Strain-Driven Corrosion Crack Growth

A pilot study of intergranular stress corrosion cracking

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Abstract

This work proposes a model for corrosion driven crack growth. The model poses a moving boundary problem, where a chemical attack removes material from the body. The rate of the chemical attack is a function of the strain along the body surface. No crack growth criterion is needed for the analysis. A finite strain formulation is used and the material model is assumed hyperelastic. The problem is stated for a large body, containing a large crack. A low frequency cyclic loading is considered. Thus, corrosion is assumed to dissolve material with a rate, approximately proportional to the strain rate. The problem is solved using finite element method based program, enhanced with a procedure handling the moving boundary. Parametric studies are performed for a series of different initial shapes of the near-tip region. Presented results show that the crack growth rate is largely dependent on the initial crack geometry. For a set of initial shapes and load levels steady-state conditions of growth are achieved, while for the others the cracks show tendency to branch.

Keywords: Stress-corrosion crack growth; Crack tip geometry; Finite strains; Finite elements; Inter-phase thickness.

Nomenclature

t_0	characteristic time in corrosion cavity growth
t	apparent time in corrosion cavity growth
v_0	characteristic penetration rate in corrosion cavity growth
v	apparent penetration rate in corrosion cavity growth
p	kinetics coefficient in the power law of cavity growth
ε_f	rupture strain of the surface passive film
$\dot{\varepsilon}_f$	auxiliary rupture strain rate of the surface passive film (ε_f / t_0)
$\dot{\varepsilon}$	crack tip strain rate
a	crack length
$\dot{a}$	crack growth rate
$\dot{a}_{av}$	average crack growth rate in Ford's model
$\hat{\varepsilon}$	surface strain measure in the simplified penetration model
$\mathcal{R}$	region occupied by the body in its undeformed (reference) configuration
$\mathbf{X}$	coordinates describing the undeformed (reference) configuration of the body
C	region occupied by the body in its deformed (current) configuration
$\mathbf{x}$	coordinates describing the deformed (current) configuration of the body
φ	deformation map

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$\mathbf{F}$	deformation gradient
$\mathbf{R}$	rotation tensor in the polar decomposition of $\mathbf{F}$
$\mathbf{V}$	stretch tensor in the polar decomposition of $\mathbf{F}$
$\mathbf{e}^{(n)}$	generalised spatial strain measure of order n
$\mathbf{T}$	unit tangent vector to the undeformed crack surface
$\mathbf{t}$	unit tangent vector to the deformed crack surface
$\mathbf{t}^*$	vector to which $\mathbf{T}$ is transformed by the deformation map φ
$\mathbf{N}$	unit normal vector to the undeformed crack surface
$\mathbf{n}$	unit normal vector to the deformed crack surface
$\mathbf{n}^*$	vector to which $\mathbf{N}$ is transformed by the deformation map φ
$\mathbf{N}^*$	vector to which $\mathbf{n}$ is transformed by the inverse deformation map φ^{-1}
$\hat{\mathbf{N}}$	unit direction of penetration with respect to the undeformed configuration
$\hat{\mathcal{R}}$	undeformed crack surface
$\mathcal{S}$	natural coordinate along the undeformed crack surface
$\hat{\mathcal{C}}$	deformed crack surfaces
s	natural coordinate along the deformed crack surface
Λ	surface stretch
Ψ	hyperelastic strain energy function
J	Jacobian of the deformation gradient
$\mathbf{b}$	left Cauchy-Green strain tensor
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\mathbf{u}$	displacement vector
λ, μ	Lame coefficients of the material
E, ν	Young's modulus and Poisson's ratio of the material
K_I	applied stress intensity factor
R	outer radius of the boundary layer problem
D	depth of the crack tip profile
H	half-thickness of the crack tip profile
k	power coefficient in the algebraic curve describing the crack tip profile
γ	coefficient of shallowness ($D / 2H$)
κ	dimensionless load parameter ($\kappa = K_I / (E \sqrt{H})$)
ω	normalised penetration rate (v / v_0)
$\underline{\omega}$	steady-state value of the normalised penetration rate
α	normalised crack extension ($\Delta a / H$)

1. Introduction

During the last three decades intense research has been dedicated to the phenomenon of environmentally assisted cracking (EAC). The motivation is that EAC is a cause for many failures of structures, such as light water reactors in nuclear power plants. In Sweden for example, EAC is responsible for as much as one fourth of all unexpected cracks in plants (Bergman *et al.* [1]). Most of the discussions on the topic have been held in the electrochemical and corrosion scientific communities, without essential

support from the solid and fracture mechanics researchers. All investigations, to the authors knowledge, have treated the crack tip as a point, characterised by a single parameter – either the stress intensity factor, K , or the J-integral, or the crack tip opening displacement. This description provides only one feature of the near-tip region, e.g. the strain energy release rate during crack growth. The consequence is that all details, such as stresses, strains, displacements, are uniquely controlled by the chosen parameter, which does not allow the interaction between the environmental attack and the mechanics to be taken into consideration.

It seems that mechanics is indebted to this important area, even if the leading processes in EAC are believed to be of electrochemical nature. The effect of the environmental exposure is that material is removed from the near-tip region, which will effect the distribution of the strains. The treatment of this problem demands a model, where the boundaries of the body are moving. This work utilises such a model to study one of the possible influences that mechanics may have on the stress corrosion crack growth. It presumes that the shape of the crack near-tip region, before the chemical attack, has significance for the evolution of the corrosion driven crack. A plane geometry for the body with the crack and a low frequency cyclic loading are considered. During the closing part of the load cycle, a passive film is assumed to build on the crack surfaces. This film protects the surfaces from corrosive attack. The following increase of the load is assumed to break the film and expose bare metal surface to the environment. This type of loading results in a corrosion model depending on the surface strain, rather than strain rate as in classical models. In addition the material is assumed elastic, which limits the applicability of the quantitative results to real situations, but the qualitative conclusions are believed to be valid also for elastic-plastic materials. Thus, the work is considered to be a pilot investigation, because of the limitations posed by the material model. Even with those simplifications, the model is too complex to be treated analytically, so a finite element based application has been used to build on the simulation of material loss due to corrosion.

The subsection 2.1 discusses briefly some of the electrochemical aspects of stress corrosion cracking, referring both to well-known theoretical works and to the latest reports, containing large amount of experimental data. It explains also the choice of cyclic load condition to achieve strain driven corrosion crack growth. Mechanical aspects of the problem are discussed in subsection 2.2, where only the necessary facts from finite strains kinematics are given. An appropriate choice of surface strain measure is proposed also there.

The third section defines the problem with respect to material, geometry and boundary conditions. The fourth section is devoted to the finite element method (FEM) implementation of the strain driven corrosion crack growth, with emphasis only on the non-trivial issues. Results of parametric studies for various shapes of the near-tip region are given in the fifth section. The last two sections discuss the outcome of the study and draw the major conclusions of this work.

2. Corrosion model

2.1 Electrochemical considerations

The majority of electrochemical experiments on pitting corrosion in the absence of mechanical straining have shown that the characteristic pit size and penetration rate follow a power law dependence on time, t . These observations have been elaborated

theoretically by Engelhardt *et al.* [2], where the derivation has lead to an expression for the cavity growth rate v in the form:

$$v = v_0 \left(\frac{t_0}{t} \right)^p \quad \text{for } t > t_0 \quad (1)$$

In the above formula: v_0 is a characteristic penetration rate, which depends solely on the metal composition and applied potential and reflects only the dissolution process; t_0 is a characteristic time, which depends additionally on the solution chemistry and diffusivity of the dissolved metal species and thus reflects both dissolution and repassivation kinetics; $0 < p < 1$ is a coefficient depending on the kinetics of the anodic dissolution process. For given metal composition and electric potential on the metal surface, v_0 offers the maximum possible penetration velocity, i.e. the velocity achieved at bare metal conditions. The characteristic time can be identified as the time elapsed prior to full refilming of the metal surface. It is important to stress, that equation (1) is valid for times larger than the characteristic time, while for smaller times the penetration rate, v , can be assumed constant and equal to the characteristic rate, v_0 .

An extension to stress corrosion has been proposed in a later work by the same authors (Engelhardt *et al.* [3]). In essence, the crack growth rate is obtained from equation (1) by assuming that the time variable can be written in the form $t = \varepsilon_f / \dot{\varepsilon}$, where the material parameter ε_f is the rupture strain of the passive film covering the metal surface, and $\dot{\varepsilon}$ is the strain rate at the crack tip, given in the sense of material derivative. Thus the penetration rate (1) at the crack tip, i.e. the crack growth rate $\dot{a}$, is written:

$$\dot{a} = v_0 \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_f} \right)^p \quad (2)$$

where the notation $\dot{\varepsilon}_f = \varepsilon_f / t_0$ is introduced for convenience.

A widely discussed stress corrosion cracking mechanism among the electrochemists is the cyclic anodic dissolution, where the strain rate causes rupture of the passive film, followed by dissolution with decreasing rate until full passivation and a new rupture of the film due to strain rate, which closes the cycle. Naturally, the period of one cycle is the characteristic time, t_0 , and upon integration of (2) over one such cycle one arrives at the average velocity of stress corrosion crack growth, which represents essentially the well-known Ford model (see e.g. Ford [4]):

$$\dot{a}_{av} = \frac{v_0}{1-p} \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_f} \right)^p \quad (3)$$

In practice, equation (3) is used to construct a point model of crack extension. Although, the crack tip region is presented as a linear segment, usually of the size of the crack tip opening displacement, the crack tip is allowed to grow only as a point straight ahead. Further, the crack tip strain rate $\dot{\varepsilon}$ is calculated using simplified relations, derived from the HRR-field solution for a stationary crack. The expression for the strain

rate engages the applied stress intensity factor and the yield stress of the material (see e.g. Engelhard *et al.* [3]).

As opposed to that, the present work equips the crack tip region with a curved shape and investigates the influence of the shape on crack growth. Moreover, the penetration velocity at each surface point is assumed to be a vector, normal to the surface at that point and having amplitude (penetration rate) given by a constitutive law. A schematic of such a model is shown in Figure 1. Because of the continuum nature of the mechanical analysis, a constitutive law similar to (2) has to be used, instead of the averaged version (3).

It is worth noting, that both in (2) and (3) the strain rate must be calculated as material derivative of the surface strain. A continuum mechanical model may be established by using (2) as an equation for the penetration rate, with the help of two additional physical observations. At the first place, whenever the strain rate at given surface point is negative, dissolution should not occur there, since no new bare metal has been brought to the surface. At the second place, even if the strain rate is positive, the strain itself must be larger than the rupture strain of the film, in order to have metal exposed to corrosion. The following modification of (2), as a constitutive law for the penetration rate, would reflect those observations in an appropriate manner:

$$v = v_0 \left(\frac{\dot{\varepsilon}}{\dot{\varepsilon}_f} \right)^p H(\dot{\varepsilon}) H(\varepsilon - \varepsilon_f) \quad (4)$$

where $H(x)$ is the Heaviside step function.

Up to date, however, there is a controversy about the evaluation of the power coefficient in equations (1) - (4). Although, an implementation of a constitutive law in the form (4) does not create essential technical problems, the results would be questionable before a generally accepted approach for identifying this parameter appears. Even in such case, the analysis would be specific for any particular system of water chemistry and metal composition. A model of type (4) might be a subject of a future study in closer collaboration with electrochemical experts.

For this study of the influence of crack tip geometry on the corrosion induced crack growth, it suffices to assume a simpler model for the penetration rate at each point of the crack surface in the form:

$$v = v_0 \hat{\varepsilon} H(\hat{\varepsilon} - \varepsilon_f) \quad (5)$$

where $\hat{\varepsilon}$ is an appropriately chosen surface strain measure, ε_f is the rupture strain of the passive film, and v_0 is the maximum possible corrosion rate, that would be achieved if a bare surface condition is maintained under the existing metal potential. Figure 2 shows schematically the behaviour of the passive film. It is assumed that the film is continuously covering the crack surfaces when the cracked body is undeformed. During application of a load, the passive film deforms elastically until the strain parallel to the surface reaches the rupture strain, ε_f . After that the film brakes and at full load a number of film fragments separated by gaps of bare metal are created. We assume that the film fragments relax after the rupture. Then if S is the length of a surface arc before the deformation, and s denotes its deformed length, the fraction of the gaps created along the arc is accepted as definition for the surface strain measure: $\hat{\varepsilon} = (s - S) / s$.

Apparently, because of the instantaneous repassivation of the surface, the model (5) would not work under constant load conditions since the necessary cause for new rupture of the film is absent. But a model of the form (4) would also lead to a rapidly decreasing penetration rate and eventually crack arrest if the load is kept constant. Such behaviour is in agreement with the latest experimental data available in the literature. Kussmaul *et al.* [5] report results of tests, performed under constant load conditions and with step-wise increasing load. The initiation of crack growth was observed after the application of the load. All the experiments, in which the load was kept constant after the initial application, showed rapid decay in crack advance and arrest within short times. Heldt and Seifert [6] make the same observation after a large series of experiments under constant and active loading and conclude that corrosion-assisted crack growth can be only initiated and maintained by active loading within the water environment. The active type of loading used in the testing series was a slow monotonically rising load. The magnitudes of the testing loads were corresponding to stress intensity factors from $20 \text{ MPa}\sqrt{\text{m}}$ up to $100 \text{ MPa}\sqrt{\text{m}}$, with upper limits close to the fracture toughness of the material. Clearly, the supply of new bare metal surface through additional straining is an essential prerequisite for maintaining corrosion-induced crack growth. Therefore, to make the model (5) working under constant load conditions one must think of the load as being applied in a cyclic manner. When the nominal value of the load is applied, the strains on the crack surface near the tip cause film rupture, which exposes certain amount (proportional to the strain) of bare metal to the aggressive water chemistry. Corrosion penetrates the material with a speed given by (5), causing material loss and reshaping the geometry of the near-tip region. The new shape will bring new surface strain distribution, but because of the repassivation the load must be removed and applied again to the same nominal value to let the new surface strains cause new rupture. Eventually, this procedure would lead to a steady-state geometry and growth rate of the crack. In practice the procedure resembles corrosion fatigue loading conditions, but the short-term effect, that the decreasing penetration rate from (4) would bring, is levelled out. In other words, the period of one cycle of loading is chosen to be not larger than the characteristic time of the system. Since the surface strains are determining the penetration speed and geometry evolution, “strain-driven corrosion cracking” seems a justifiable definition for the pilot study presented in this work.

2.2 Surface kinematics

The first observation to be mentioned is that a small strain continuum analysis would be an inappropriate way to approach the problem. The small strain elastic solution in case of a sharp crack with traction free faces, for example, gives vanishing strains along the crack surfaces with a sudden jump to infinity when the crack tip is reached. Even when the near-tip region is assigned a curved shape and a small strain analysis would give non-zero surface strains in a certain segment of the profile close to the tip, such a solution is inaccurate, because that segment in reality would be embedded in an area where large strains are present. To illustrate the error, that may be introduced using small strain formulation, an example comparing small strain and finite strain results is given in an Appendix, but it should be consulted after reading the results section. Moreover, the very nature of the problem requires a distinction between one reference (undeformed) configuration of the solid, which evolves in time due to changing boundary, and one current (deformed) configuration, which evolves correspondingly to

the reference configuration, but also determines its future evolution. Such a distinction calls for finite strain formulation and analysis.

Consider an elastic solid body, occupying region $\mathcal{R}$ with coordinates $\mathbf{X}$ in its undeformed state, and region $\mathcal{C}$ with coordinates $\mathbf{x}$ in its deformed state. The deformation map $\varphi: \mathbf{X} \rightarrow \mathbf{x}$ is assumed continuous with deformation gradient $\mathbf{F} = \nabla_{\mathcal{R}} \mathbf{x}$ throughout $\mathcal{R}$ and inverse $\mathbf{F}^{-1} = \nabla_{\mathcal{C}} \mathbf{X}$ throughout $\mathcal{C}$. In components $F_{iJ} = \partial x_i / \partial X_J$ and $F_{Ji}^{-1} = \partial X_J / \partial x_i$.

If $\mathbf{T}$ is a unit tangent vector at point $\mathbf{X}$ of a material curve, then $\mathbf{F}$ transforms $\mathbf{T}$ into a tangent vector $\mathbf{t}^* = \mathbf{F}\mathbf{T}$ at point $\mathbf{x}$ of the deformed material curve. The length of $\mathbf{t}^*$ is defined as the stretch at point $\mathbf{x}$, which the material curve experiences during the deformation φ . The stretch is denoted hereafter by Λ . If $\mathbf{t}$ is the unit length vector along $\mathbf{t}^*$ this operation is written as:

$$\Lambda \mathbf{t} = \mathbf{F}\mathbf{T} \quad (6)$$

If point $\mathbf{X}$ of the material curve is belonging to a boundary of the body, the deformation gradient used in (6) must be understood as the limiting value of the deformation gradient, when the boundary is approached from the interior of $\mathcal{R}$.

In contrast to the tangent, if $\mathbf{N}$ is the unit normal vector at point $\mathbf{X}$ on a material surface, then generally $\mathbf{F}$ transforms $\mathbf{N}$ into a non-normal vector $\mathbf{n}^* = \mathbf{F}\mathbf{N}$ at point $\mathbf{x}$ on the deformed material surface. Non-normality is a manifestation of existing shear deformation. For our purposes, it is preferable to write the inverse version of this operation, denoting by $\mathbf{n}$ the unit normal vector at point $\mathbf{x}$ on a deformed material surface:

$$\mathbf{N}^* = \mathbf{F}^{-1} \mathbf{n} \quad (7)$$

Note that $\mathbf{N}^*$ is generally a non-unit, non-normal vector at point $\mathbf{X}$ on the undeformed material surface. It is the vector, to which the unit vector $\mathbf{n}$ is carried by the inverse deformation map φ^{-1} , e.g. during unloading. Again, if point $\mathbf{x}$ is belonging to a boundary of the body, the inverse deformation gradient used in (7) must be understood as the limiting value of the inverse deformation gradient, when the boundary is approached from the interior of $\mathcal{C}$. Equations (6) and (7) are sufficient for describing surface kinematics for plane problems. In case of three-dimensional problem, we refer to Norris [7] for a full discussion, while here we specialise to plane body with a crack.

Figure 3 shows schematically a portion of the plane body surrounding the crack tip in its reference state $\mathcal{R}$ and in its current state $\mathcal{C}$. The boundaries, $\hat{\mathcal{R}}$ and $\hat{\mathcal{C}}$, are plane curves, which are parameterised with their natural coordinates, S and s respectively, measured from an arbitrary origin, i.e. $\hat{\mathcal{R}}: S \rightarrow \mathbf{X}$ and $\hat{\mathcal{C}}: s \rightarrow \mathbf{x}$. Then the unit tangent vectors along the two surfaces are given simply by the first derivatives of the position with respect to the natural coordinates: $\mathbf{T} = \mathbf{X}'(S)$ and $\mathbf{t} = \mathbf{x}'(s)$. For convenience, we define the unit normal $\mathbf{n}$ as a vector perpendicular to the tangent $\mathbf{t}$ and directed inwards the material.

Consider now a situation, where the mechanical problem for the plane body with a crack is solved at given moment of time, i.e. we have at our disposal description of the deformed body $\mathcal{C}$ and its surface $\hat{\mathcal{C}}$ in terms of coordinates $\mathbf{x}$ and the inverse

deformation gradient $\mathbf{F}^{-1}$ throughout $\mathcal{C}$. This knowledge is sufficient to serve the corrosion model accepted in the previous subsection, because the penetration is driven by the current surface strains and is directed along the current normal vector at any surface point. It is used to determine the reference configuration of the body for the next time step or load cycle. The tangent, $\mathbf{t}$, and the normal, $\mathbf{n}$, to the deformed surface $\hat{\mathcal{C}}$ are obtained as discussed above. The inverse of the stretch at given surface position is obtained from the inverse version of (6) as:

$$\frac{1}{\Lambda} = \left| \mathbf{F}^{-1} \mathbf{t} \right| \quad (8)$$

The change of the reference profile for the next load cycle has a unit direction obtained from (7):

$$\hat{\mathbf{N}} = \frac{\mathbf{F}^{-1} \mathbf{n}}{\left| \mathbf{F}^{-1} \mathbf{n} \right|} \quad (9)$$

Note, that the unit vector $\hat{\mathbf{N}}$ may coincide with the unit normal vector $\mathbf{N}$ to the reference profile, for example when the surface is traction free and the material is homogeneous and isotropic. Note also, that using equation (8) and (9) does not require explicit knowledge of the reference state for the current configuration. We prefer to keep this approach, because it is suitable for material models with unrecoverable deformations, such as plasticity. This possibility is given a word in the discussion section of the paper. We refer to Wu [8] and Freund [9] for additional reading concerning plane surface kinematics.

The last issue to be addressed in this section is the choice of local surface strain measure. Considering the polar decomposition of the deformation gradient $\mathbf{F} = \mathbf{V} \mathbf{R}$ in terms of a rotation tensor $\mathbf{R}$, followed by the stretch $\mathbf{V}$ in the spatial configuration, the generalised spatial strain measures are given by:

$$\mathbf{e}^{(n)} = \frac{1}{n} \left(\mathbf{I} - \mathbf{V}^{-n} \right) \quad (10)$$

where $\mathbf{I}$ is the unit second-rank tensor and n is the order of the measure. An appropriate choice of surface strain measure to reflect the physics of the model (5) is the linear measure, i.e. the one obtained from (10) for $n=1$. For the plane geometry, considered in this work, the surface strain is a scalar, which with the chosen strain measure and accounting for (8) takes the form:

$$\hat{\varepsilon} = 1 - \frac{1}{\Lambda} \quad (11)$$

The motivation for using strain measure (11) is that the penetration speed is limited by the maximum rate of corrosion v_0 . This has a sound physical ground, because however large the strain is, in reality it may cause at most 100% destruction of the passive film, which is the bare metal condition of the surface. Thus, for very high loads the strain approaches unit and the penetration speed becomes the bare metal corrosion rate, a fact that has been experimentally observed (see e.g. Heldt [6]). The rupture strain of the passive film ε_f has no influence on the behaviour of the near-tip region for high

loads, since its experimental value is of the order of 10^{-3} , albeit variable for different metal compositions. The role of ε_f may be seen as determining the boundary of the surface segment, over which the corrosion acts.

3. Problem description

The constitutive material model adopted is a hyperelastic neo-Hookean, with elastic strain energy function defined by:

$$\Psi = \frac{\mu}{2} (\text{tr}[\mathbf{b}] - 3) - \mu (\ln J) + \frac{\lambda}{2} (\ln J)^2 \quad (12)$$

where $\mathbf{b} = \mathbf{F}\mathbf{F}^T$ is the left Cauchy-Green tensor, $J = \det[\mathbf{F}]$ is the Jacobian of the deformation gradient, and λ and μ are the small-strain Lamé coefficients. The relationship between the Cauchy stress and strain is then derived as:

$$\boldsymbol{\sigma} = \frac{\partial \Psi}{\partial \mathbf{b}} = \frac{\mu}{J} (\mathbf{b} - \mathbf{I}) + \frac{\lambda}{J} (\ln J) \mathbf{I} \quad (13)$$

Note, that this model is approaching linear elasticity in the limiting case of vanishing strains (see e.g. Bonet and Wood [10]) and will properly describe the material behaviour in the body outside the near-tip region.

A large body with a large crack is considered. Figure 4 shows the near tip region and introduces Lagrangian coordinate systems. Far away from the coordinate origin linear elastic behaviour prevails, which allows us to formulate a boundary layer problem for a circular disk with centre at the origin and sufficiently large outer radius R . In the initial configuration, the crack occupies a narrow strip $X_1 \leq 0$, $|X_2| < H$, parallel and symmetric with respect to the negative X_1 -axis. In the region $0 < X_1 < D$ lies the initial head of the crack with a boundary described by an algebraic curve with equation:

$$\left(\frac{X_1}{D} \right)^k + \left(\frac{X_2}{H} \right)^k = 1 \quad (14)$$

Plane strain conditions are considered, since the body is assumed large in the direction perpendicular to the X_1 - X_2 plane. The crack surfaces are assumed traction free. The displacements at the outer boundary $r = R$, $|\theta| < \pi$ are given by the leading terms of the so called Williams expansion:

$$\begin{aligned} u_1 &= \frac{(1+\nu) K_I}{4 \pi E} \sqrt{2 \pi R} \left[(5-8\nu) \cos \frac{\theta}{2} - \cos \frac{3\theta}{2} \right] \\ u_2 &= \frac{(1+\nu) K_I}{4 \pi E} \sqrt{2 \pi R} \left[(7-8\nu) \sin \frac{\theta}{2} - \sin \frac{3\theta}{2} \right] \end{aligned} \quad (15)$$

where E and ν are the modulus of elasticity and Poisson's ratio respectively and K_I is the applied stress intensity factor. The two limits for θ are approximate, because of the

slot formed by the crack, which confines the bulk to $|X_2| > H$ close to $X_1 = -R$. The symmetry of the load and geometry allow us to treat only the upper half of the body.

The load is applied in cycles. During the loading part of a cycle, the displacements (15) are imposed to their nominal values. The deformed configuration is found and the rate of corrosion penetration is calculated from (5), using equations (8) and (11). The body is unloaded and the boundary of the undeformed body is changed in those regions, where corrosion causes material loss. The direction of the boundary motion is given by (9) and the amplitude by the calculated penetration rate. Thus, the reference configuration for the next load cycle is established.

4. FEM implementation

The nature of the problem to be modelled requires a frequent update, after each increment of time or load cycle, of the unloaded configuration of the body. The available commercial codes turned out to be unsuitable for such a procedure mainly because the needed parts of the code are hidden from the user. Therefore, an in-house finite element processor for finite strain continuum analysis is used in this work as a basic solution tool. The processor uses updated Lagrangian formulation, i.e. the mesh is defined over the reference configuration and follows the deformation of the material, but all the relations between the basic thermodynamic variables are defined in the current configuration. Additionally, procedures modelling the material loss in the corrosion process, reshaping the crack tip surface and re-meshing the new updated body are incorporated into the program. Re-meshing process is inevitable, because the purpose of the analysis is to follow the crack growth up to a steady-state condition whenever that is possible, and that may require a considerable crack advance to achieve. Basically, the simulation procedure for one time interval or load cycle follows the steps:

- i. Applying the nominal load in one or, if necessary, several load steps and finding the mechanical equilibrium of the body;
- ii. Parameterising the deformed crack surface and obtaining the spatial tangent and normal vectors at each node along the surface;
- iii. Calculating the surface strain measure and the penetration speed at each node;
- iv. Removing the load and updating the unloaded configuration by moving the surface nodes with the speed found in the previous step and along the transformed back spatial normal vectors;
- v. Re-meshing the updated configuration of the body and accepting it as a reference configuration for the next time interval.

The first step is standard mechanical analysis, based on the chosen constitutive material model. In the second step, parameterisation is done using natural coordinate s along the crack surface. Figure 5 shows a schematic picture of the near-tip region in the deformed configuration. The natural coordinate assumes its zero value at the crack tip and increases when following the crack faces towards the crack mouth. The position of every node n_j on the surface is then given by its radius vector in the form:

$$\mathbf{r}(n_j) = [x_1(s_j), x_2(s_j)] \quad (16)$$

where s_j is the natural coordinate of the node. The coordinate functions $x_1(s)$ and $x_2(s)$ are interpolated using cubic splines. The unit tangent vector at each node of the

deformed crack profile and in the direction of increasing natural coordinate is obtained by numerical differentiation of the radius vector

$$\mathbf{t}(n_j) = [x'_1(s_j), x'_2(s_j)] \quad (17)$$

and the unit inward normal vector is simply taken perpendicular to the tangent

$$\mathbf{n}(n_j) = [x'_2(s_j), -x'_1(s_j)] \quad (18)$$

To obtain the stretch of the surface at given node n_j , the inverse deformation gradients at the Gauss points closest to that node from the two neighbouring elements, say e_i and e_{i+1} , may be used in practice (cf. Fig. 5). In this work, the stretch at n_j is calculated from (8), using the unit spatial tangent vector (17) and the inverse deformation gradient $\mathbf{F}_{i+1}^{-1}$, i.e. the value found in the element positioned in the direction of increasing natural coordinate. Then the surface strain, determining penetration rate is calculated from (11). The direction of penetration in the unloaded configuration is obtained from (9) using the spatial normal vector (18) and again the inverse deformation gradient $\mathbf{F}_{i+1}^{-1}$.

Summarising the corrosion model, the velocity of penetration at each surface node is written in terms of known solution variables and material parameters:

$$\mathbf{v} = v_0 \left(1 - |\mathbf{F}^{-1} \mathbf{t}|\right) H \left(1 - |\mathbf{F}^{-1} \mathbf{t}| - \varepsilon_f\right) \frac{\mathbf{F}^{-1} \mathbf{n}}{|\mathbf{F}^{-1} \mathbf{n}|} \quad (19)$$

The technicalities of the last two steps of the time interval procedure will not be discussed.

5. Crack growth results

We introduce the normalised crack growth rate $\omega = v / v_0$, as the ratio between the apparent and the maximal crack growth rates at any moment of time, and denote by $\underline{\omega}$ its value when steady-state conditions of growth are achieved. Further, we introduce a dimensionless load parameter defined by:

$$\kappa = \frac{K_I}{E \sqrt{H}} \quad (20)$$

The deepness or the shallowness of the near tip profile is controlled by the ratio $\gamma = D / 2H$, where $\gamma > 1$ represents deep crack heads, while $\gamma < 1$ represents shallow crack heads. The sharpness or the bluntness of the tip is controlled by the power of the algebraic curve (14). For the limiting case $k = 2$, the profile of the crack head assumes an elliptic form and the curvature at the crack tip assumes a finite value. Cases with $k < 2$ result in sharp crack tips with infinite curvatures, while for $k > 2$ the crack tips are blunted and have zero curvatures.

For all the cases analysed in this work, the ratio R / H between the outer radius of the disk and the crack half-thickness has been kept larger than 10^5 , which is believed sufficiently large to justify the boundary layer formulation (15).

This section presents the results for the steady-state crack growth rate as a function of the applied load. Simulations have been performed for a series of different crack tip shapes. The crack tip shape with $\gamma = 1$ and $k = 2$ is accepted as a basis for comparative purposes. For rupture strain of the passive film, the value $\varepsilon_f = 10^{-3}$ has been used throughout the calculations. As commented at the end of Section 2, ε_f has no influence on the behaviour of the near-tip region for the range of load parameters considered in this work.

Figure 6 illustrates the near-tip region for the basic shape and the loading $\kappa = 0.2$. The initial mesh is given as an underlying grid. The solid region describes the reference configuration after the crack has grown more than ten times the crack half-thickness. Figure 7 shows the corresponding evolution of the crack growth rate ω as a function of the crack extension $\alpha = \Delta a / H$. As seen from the figure, a transient region of growth exists, where the profile of the crack head is in a reshaping mode until it reaches a steady-state form. The transient region is typical for all initial shapes and load intensities and starts with initial blunting of the crack head. This blunting leaves the wake behind the crack front seen in Figure 6.

Not for all shapes and loads, however, the crack grows straight ahead in its initial plane. Figure 8 shows the same region as Figure 6, but the load $\kappa = 0.4$. The crack head shows a tendency of branching and there is a competition between the original direction and two symmetric possibilities of growth. For the case in Fig. 8 the growth rate of the main crack is higher and after a growth of several H it remains the only growing branch. Calculations for larger loads have resulted in arrest of the main crack.

Very similar development of branches is observed for cracks with initially shallow profiles, i.e. $\gamma < 1$, but the branching starts at lower load levels. Cracks with initially blunted tips, i.e. $k > 2$, in all studied cases branch during the transient reshaping mode. In general, branching occurred for all cases with vanishing crack tip curvature of the deformed shape. In those cases the largest surface strain is found over a segment at a distance about $D/2$ from the crack tip. All such situations are numerically unstable and require a small perturbation to determine the preferable direction of growth.

Figure 9 shows the steady-state values of the normalised crack growth rates, ω , as a function of the load, κ , for constant $\gamma = 1$ and different values of the power coefficient, k . Results for $k > 2$, i.e. initially blunted crack heads, are not shown here, because all of them lead to crack branching. The curve for $k = 2$ is the only one given in full with solid line. For other values of k , the results for two values of ω are shown with points, for $\kappa = 0.2$ and $\kappa = 0.4$.

Figure 10 shows the same solid curve as Figure 9, but now compared with the results for varying parameter γ and constant $k = 2$. For some γ only the results for the two load levels, same as in Figure 9, are given. Because of the comparatively larger differences, one more curve for $\gamma = 1.5$ is given in full with dashed line. Shapes with $\gamma \leq 0.5$, i.e. shallow crack heads, also lead to blunting even for the lower of the two load levels, and therefore are not given.

6. Discussion

In the framework of intergranular stress corrosion, the crack is considered growing in the inter-phase between metal crystal domains. The inter-phase thickness sets a natural upper limit for the parameter $2H$, introduced as crack thickness in this work. In reality the thickness of the inter-phase is of the order of several microns. To illustrate its significance for the crack growth rate, we choose two values for the crack half-thickness: $H = 1.0 \mu\text{m}$ and $H = 10 \mu\text{m}$. It should be noted, that these values are not considered here as scatter limits for the inter-phase thickness. They should be seen as two average values of H over certain distance of crack growth.

For the basic crack head shape, $\gamma = 1$ and $k = 2$, the solid line given in both Figures 9 and 10 splits into two curves if the normalised steady-state crack growth rate, $\underline{\omega} = v / v_0$, is plotted against the applied stress intensity factor, K_I , for the two chosen values of crack half-thickness. Figure 11 shows those curves in a broader range of the applied K_I than the previous figures. However, the crack growth rate at large loads should be taken with caution because the fracture toughness of a particular material sets a limit for K_I , above which the crack will propagate for purely mechanical reasons.

It is seen from the figure that the inter-phase thickness has a significant influence on the crack growth rate. This could explain part of the tremendous scatter that has been observed in measured stress-corrosion crack growth rates under equal applied stress intensity factors. Experiments show that the crack growth rate may vary from $30 \mu\text{m}$ up to 3 m per year (see e.g. Ford and Andresen [11]). Kussmaul et al. [5] comment that the scatter may be due to insufficient control of loading and environmental conditions. This work adds the possibility that part of the scatter may be due to statistical reasons – unpredictable inter-phase thickness and starting crack tip geometry. For example in the load range that is of practical interest for the boiling water reactors in power plants, $K_I < 100 \text{ MPa}$, the crack with $H = 1.0 \mu\text{m}$ will grow about three times faster than the crack with $H = 10 \mu\text{m}$ at steady-state condition for one and the same load.

It is seen from Figure 9, that the largest deviation in the steady-state crack growth rate, when varying the initial sharpness with k , is less than 20% in the load interval under consideration. As expected, the sharper the initial profile the faster the crack growth, but this influence is very small compared to the influence of the inter-phase thickness. That small influence may be explained with the fact, that for all cases the transient interval of reshaping begins with crack head blunting, which damps down the effect of the initial sharpness.

Figure 10 shows that the deviation in the steady-state crack growth rate, $\underline{\omega}$, when varying the initial deepness γ is as much as 40%. The interesting feature, seen in this figure, is the tendency of the initially deeper cracks to grow slower at steady-state condition than initially shallower cracks. That may seem surprising, but it again indicates the importance of the transition period, which for real cracks could yield unpredictable shapes.

The simulations in this work, that have lead to tendencies of branching, show that the separation line between shapes leading to branching and non-branching cracks lies around the chosen basic shape for the considered loading parameter interval. More blunted and shallower initial profiles tend to branch. However, any increase of the loading parameter, either by larger applied stress intensity factor or smaller apparent

inter-phase thickness, shifts the separation line in the direction of sharper and deeper initial crack head profiles. That is because the largest surface strain is not any more found at the tip, but close to the surface point of largest curvature. Experimentally, branching has often been observed for high load levels (see e.g. Heldt [6]), but the authors also report that some specimens tested at low K_I values revealed significant macro-branching with paths inclined at ca. 45° to the initial path. That may be explained by different profiles of the prefabricated cracks prior to testing and brings a statistical uncertainty into the analysis, since the profile cannot be known in advance.

A comment on modelling the moving boundary by updating the unloaded configuration after each load cycle is due. In case of constitutive material model with recoverable deformations, like hyperelasticity, the unloaded configuration coincides with the reference configuration from the beginning of the step. This makes the updating procedure easy to implement. The situation of inelastic material model is considerably more difficult. The unloaded body does not occupy its reference configuration from the beginning of the current time step, because of possible unrecovered deformations. The directions of penetration must be found again by transforming back spatial normal vectors at each surface node, but now using only the elastic part of the inverse deformation gradient. Although this is possible to be handled by the used finite element program, a significant amount of additional work would be needed because of the necessity to re-map the residual stress and strain fields onto the new elements.

7. Conclusions

A moving boundary technique can be used to analyse corrosion-driven crack growth. The cracks analysed here are large and modelled with a finite crack tip. The initial geometry of the tip is given by a shape and a length parameter, e.g. the notch half-width, H .

The crack growth rate is a function of the stress intensity factor, K_I , the modulus of elasticity, E , and the half notch width, H , via the parameter $\kappa = K_I / (E\sqrt{H})$. For small loads the crack growth rate is proportional to κ . The meaning of this is that the steady state growth, approximately assumed after a crack advance of say $3H$ – $5H$, is controlled by the initial conditions. This is in agreement with experimental observation of cracks that, under seemingly identical conditions, may grow with different speeds.

The crack growth rate seems to be extremely sensitive to the initial shape of the crack tip. The shapes used in the present study were varied only to a limited extent, within a class of strongly restricted crack shapes. Still the variation of the crack growth rate at steady state was as much as 50% and the largest differences were between virtually similar shapes. The variation among real cracks will probably display a much larger shape variation due to the history of the pre-crack, material non-homogeneities, orientation of grains etc. This offers an explanation of the very large scatter in experimental results that is frequently observed. However, pure geometrical considerations to foresee the resulting crack growth rate at steady state could not be found. The apparent sharpness or bluntness could not be used for this kind of judgement.

For some of the crack tip shapes branching occurred. The tendency was enhanced at large loads. Although no definite answer could be given, branching seems to be triggered

by the bluntness of the crack. The analysis was not carried any further than to the initiation of branching in these cases.

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Appendix

The surface strain measure introduced by equation (11), may be written in a different way using the reference, S , and the current, s , lengths of the line segment at given surface point:

$$\hat{\varepsilon} = \frac{s-S}{s} = 1 - \frac{1}{\Lambda} \quad (\text{A1})$$

Since the small strain is defined, with respect to the reference length by:

$$\varepsilon = \frac{s-S}{S} \quad (\text{A2})$$

the surface strain measure is derivable from the small strain as follows:

$$\hat{\varepsilon} = \frac{\varepsilon}{1 + \varepsilon} \quad (\text{A3})$$

Figure 12 shows the surface strain at the crack tip as a function of the loading parameter, κ , for the basic crack head shape, $\gamma = 1$ and $k = 2$. The surface strain curve at finite strains is obtained using equation (A1) and is identical to the one shown in the main text. The dashed line marks the crack tip strain at small strains, which is used with equation (A3) to produce the curve for surface strain at small strains. It is seen from the graph, that the small strain solution would underestimate the apparent surface strain and thus the crack growth rate in the proposed model. The error that would be introduced by using a small strain analysis is shown in Figure 13 for completeness. It should be underlined once again, that those curves must be taken as illustrations and should not be trusted for large values of the loading parameter. It may be concluded, however, that even in the interval of reasonably low loading parameter, the error introduced by the small strain approximation is unacceptably large.

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Figure captions:

- Figure 1. Surface model of crack extension.
- Figure 2. Schematic of the passive film rupture.
- Figure 3. Deformation of the near-tip region.
- Figure 4. Geometry of the near-tip region.
- Figure 5. Deformed near-tip region in finite element formulation.
- Figure 6. Initial mesh and unloaded configuration at steady-state for $\kappa = 0.2$.
- Figure 7. Evolution of $\omega = v / v_0$ as a function of $\alpha = \Delta a / H$.
- Figure 8. Initial mesh and unloaded configuration at steady-state for $\kappa = 0.4$.
- Figure 9. $\underline{\omega}$ versus κ : constant crack head deepness, $\gamma = 1$; varying crack head sharpness $k \leq 2$.
- Figure 10. $\underline{\omega}$ versus κ : varying crack head deepness γ ; constant crack head sharpness, $k = 2$.
- Figure 11. $\underline{\omega}$ versus K_I for two values of the crack half-thickness: $\gamma = 1$; $k = 2$.
- Figure 12. Crack tip surface strain $\hat{\epsilon}$ versus κ : comparison between small strain and finite strain formulations.
- Figure 13. Error in the small strain results for the crack tip growth rate.

Figure 1

Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7

Figure 8

Figure 9

Figure 10

Figure 11

Figure 12

Figure 13