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Strain gradient plasticity-based modeling of hydrogen environment assisted cracking

Emilio Martínez-Pañeda [a,*], Christian F. Niordson [b], Richard P. Gangloff [c]

[a] Department of Construction and Manufacturing Engineering, University of Oviedo, Gijón 33203, Spain
[b] Department of Mechanical Engineering, Solid Mechanics, Technical University of Denmark, Kgs. Lyngby DK-2800, Denmark
[c] Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA 22904, USA

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ABSTRACT

Finite element analysis of stress about a blunt crack tip, emphasizing finite strain and phenomenological and mechanism-based strain gradient plasticity (SGP) formulations, is integrated with electrochemical assessment of occluded-crack tip hydrogen (H) solubility and two H-decohesion models to predict hydrogen environment assisted crack growth properties. SGP elevates crack tip geometrically necessary dislocation density and flow stress, with enhancement declining with increasing alloy strength. Elevated hydrostatic stress promotes high-trapped H concentration for crack tip damage; it is imperative to account for SGP in H cracking models. Predictions of the threshold stress intensity factor and H-diffusion limited Stage II crack growth rate agree with experimental data for a high strength austenitic Ni-Cu superalloy (Monel®K-500) and two modern ultra-high strength martensitic steels (AerMet™100 and Ferrium™M54) stressed in 0.6 M NaCl solution over a range of applied potential. For Monel®K-500, K_{TH} is accurately predicted versus cathodic potential using either classical or gradient-modified formulations; however, Stage II growth rate is best predicted by a SGP description of crack tip stress that justifies a critical distance of 1 μm. For steel, threshold and growth rate are best predicted using high-hydrostatic stress that exceeds 6 to 8 times alloy yield strength and extends 1 μm ahead of the crack tip. This stress is nearly achieved with a three-length phenomenological SGP formulation, but additional stress enhancement is needed, perhaps due to tip geometry or slip-microstructure.

1. Introduction

Multi-scale model predictions of material properties are important for alloy and process development, material life-cycle optimization, and component performance prognosis [1]. Interdisciplinary advances in deformation processing [2], fatigue [3], stress corrosion cracking (SCC) [4], and hydrogen embrittlement [5] illustrate this cutting-edge approach. Internal hydrogen and hydrogen environment assisted cracking (IHAC and HEAC, respectively) degrade high toughness alloys in fracture-critical aerospace, ship, energy, and ground transportation structures [6]. Moreover, hydrogen-stimulated damage is a primary mechanism for SCC of titanium, iron, nickel and aluminum-based alloys [7]. Models based on hydrogen-enhanced decohesion (HEDE) [8], interacting with hydrogen-enhanced localized plasticity (HELP) [9], predict trends in the subcritical crack growth rate properties of alloys stressed in environments that produce atomic hydrogen (H) via chemical and electrochemical reactions on crack tip surfaces [7,10]. However, improvements are required; local crack tip stress and dislocation configuration, as well as crack opening profile, are particularly important [11,12].

Building on elastic stress intensity factor (K) similitude for subcritical crack propagation [10], a diversity of IHAC and HEAC models [13–21] employ a crack tip stress field from classical continuum fracture mechanics [10,22], including finite-strain blunting [23], to predict growth threshold (K_{TH}) and rate (da/dt) properties. Alternative modeling is based on dislocation shielding of elastic crack tip stresses [24–27]. The difference between these two approaches centers on the magnitude and distribution of crack tip stresses, which define the location and severity of crack tip H-damage in the fracture process zone (FPZ). Continuum plasticity modeling shows that the maximum opening-direction tensile stress is 3–5 times alloy yield strength and located at 1–2 blunted

* Corresponding author.
E-mail address: mail@empaneda.com (E. Martínez-Pañeda).

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crack tip opening displacements (of order 2–20 μm) ahead of the crack tip surface [23]. Dislocation-based models predict crack opening-direction stresses of 12–25 times yield strength and located much closer to the crack tip [24,25]. This difference is important because HEDE defines cracking as the balance between local tensile stress and H-concentration-reduced interface strength [8] (or reduced-total work of fracture [14,15]). Crack tip H concentration increases exponentially with rising hydrostatic stress [28,29], the crack tip stress gradient affects H diffusion [20,21], and dislocation density impacts the H flux via reversible-H trapping [21]. Next generation H-cracking models require an improved-quantitative description of the crack tip stress field between the extremes represented by classical continuum plasticity and dislocation shielding.

Extensive research has focused on the *smaller is harder* behavior of metals [30–35]. This size effect is attributed to geometrically necessary dislocations (GNDs), which accommodate lattice curvature due to non-uniform plastic deformation. Since classical plasticity lacks a material length, strain gradient plasticity (SGP) theories have been proposed to capture size effects. Isotropic SGP formulations are phenomenological (PSGP) [31] or mechanism-based (MSGP) [33,34]. These theories bridge the gap between length-independent continuum plasticity and discrete dislocation modeling by linking statistically stored and geometrically necessary dislocation densities to the mesoscale plastic strain/strain gradient and strain hardening. Since the plastic zone is small, with a large spatial gradient of high-strain deformation [23], it is imperative to account for GNDs in modeling crack tip stress and strain. Critically important for IHAC and HEAC, SGP modeling has consistently shown that increased GND density at the crack tip leads to: (a) higher local stresses, (b) a contraction in the breadth of the crack tip stress distribution, and (c) reduced blunting; each compared to classical plasticity [36–38]. SGP must be quantitatively implemented in material-damage models [39], as recognized for cleavage [40], interface fracture [41], layered-structure damage [42], ductile-microvoid fracture [43], fatigue [44], and H-enhanced cracking [7,45].

Recent SGP advances are relevant to finite element analysis (FEA) of crack tip stress and strain. PSGP theory with the full complement of three-gradient terms predicts high stresses that persist to a 10-fold larger distance ahead of the sharp crack tip compared to predictions from a single-length formulation [36]. However, this FEA was based on infinitesimal strain [31,36]. A large-strain FEA analysis of a blunting crack tip demonstrated that PSGP and MSGP formulations each predict elevated crack tip tensile stress and reduced crack tip opening compared to classical plasticity [37,38]. The distance over which this stress elevation persists is up to tens of micro-meters, sufficient to engulf the FPZ for HEAC [7], before merging with classical predictions at larger distances within the plastic zone. While classical plasticity predicts a stress maximum located at 1–2 blunted openings in front of the crack tip [22,23], large-strain SGP-enhanced stresses are highest at the smallest-FEA-modeled distance (100 nm) ahead of the tip, with no evidence of a stress maximum. Finally, SGP promotes stress elevation that depends on applied load, in sharp contrast to the K_I independence of maximum stress predicted by classical plasticity [23]. The crack tip stress distribution is affected by both the SGP model used and value(s) of the material length(s). Uncertainties remain regarding: (a) the constitutive prescription that best captures increased GND density associated with a plastic strain gradient [32], and (b) the absolute values of material-dependent length(s) dependent on test method (e.g., nano-indentation) and SGP-model analysis of such measurements [36,38].

2. Objective

The objective of this research is to implement and validate the coupling of a large-strain FEA-SGP analysis of crack tip stress with HEDE-mechanism-based models that predict HEAC propagation threshold and kinetics properties. Specific aims are to: (1) improve the basis for HEAC models using SGP inputs and insights, (2) predict H-cracking properties with fewer model parameters, (3) contribute insight into the role of GNDs ahead of a crack tip, and (4) experimentally assess the proper continuum-SGP formulation of crack tip stresses.

Model assessment is based on measurements of da/dt versus K_I for HEAC in a Ni-Cu superalloy [46,47] and two ultra-high strength martensitic steels [48,49], each stressed in a chloride solution. Electrochemistry measurements and modeling yielded diffusible crack tip H concentration versus bold-surface applied potential (E_{APP}) [46,50], as well as trap-affected effective H diffusivity (D_{H-EFF}) for each alloy [51–53]. The E_{APP} dependencies of K_{TH} and the H-diffusion limited Stage II crack growth rate (da/dt_{II}) were originally modeled [46–49] using crack tip stress expected from blunt-crack [23] and dislocation shielding [24] analyses. This database and the HEDE-modeling approach are reanalyzed using crack tip stress distributions from new FEA that incorporates: (a) the finite strain framework for both PSGP and MSGP [38], and (b) specific alloy-dependent properties and load levels that create H cracking.

3. Experimental procedure

Three high strength alloys were modeled: (a) an austenitic Ni-Cu superalloy hardened by spherical γ' precipitates ($Ni_3(Al,Ti)$; 5 nm radius, 0.08–0.1 vol fraction, and 150000 to 190000 precipitates/μm^3 [54]), and (b) two martensitic ultra-high strength steels strengthened by needle-shaped carbide precipitates ($(Cr,Mo)_2C$; 1 nm radius, 5–8 nm length, volume fraction of order 0.03, and about 150000 precipitates/μm^3 [52,55,56]). The heat treatment and microstructure of the superalloy, Monel®K-500 (Ni-28.6Cu-2.89Al-0.45Ti-0.166C by wt pct), are described elsewhere [46,51,54]: 0.2% offset yield strength (σ_{YS}) is 773 MPa, elastic modulus (E) is 183.9 GPa, and ultimate tensile strength (σ_{UTS}) is 1169 MPa from tensile testing; Ramberg-Osgood flow constants [57] from compression testing are $n = 20$, $\alpha = 0.39$, $E = 185.7$ GPa and $\sigma_o = \sigma_{YSc} = 786$ MPa; and plane strain fracture toughness (K_{IC}) is 200–340 MPa$\sqrt{m}$. The two similar quenched and aged block-martensitic alloy steels, AerMet™100 (Fe-13.4Co-11.1Ni-3.0Cr-1.2-Mo-0.23C by wt pct) and Ferrium™M54 (Fe-7.0Co-10.1Ni-1.0Cr-2.1Mo-1.3-W-0.1V-0.30C by wt pct), are described elsewhere [48,49,52,55,56]. For AerMet™100 and Ferrium™M54, respectively, σ_{YS} is 1725 MPa and 1720 MPa and σ_{UTS} is 1965 MPa and 2020 MPa from tensile testing; Ramberg-Osgood constants are $n = 13$ and 14, $\alpha = 1.0$, $E = 194$ and 198 GPa, $\sigma_o = \sigma_{YSc} = 1985$ MPa and 1951 MPa; and K_{IC} is 130 MPa$\sqrt{m}$ and 126 MPa$\sqrt{m}$.

The kinetics of HEAC were measured for Monel®K-500, AerMet™100, and Ferrium™M54 using precracked fracture mechanics specimens stressed under slow-rising K_I while immersed in an aqueous solution of 0.6 M NaCl and as a function of E_{APP}, as detailed elsewhere [5,46–49]. The da/dt versus K_I results for each alloy are typical of HEAC in high strength metals [7]. Two material properties characterize these data; specifically, the K_{TH} for the onset of resolvable crack propagation under slow-rising K_I, which rapidly accelerates in Stage I then transitions in Stage II to K-independent growth at a plateau level (da/dt_{II}) due to chemical reaction or mass transport limitation [10]. The measured E_{APP} dependencies of K_{TH} and da/dt_{II} (taken at a fixed K_I of 40–50 MPa$\sqrt{m}$ within Stage II) are used to assess the predictions of HEAC models that incorporate either MSGP or PSGP. All potentials are expressed with respect to