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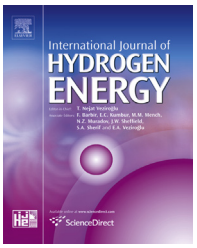

Modelling of stress-corrosion cracking by using peridynamics

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ABSTRACT

We present for the first time a numerical multiphysics peridynamic framework for the modelling of adsorbed-hydrogen stress-corrosion cracking (SCC), based on the adsorption-induced decohesion mechanism. The material is modelled at the microscopic scale using microstructural data. First-principle studies available in the literature are used for characterizing the process of intergranular material strength degradation. The model consists of a polycrystalline AISI 4340 high-strength low-alloy (HSLA) thin, pre-cracked steel plate subjected to a constant displacement controlled loading and exposed to an aqueous solution. Different values of stress intensity factor (SIF) are considered, and the resulting crack propagation speed and branching behaviour are found to be in good agreement with experimental results available in the literature.

Introduction

SCC can be defined as the progressive fracturing of the material due to the presence of non-cyclic tensile stress and the exposure to some gaseous and/or liquid environments. SCC can develop in brittle and non-brittle materials, metals and non-metals and can have different morphologies such as intergranular SCC (I-SCC) and transgranular SCC (T-SCC). Crack branching is common in SCC-damaged materials and, in certain cases, the tensile stress necessary to trigger the phenomenon can be as low as 5% of the yield stress [20]. Due to the substantial number of SCC critical environment–material combinations, a wide range of systems related to different industries are affected by this phenomenon such as pipelines, nuclear power systems, aerospace vehicles, boilers, cooling water systems and oil and gas drilling and production systems [37].

The first catastrophic failures due to SCC occurred in the first years of the 19th century: boiler explosions cost the loss of a large number of human lives. The phenomenon was first recognized in 1873 by W. H. Johnson in a laboratory experiment [20]. Despite the resources and efforts dedicated to the study of this problem, catastrophic failures due to SCC

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Nomenclature

SCC	Stress-corrosion cracking
AIDEC	Adsorption-induced decohesion
SIF	Stress intensity factor
HSLA	High-strength low-alloy
CZM	Cohesive zone model
FEM	Finite element method
CCM	Classical continuum mechanics
PD	Peridynamics
BCC	Body-centered cubic
DFT	Density functional theory
UBER	Universal binding energy relation
H_x	Horizon of a generic particle **x**
δ	Radius of the horizon [m]
f	Mechanical response function [N/m^6]
f_d	Hydrogen concentration response function [mol/m^{6}s]
$C(\mathbf{x}, t)$	Hydrogen concentration field [mol/m^3]
$\dot{C}(\mathbf{x}, t)$	Time derivative of hydrogen concentration field [mol/m^{3}s]
c	Mechanical bond constant [N/m^6]
d	Hydrogen bond constant [m^{-2} s^{-1}]
s	Bond stretch
s_0	Critical stretch
x	Vector defining the position of a generic particle **x**
x'	Vector defining the position of a generic neighbour of particle **x**
y	Vector defining the position of particle **x** in the deformed configuration
y'	Vector defining the position of particle **x'** in the deformed configuration
$\mathbf{b}(\mathbf{x}, t)$	Body force density field [N/m^3]
K_{IC}	Fracture toughness [MPa $\sqrt{\text{m}}$]
h	Plate's thickness [m]
L	Plate's length [m]
W	Plate's width [m]
E	Young's modulus [N/m^2]
ν	Poisson's ratio
G_c	Critical energy release rate [N/m]
u	Enforced displacement applied to the plate [m]
C_{ij}	Elastic moduli of the local stiffness matrix [N/m^2]
[C]	Local stiffness matrix
SHC	Surface hydrogen concentration [mol/m^2]
SHCSV	Surface hydrogen concentration saturation value [mol/m^2]
Δx	Grid spacing [m]
dt	Time step size [s]
c_{T1}	Bond constant type-1 [N/m^6]
c_{T2}	Bond constant type-2 [N/m^6]
ξ_{ij}	Undeformed bond length between particles i and j [m]
θ	Bond angle with respect to the crystal orientation angle [rad]
V_j	Volume of a generic neighbouring particle j [m^3]
q_A	Number of peridynamic bonds along A directions
q_B	Number of peridynamic bonds along B directions
D_{gb}	Grain boundary diffusion coefficient [m^2/s]
ψ	Hydrogen grain boundary coverage
$\mathbf{u}(\mathbf{x}, t)$	Displacement field at **x** [m]
$\mathbf{u}(\mathbf{x}', t)$	Displacement field at **x'** [m]
$\rho(\mathbf{x})$	Mass density at **x** [Kg/m^3]
$\ddot{\mathbf{u}}(\mathbf{x}, t)$	Acceleration vector field [m/s^2]
$dV_{\mathbf{x}'}$	Volume of a generic neighbouring particle **x'** [m^3]

still occur. Moreover, hydrogen is deemed one of the potential candidates to replace fossil fuels. SCC remains, thus, the object of continuous study by academic, industry and other institutions, aimed at, for instance, SCC prediction, SCC monitoring, designing of SCC environmental control procedures and designing of better SCC-resistant materials.

As comprehensively described in Ref. [20], various theoretical models are available in the literature for explaining the mechanisms that lead or just contribute to SCC. However, there is not much agreement about which mechanisms are more appropriate for particular material–environment combinations. The published literature abounds with SCC experimental data such as those reported in Refs. [7,13,15,16,23,28,48,50], but their usefulness is limited by the large amount of parameters contributing to the phenomenon. Moreover, the number of SCC numerical models is increasing in the scientific literature, and many of them are based on the coupling of fracture mechanics and classical continuum mechanics (CCM) theory within the finite element method (FEM) via implementation of the cohesive zone model (CZM) by using cell mesh cohesive elements. Some studies of this kind are described in Refs. [1,9,38,40,42], where hydrogen assisted SCC in high-strength steels is modelled. A similar approach is used in Refs. [2,49] and [3] for the modelling of hydrogen embrittlement in steel pipelines. Studies based on atomistic simulations, such as [5] and [19], are also available. Despite the worthy prediction capabilities and the resulting important insights provided by the use of these numerical techniques, there are various limiting factors. First of all, due to the lack of enough computational power, the current timescales and length scales that can be considered in atomistic simulations are far from those needed in practical engineering applications. Secondly, FEM cell mesh cohesive elements do not allow the analysis of arbitrary crack paths and often lead to mesh dependence and numerical convergence issues. Furthermore, if adaptive remeshing procedures are adopted, numerical errors can arise and computational cost will increase. As mentioned in Ref. [34], another issue is related to the possible overestimation of the fracture energy in the case of crack path not coincident with the element boundaries. Therefore, the past decades have seen the introduction, development, further refinement and application of more advanced numerical techniques suitable for the reproduction of complex fracture behaviours observed in

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