientations are representative of those used in the experiments.

Nodal data from the first three nodes ahead of each crack tip (Fig. 16b) were recorded, and averages were taken for the hydrostatic stress (MPa) and the phase field parameter, Φ . As mentioned previously, hydrostatic stress generally degrades as a function of Φ (as the crack extends). In contrast, crack shielding leads to stagnation of the hydrostatic stress for the shorter crack, as shown in Fig. 17a, b,

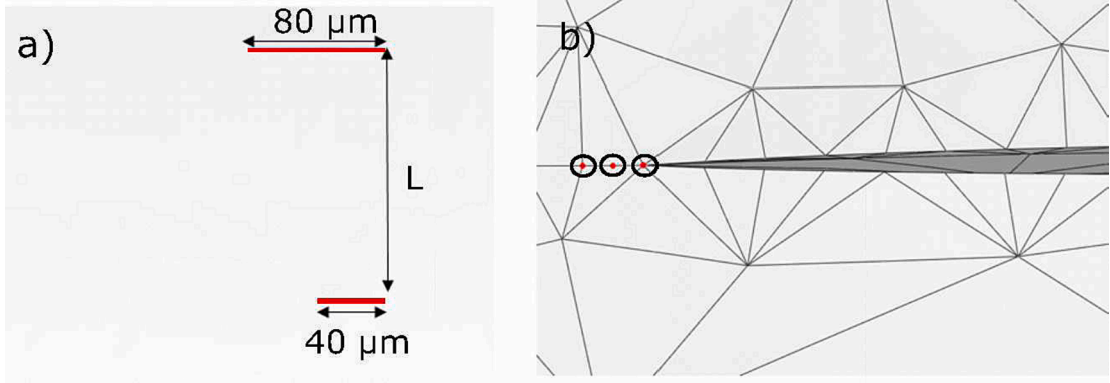


Fig. 16. A) predefined crack size and positioning for the given simulation and b) nodes from which data were extracted.

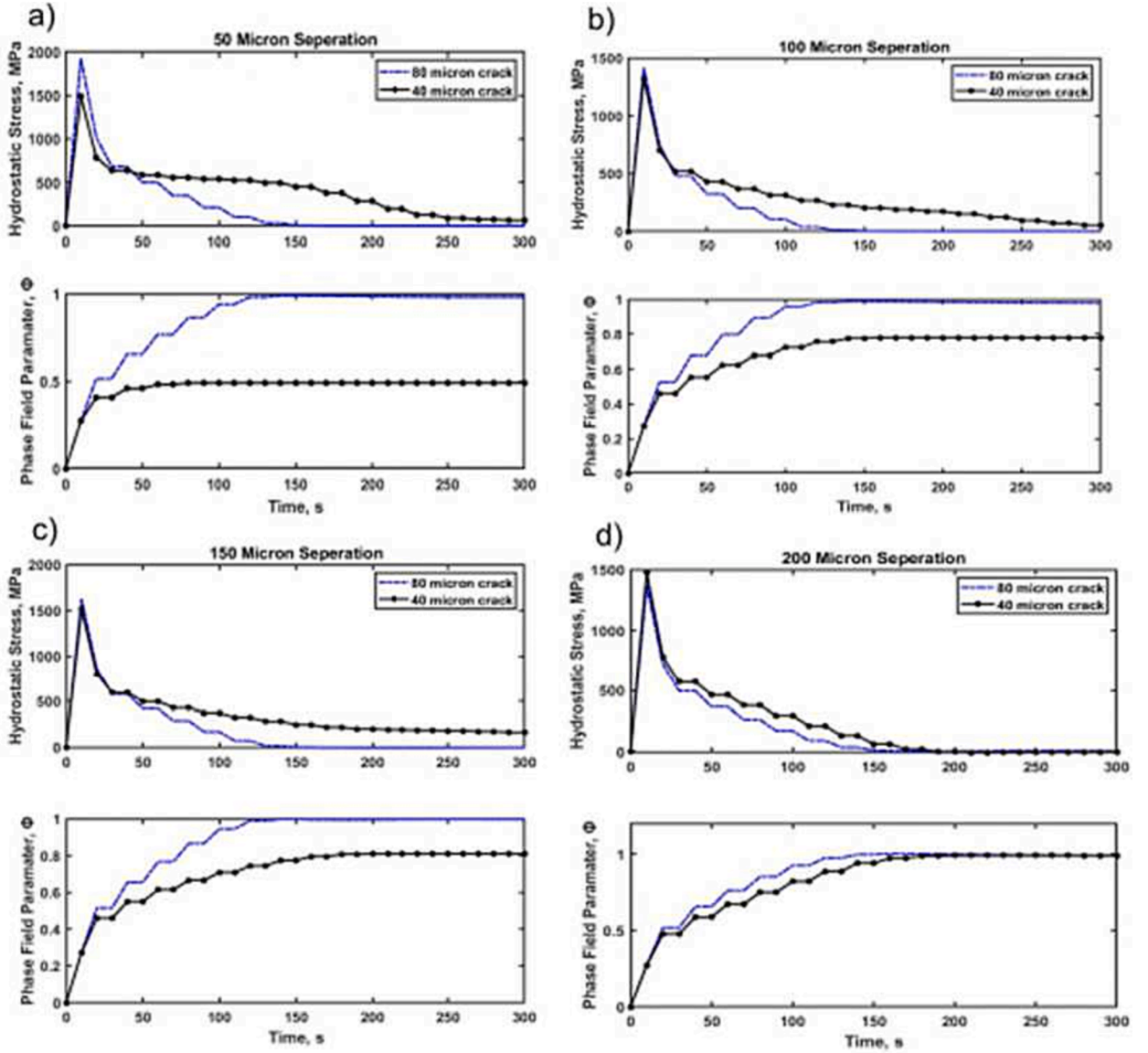


Fig. 17. Hydrostatic stress (MPa) and phase field parameter (Φ) for two parallel cracks separated by 50, 100, 150, and 200 μm .

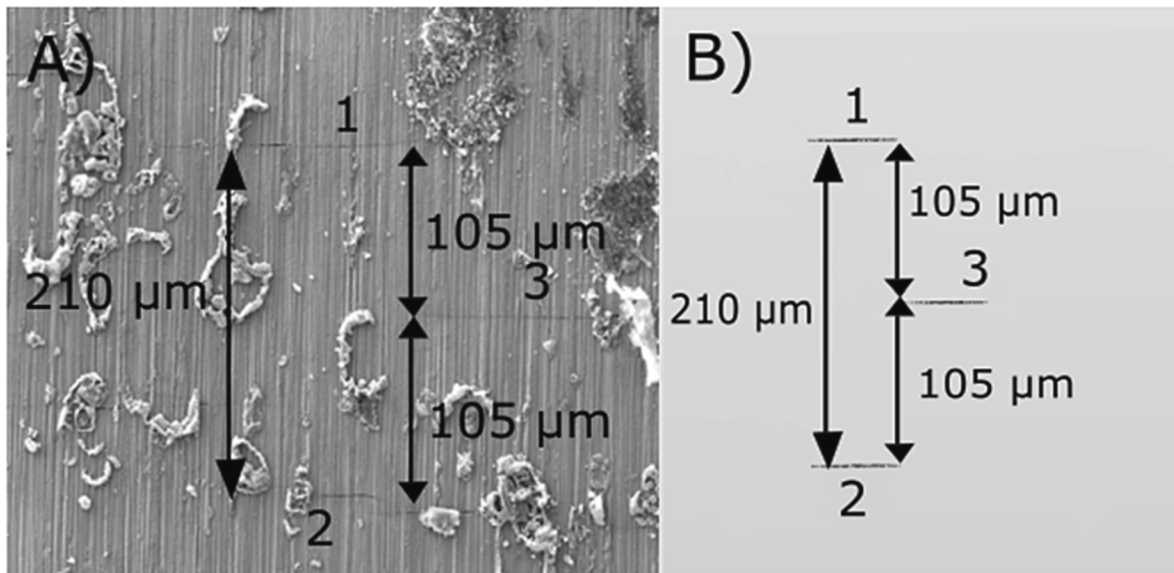


Fig. 18. A) sem image representing the crack shielding mechanism and b) the crack layout used in the simulation to replicate this scenario.

and c. Here, a normal distance of 50 μm between cracks results in shielding and eventually arresting the shorter crack (Φ for the shorter crack halts at 0.45, whereas it reaches 1 for the longer crack). Fig. 18.

For separations of 100 and 150 μm , the phase field parameter progressed significantly further, reaching a value of $\Phi = 0.8$. Crack shielding effects at these separations are similar, with the only significant difference being the higher hydrostatic stress for a 150 μm separation. With a further normal distance of 200 μm , the propagation remained unaffected and completely cracked ($\Phi = 1$) for both instances without any interference.

An example of the crack morphology in the experiments is shown in the SEM image in Fig. 18a. A simulation was performed to replicate this configuration (Fig. 18b), in which three cracks (50 μm) were placed in a similar configuration. Cracks #1 and #2 were separated by a total distance of 200 μm , whereas crack #3 was separated by 100 μm on either side. As the simulation progressed, crack #3 eventually stopped propagating to the left as the surrounding cracks initiated a stress shielding effect. Propagation to the right can continue without interaction, owing to the positioning in relation to the surrounding cracks. Cracks 1# and #2 are at a sufficient separation distance to prevent crack shielding and allow unaffected propagation. Fig. 19 presents the final configuration after 300 s (5 min or 15 min total, including initiation time) of exposure. Fig. 20 further presents the development of the phase field parameter, Φ , which was recorded at three sites (P1, P2, and P3 in Fig. 19b) for crack #3. Positions P1 and P2 can eventually reach $\Phi = 1$ without interaction; however, P3 is now in the vicinity of the surrounding cracks and, as a result, encounters shielding. This onset of stress shielding occurred after 20 s, as Φ for P3 did not exceed 0.8

The analysis of crack configurations that matched the experiments demonstrated that closely spaced cracks coalesced and merged to sustain the crack propagation. Fig. 21b shows another example of this mechanism, in which cracks #1 and #2 merge, while cracks #2 and #3 seem to start converging towards each other. The normal distance between cracks is a critical factor that determines

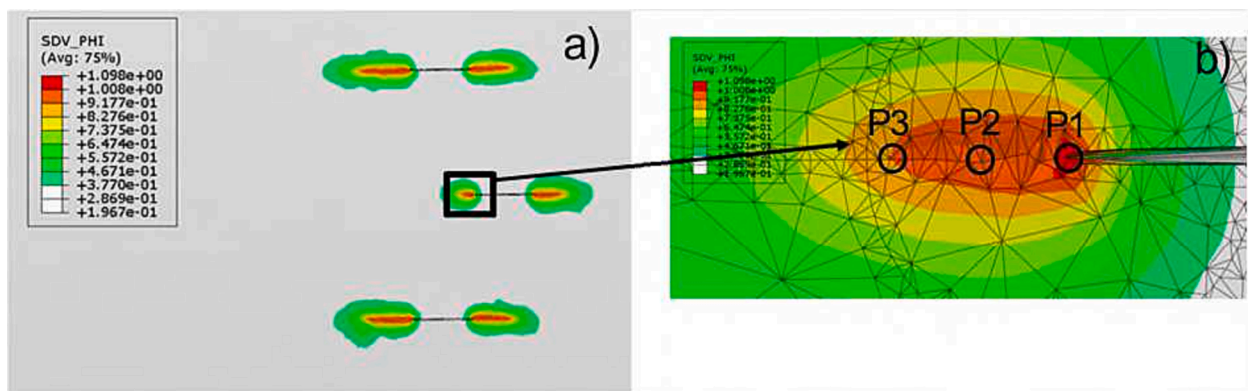


Fig. 19. A) simulation results showing crack morphology and total crack lengths and b) 3 points from which data was extracted.

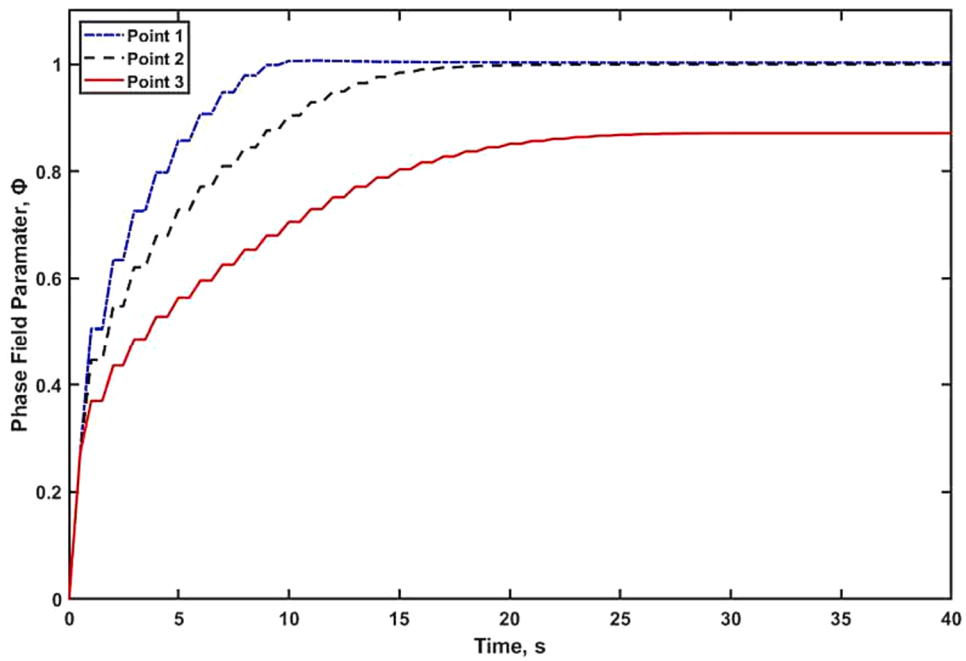


Fig. 20. Plot representing stagnation of propagation as a result of stress shielding at three different points ahead of the crack tip.

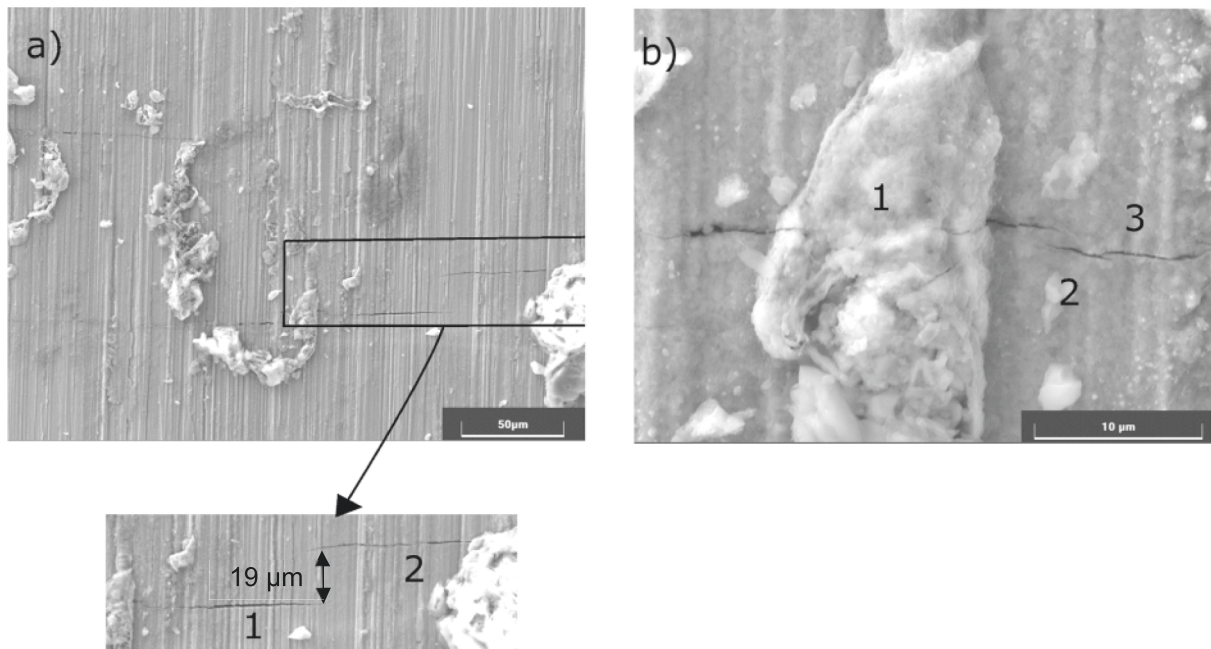


Fig. 21. A magnified SEM image representing crack tip convergence and coalescence.

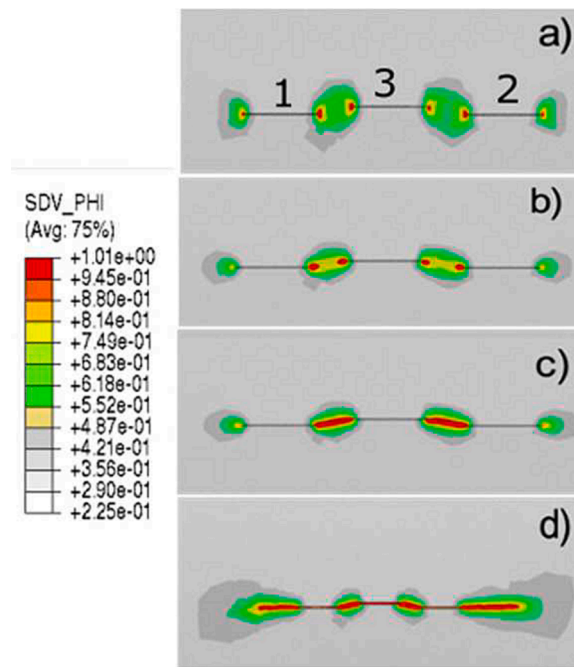


Fig. 22. Simulation results representing effects of crack coalescence between off-parallel cracks with a separation distance of 10 μm or less.

whether cracks encounter shielding, coalesce, or grow without interaction. Off-parallel cracks spaced at 10 μm or less resulted in the coalescence of multiple surrounding cracks. On the contrary, Fig. 21a highlights that the separation distance between cracks #1 and #2 was approximately 19 μm , and hence, crack shielding mechanisms dominated.

The simulation in Fig. 22 approximates the experimental configuration presented in Fig. 21b. Here, three cracks near the apex had equal dimensions (50 μm in length and depth of 20 μm), with the central crack being separated by a vertical distance of 10 μm . The results show that the phase field parameter increases between cracks, demonstrating an active coalescing mechanism. The same simulation was then run twice over, each time increasing the separation distance (to 50 and 100 μm , respectively) and found that at these distances shielding then became the dominant interaction mechanism. This is represented in Fig. 23, which shows that an increase in crack spacing results in shielding, with the stagnation of both the hydrostatic stress and phase field parameters.

5. Discussion

A combination of experimental and computational studies has shown that the interaction of several length scales plays a role in both the slowing and enhancement of crack propagation in superalloys at high temperatures and in corrosive environments. The models were parameterised to match the stress and time required to initiate cracks on the C-Ring surfaces, which resulted in a calibration robust enough to independently predict crack interactions and spacing. Hence, phase field modelling successfully demonstrated the extent of the crack interaction independent of the corrosion mechanism.

The positioning and separation of the distance between multiple cracks are critical parameters that determine the extent of damage. Multiple parallel cracks separated by 150 μm or less resulted in shielding, which slowed down or arrested the crack growth. In these situations, longer cracks dominate and shut down any further propagation of shorter cracks owing to a reduction in crack tip stresses. This phenomenon is therefore relevant to SCC, as many initiation sites on the components may interact and shield prematurely, preventing catastrophic cracking. Hence, a high density of small cracks could be less detrimental than a single small crack that has the potential to grow unbound. However, models and experiments have shown that cracks located within tens of microns result in stress intensification that coalesces into longer cracks. This may result in cracks with sufficiently high stress intensity factors to allow rapid propagation, eventually passing from short cracks to long crack regimes.

The time required to embrittle the material over a certain length scale was controlled by the diffusivity of the species. By comparing this to the diffusivity of other species, we can obtain further insights into the mechanisms actively involved in embrittlement. Because databases for the diffusion coefficients of impurities in single-crystal CMSX-4 are scarce, we consider diffusivity coefficients for pure nickel (Table 4). Interestingly, the diffusivity employed in the simulations closely matches that of sulphur, which reinforces the detrimental role of this element [17].

It should be noted that the underlying physics of the model needs improvement to better capture the corrosion process; however, this is difficult to do, although it is still unclear from the experiments what is occurring. Instead, the scope of this study was to highlight

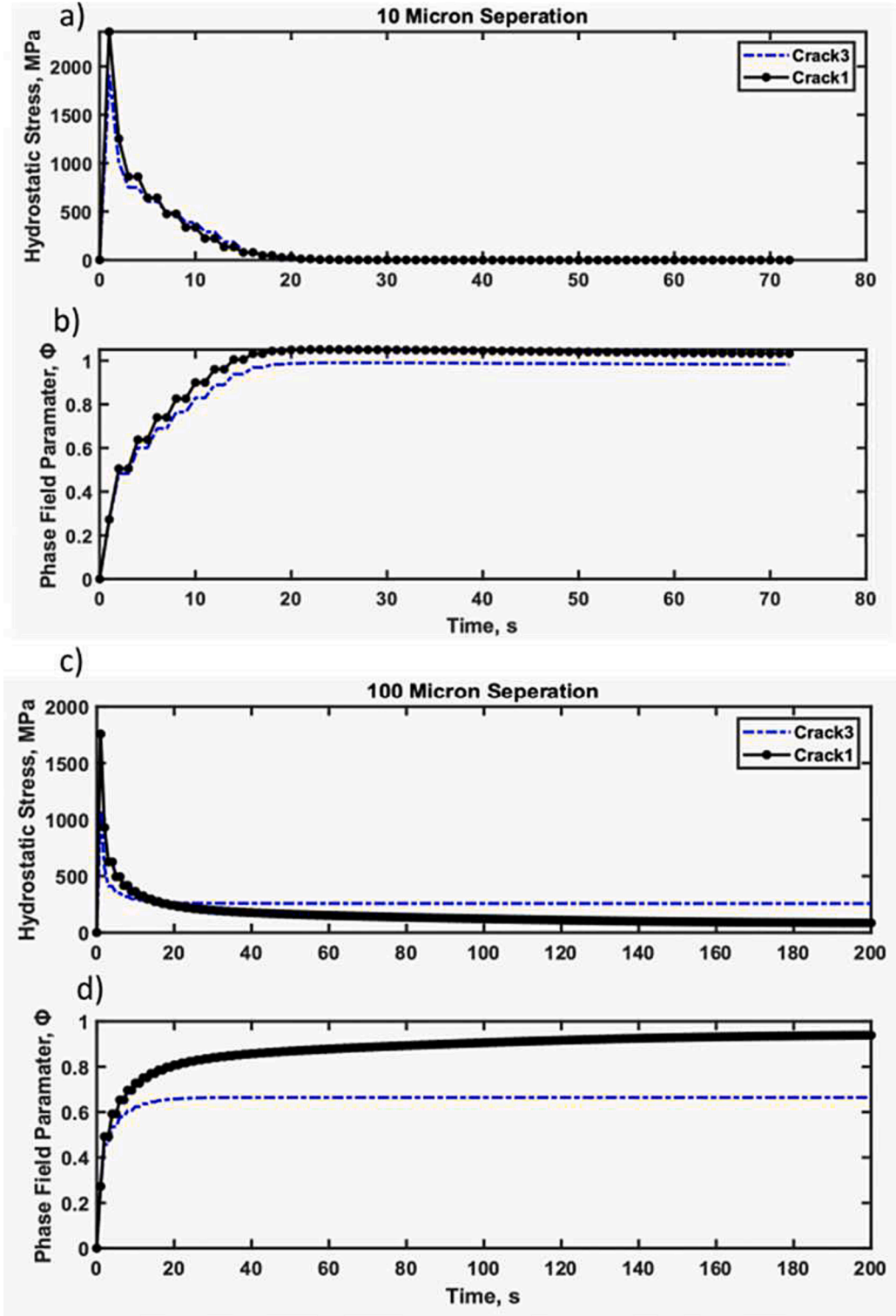


Fig. 23. Plots which show the stress intensification and merging of cracks represented by $\Phi = 1$ because of the coalescence of both cracks (a and b) and the stagnation in both stress and Φ when shielding occurs (c and d).

Table 4

List of known diffusivity coefficients for pure Ni. The estimated diffusivity used in the phase field model closely matches that of sulphur.

Element	Diffusion Coefficient (mm ² /s)
Hydrogen	3.573x10 ⁻³ [12]
Oxygen	9.358x10 ⁻⁶ [12]
Sulphur	1.403x10 ⁻¹⁰ [45]
Aluminium	2.576x10 ⁻¹⁴ [45]
Tungsten	1.32x10 ⁻²⁶ [45]

the detrimental role of crack interactions in SCC, and the results clearly showed that. Finally, the integration of phase field modelling with experiments results in a better understanding of crack interaction and allows for better design of testing configurations that can reveal the underlying mechanisms.

6. Conclusions

The integration of experiments, microscopy, and modelling has revealed the nature of SCC in high-temperature superalloys. From our analysis, we conclude the following.

- 1) The position and magnitude of the peak stress are highly sensitive to the crystal orientation, which affects the crack-growth rate. Beyond a given point in C-Rings, crack propagation is not feasible due to the low levels of stress,
- 2) Cracking is time- and stress-dependent and relies on the diffusion of impurities to a critical concentration, which degrades the energy release rate. Lower stresses require longer times to achieve higher concentrations and increase degradation.
- 3) Under the experimental conditions considered, crack propagation occurred for cracks separated beyond 150 μm . Below this characteristic distance, which is determined by the kinetics of diffusion, crack shielding plays a significant role in arresting the crack propagation. However, cracks within a perpendicular distance of 10 μm dominated the crack coalescence.
- 4) Our analysis suggests that the time-dependent nature of cracking is controlled by a mechanism whose kinetic response matches the diffusion of sulphur, which is one of the possible mechanisms proposed in the literature.

7. Data availability statement

Data supporting this study cannot be made available due to commercial and intellectual property restrictions.

CRediT authorship contribution statement

Mustafa Elsherkisi: Writing – review & editing, Writing – original draft, Methodology, Formal analysis, Data curation. **Fabian Duarte Martinez:** Data curation, analysis, Writing – review and editing. **Julian Mason-Flucke:** Supervision, Project administration, Conceptualization. **Simon Gray:** Writing – original draft, Supervision, Methodology, Funding acquisition, Conceptualization. **Gustavo M. Castelluccio:** Writing – original draft, Supervision, Project administration, Methodology, Conceptualization.

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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Appendix A

To further validate the length scale parameter study, two c-ring simulations were run to strengthen the hypothesis that in the case of crack propagation in metals, more physical meaning can be assigned to l .

In both cases, all loading conditions and material parameters (including l with a value of 0.04 mm) were kept the same, the only thing to change was the mesh. In case #1 the mesh size was 8 times smaller (0.005 mm) than the length scale (just as with the simple 3D block in the original manuscript) and for case #2 a coarser mesh (0.08 mm, now twice the size of l) was used.

The plot below shows that even in this case, by fixing the parameter l , minor deviations in the mesh size had little effect on the

result, and highlights that the physical meaning behind l will provide a more accurate representation when compared to a numerical justification. In some cases, this may be sufficient; however, in the case of crack propagation, we believe that CTOA/CTOD is a great example of a more physical meaning. CTOA/CTOD is known to remain constant during steady crack propagation in metals, and as such, would make sense to relate it to the width of a smear crack for modelling purposes.

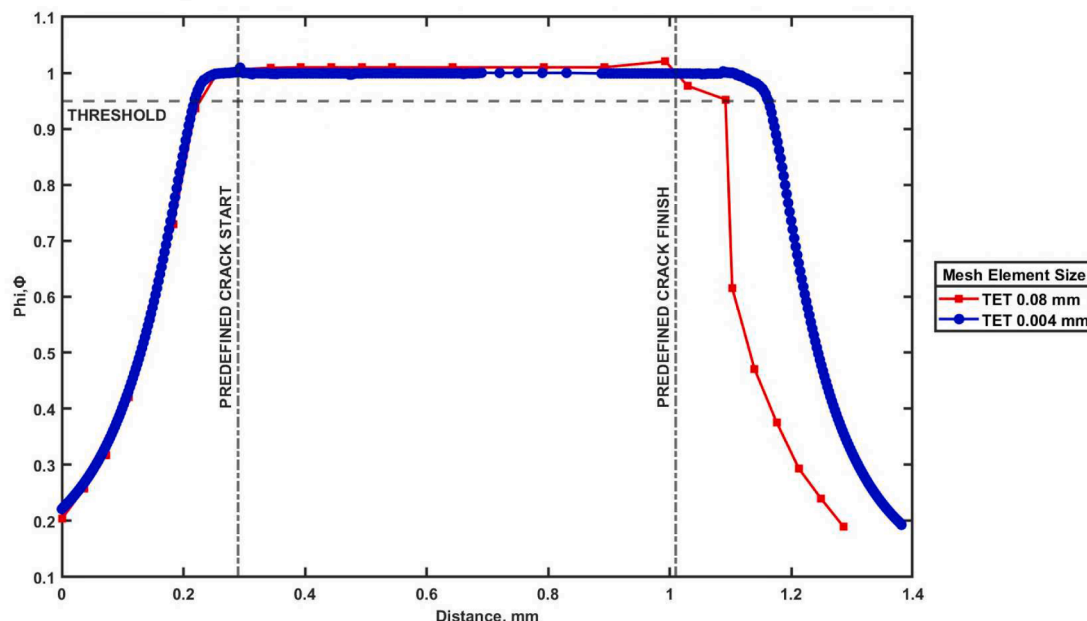


Fig. 24. Length scale parameter study performed using two C-Ring tests.

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Interaction of stress corrosion cracks in single crystals Ni-Base superalloys

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