Meshless Peridynamics Method for Modeling Corrosion Crack Propagation

Srujan Rokkam
Advanced Cooling Technologies, Inc. (ACT), Defense-Aerospace Group, Lancaster, PA – 17601, U.S.A.
Srujan.Rokkam@1-act.com, https://orcid.org/0000-0001-9029-7837

Nam Phan
Structures Division, Naval Air Systems Command – Patuxent River, MD - 20670, U.S.A.
Nam.Phan@navy.mil

Max Gunzburger, Sachin Shanbhag
Dept. of Scientific Computing, Florida State University, Tallahassee, FL – 32306, U.S.A.
mgunzburger@fsu.edu, sshanbhag@fsu.edu

Kishan Goel
Structures Division, Naval Air Systems Command – Patuxent River, MD - 20670, U.S.A.
Kishan.Goel@navy.mil

ABSTRACT. Corrosion crack propagation is a result of complex interactions between electrochemical processes and stress redistribution in response to material/environment. In this work, we present a recently developed meshless peridynamics approach for modeling corrosion damage and resulting crack propagation phenomena under synergistic effects of corrosion and mechanical loading. The approach is based on non-local peridynamics theory that replaces governing equations of classical continuum mechanics with integro-differential equations that are easy to solve across discontinuities like cracks. Here we summarize the peridynamic modeling framework developed for corrosion damage scenarios and illustrate its capabilities using numerical simulations of different test scenarios. The framework is able to capture crack path propagation under synergistic influence of corrosion and mechanical loading, without the need to re-mesh the domain or special numerical treatments.

KEYWORDS. Corrosion Crack Propagation, Modeling, Peridynamics, Non-local Methods, Corrosion Damage.

INTRODUCTION

Corrosion assisted crack formation in materials is an omnipresent problem in structural components of several aerospace, industrial and defense systems which are subject to corrosive or aqueous environments. Collectively referred to as environmentally assisted cracking (EAC), the exact nature of corrosion damage depends on the interaction between the host alloy/metal and the corrosive environment, the mechanical loading conditions and metallurgy of the host alloy/metal. Examples of EAC include phenomena such as stress corrosion cracking (SCC), corrosion fatigue (CF) and

hydrogen embrittlement (HE). Common to all these phenomena is the formation of cracks due to corrosion processes or material degradation, and growth of cracks in response to mechanical load or synergetic effects. Such crack propagation and failure can affect the performance and integrity of components and jeopardize their safe and economic operation.

Early approaches for modeling corrosion crack propagation treated the crack initiation and propagation stages separately, each modeled by respective empirical laws and superimposes their results. For example, crack initiation followed a pitting corrosion model, once pit reaches a critical size the crack growth stage onsets and follows a fracture mechanics-based model. Various models have been developed to capture specific sub-processes of EAC phenomena and resulting lifetime to failure [1, 2, 3]. Later, with the advent of finite element method (FEM), crack propagation problem has been frequently modeled using solution of continuum mechanics equations where crack growth is based on fracture mechanics approach. However, classical continuum mechanics equations comprise of partial differential equations (PDEs) which do not exist on crack surfaces and other singularities. The FEM based approaches also suffer from a requirement to re-mesh the domain with propagation of cracks. These limitations led to development of extended finite element method (x-FEM) based models [4, 5], cohesive zone element method (CZM) [6], which eliminate the need for mesh regeneration. However, these methods inherit limitations arising from the PDE structure and need a kinetic relation to inject elements along likely crack path. Such information is difficult to obtain for corrosion crack dynamics, thereby limiting their model capabilities.

Peridynamics (PD) is a nonlocal continuum mechanics theory introduced by Stewart Silling [7] as a reformulation of the classical elasticity theory for modeling materials with discontinuities such as cracks. The theory generalizes the local force assumption to allow non-local forces i.e., forces which act on material points that are separated by a distance. The material mechanics is modeled by treating internal forces within the body as a network of interactions between material points. Consequently the PD theories replace the PDEs of classical solid mechanics with integro-differential equations. In the simplest case of the *bond-based* PD models, the governing equation follows local conservation of linear momentum [8] as:

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t)=\int_{H_{\mathbf{x}}}\mathbf{f}\left(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t),(\mathbf{x}'-\mathbf{x})\right)dV_{\mathbf{x}'}+\mathbf{b}(\mathbf{x},t) \tag{1}$$

where ρ is the mass density in reference configuration, $\mathbf{u}(\mathbf{x},t)$ is the displacement vector defined as $\mathbf{y}(\mathbf{x},t)=\mathbf{x}+\mathbf{u}(\mathbf{x},t)$ where $\mathbf{y}(\mathbf{x},t)$ is the spatial point in deformed configuration of material point $\mathbf{x}$. For relative position $\boldsymbol{\xi}=\mathbf{x}'-\mathbf{x}$ and relative displacement $\boldsymbol{\eta}=\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t)$, the kernel $\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})$ is the nonlocal force vector function which describes the force exerted by material point $\mathbf{x}'$ on material point $\mathbf{x}$, and $H_{\mathbf{x}}$ is the neighborhood of $\mathbf{x}$. The interactions of material points (or PD particles) beyond a spherical region of influence, called the *horizon* (radius δ) are typically assumed to vanish (as shown in Fig. 1-(a)). Since the integral can be evaluated across cracks or discontinuities, the same mathematical equations can be used to describe the mechanics behavior over the entire domain: bulk material, cracks and discontinuities. The numerical structure of the governing equation yields a meshless formulation, which facilitates simulation of crack growth problem without the need for complicated meshing or crack-tracking algorithms. While early PD formulations followed the so-called *bond-based* approach which are suitable for only linear isotropic materials with limitations on Poisson ratio, subsequent developments of PD theory led to more generalized *state-based* models, which can describe all types of material behavior [9]. The PD approach has been applied to several problems like modeling fracture [10], damage analysis of composite laminates [11, 12], electro-migration [13], transient heat conduction [14], thermomechanical fracture [15] and is gaining attention from researchers worldwide for new applications.

Motivated by the need to develop a physics-based approach for corrosion crack propagation we recently developed a PD approach for modeling corrosion damage and resulting failure without the need for re-meshing the domain or specification of crack paths [16,17]. In this paper we present a PD model for corrosion damage and crack propagation formulated by extending conventional PD mechanics and discuss its modeling capabilities using sample results.

PERIDYNAMICS MODEL FOR CORROSION DAMAGE AND CRACK PROPAGATION

In this section, we briefly discuss the extension of PD theory to model corrosion damage and crack propagation scenarios. PD approach describes a solid continua using material points which correspond to a unit differential volume element within the domain. To describe a solid body subject to corrosion we extend the PD treatment of solid continuum to a network of interacting mesoscopic material points whose interaction behavior is dependent on the extent of corrosion within each particle. Subsequently we develop PD governing equations for the material mechanics and evolution of

corrosion within the solid. Figure 1(b) describes the PD representation of a solid body containing a corrosion pit/crack. Each material point (i.e., PD particle) is a representation of a mesoscopic unit volume which could contain the pristine metal and corrosion products. For example, if the material system comprises of two types of corrosion products (α_1 and α_2) and hydrogen gas, the corresponding field variables associated with each PD material point will be $C^{\alpha_1}, C^{\alpha_2}, C^H$. These fields represent the average volumetric concentration of corrosion species (products α_1, α_2 and hydrogen, respectively) within the unit volume of PD material point. The nature of interaction between a PD material point and its neighbors (within the horizon) will be defined in terms of the micro-chemical species at interacting material points. Consequently, the force response function of Equation (1) will now take the form $\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi}) \to \mathbf{f}\left(\boldsymbol{\eta},\boldsymbol{\xi};\mathbb{C}^{\alpha_1},\mathbb{C}^{\alpha_2},\mathbb{C}^H\right)$. Here, $\mathbb{C}^{\alpha_1} = C_i^{\alpha_1} - C_j^{\alpha_1}$ is difference in concentration difference between material points at i and j of α_1 - species; similar definitions hold good for other concentration fields as well. Each PD bond between material points at i and j will be responsible for the nature of elastic interaction between those two points and also responsible for the exchange of species between the two points (example, by diffusion). Consequently, we obtain a *micro-chemically sensitive PD* framework, which is appropriate for modeling corrosion damage and crack propagation.

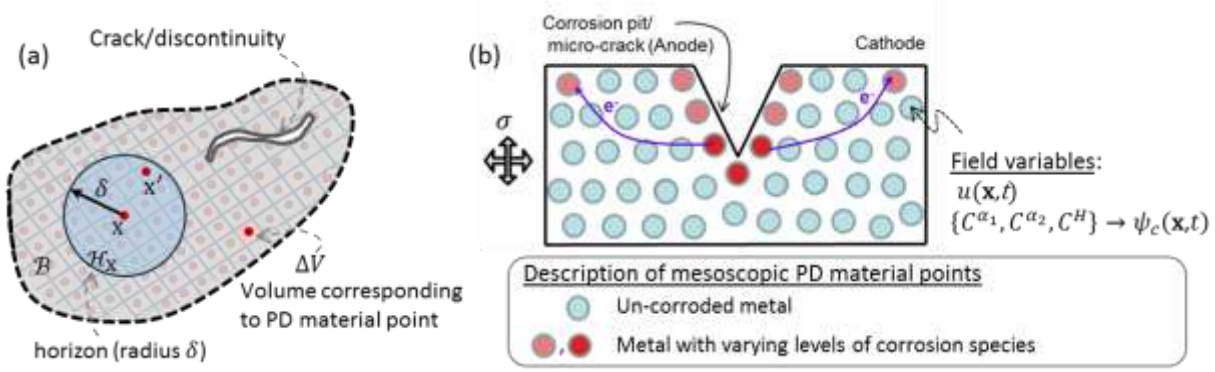

Figure 1: Schematic of: (a) PD continuum body B which is divided into finite sub-domains, each represented by a material point and (b) Description of solid continua undergoing corrosion using PD material points.

In order to demonstrate the suitability of the micro-chemically sensitive PD approach for corrosion damage modeling, we consider a simplified material system: a pure metal undergoing pitting corrosion damage. Pitting corrosion typically involves dissolution of metal at the surface, to form a pit (cavity) and metal ions, similar to Figure 1(b). The pitted regions are weakened mechanically and have a lower load carrying capacity that un-corroded regions. To capture this response of the pitting process, we devised a PD material model which is capable of weakening the material mechanics based on the extent of corrosion. For the purpose of discussion going forward, we introduce generalized *corrosion degradation field*, $\psi_c(\mathbf{x},t)$, which is indicative of the extent of corrosion within each PD particle (i.e., volume element) and lumps the behavior of all corrosion products within a material point. By design, corrosion degradation field $\psi_c(\mathbf{x},t)$ varies such that, $\psi_c(\mathbf{x},t)=0$ if the PD particle is un-corroded, $\psi_c(\mathbf{x},t)=1$ if the PD particle is fully-corroded (i.e., completely weakened) and takes a value $0<\psi_c(\mathbf{x},t)<1$ is PD particle is partially corroded.

Using a sequence of mathematical arguments [16, 17], we obtain the governing mechanics equation that accounts for the mechanistic influence of pitting corrosion as below:

$$\rho\ddot{\mathbf{u}}(\mathbf{x},t) = \int_{H_\mathbf{x}} \mathbf{f}\left(\mathbf{u}(\mathbf{x}',t)-\mathbf{u}(\mathbf{x},t),(\mathbf{x}'-\mathbf{x})\right);\theta\left(\psi_c(\mathbf{x}',t),\psi_c(\mathbf{x},t)\right)dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t), \qquad (2)$$

where, $\theta(\mathbf{x},\mathbf{x}',t) \equiv \theta\left(\psi_c(\mathbf{x}',t),\psi_c(\mathbf{x},t)\right)$ is a measure of the loss of "bond-stiffness" for the bond $\boldsymbol{\xi}$ connecting PD particles at $\mathbf{x}$ and $\mathbf{x}'$, due to occurrence of corrosion. Further, the bond between particles located at points $\mathbf{x}$ and $\mathbf{x}'$ is designed to break when,

$$s(\mathbf{x},\mathbf{x}',t) > s_\circ \nu(\mathbf{x},\mathbf{x}',t) \qquad (3)$$

Here, $\nu(\mathbf{x},\mathbf{x}',t) \equiv \nu\left(\psi_c(\mathbf{x}',t),\psi_c(\mathbf{x},t)\right)$ is a term accounting for the reduction in ability to strain or "stretch-threshold" of the material. The degradation functions $\theta(\mathbf{x},\mathbf{x}',t)$ and $\nu(\mathbf{x},\mathbf{x}',t)$ together account for the material degradation due to manifestation of pitting corrosion and modify the network of internal non-local PD forces acting between bonds connecting all pairs of PD particles $\mathbf{x}$ and $\mathbf{x}'$. The nature of degradation functions $\theta(\mathbf{x},\mathbf{x}',t)$ and $\nu(\mathbf{x},\mathbf{x}',t)$ is prescribed using a set of constraints devised to describe behavior of corroding material. At this stage of model development we do not consider corrosion electrochemistry and prescribe the evolution of corrosion degradation field as:

$$\dot{\psi}_c(\mathbf{x},t) = \int_{H_x} D_c\left(\psi_c(\mathbf{x}) - \psi_c(\mathbf{x}')\right) dV_{\mathbf{x}'} + J_c(\mathbf{x},t) \tag{4}$$

where, D_c in the effective diffusivity characteristic of corrosion propagation in a material system and J_c is a body flux representing a source of corrosion damage due to applied boundary conditions. As corrosion manifests Eq. (4) evolves the corrosion field $\dot{\psi}_c(\mathbf{x},t)$ which in-turn influences the PD mechanics Eqs. (2)-(3) and weakens the material. This weakening of material reduces the load carrying capacity of the pitted region and leads to nucleation of corrosion crack.

Discretized version of the PD evolution equations are obtained by replacing the volume integrals by a finite sum. A numerical solution framework to solve the PD corrosion damage governing equations was developed using C++ programming language. To account of the lack of a full neighborhood for PD material points near surface or boundary, a surface correction was employed to adjust the material properties of those regions. The temporal discretization of PD equations follows an explicit Euler time marching scheme.

SIMULATION RESULTS

In the following we discuss select PD simulations undertaken to illustrate the capabilities of the developed PD corrosion damage material model and simulation framework developed to numerically solve the governing equations. For the scope of this paper, simple test cases mimetic of corrosion pitting, pit growth and corrosion initiated crack propagation under external loads are simulated. The mechanical properties of the bulk solid are set to be equivalent of aluminum and corrosion based degradation parameters are chosen to demonstrate the phenomenological behavior of the PD models.

Corrosion Pitting and Incipient Crack Formation

To verify the response of coupled PD model for corrosion pit nucleation and resulting crack initiation, we simulate a scenario in which an hourglass specimen, shown in Figure 2, is subject to corrosion at two pre-defined hemi-spherical regions. This test case does not apply any external mechanical loads and mimics a scenario where corrosion manifests itself. As the simulation proceeds, corrosion seeds via corrosion damage body flux (J_c), applied as boundary condition in the selected hemi-spherical regions. Figure 2 (a)-(d) show temporal snapshots of the damage field which evolves corresponding to corrosion pit nucleation and growth. Figure 2 (e)-(h) show the evolution of displacement field $\mathbf{u}(\mathbf{x},t)$ in x-direction, with increasing simulation time. Though external loads are not applied as boundary condition, the $\mathbf{u}(\mathbf{x},t)$ field is computed since the mechanics equations are evaluated alongside the corrosion field. As the corrosion manifests (the field ψ_c increases), it inflicts damage in the material by weakening peridynamics bonds connecting material regions. The weakened region (within the pit) also loses its stretch capability, eventually leading to formation of crack precursor, illustrated in subfigure (d). As the simulation proceeds, the corrosion induced material damage develops into an incipient crack within the pitted region. In Figure 2(h), we can observe that the discontinuity in the displacement field across the incipient crack, illustrating the coupling between the PD mechanics and corrosion evolution field.

Next we consider a scenario where corrosion and tensile loads are applied simultaneously. Figure 3 (a)-(c) shows temporal snapshots from a corrosion pitting simulation in a slab specimen that was simultaneously subject to tensile loading along long ends. As the simulation proceeds, the slab also elongates under external load, as well as pits nucleate and grow on the surface where corrosion boundary condition is applied. To illustrate how the load carrying capacity of the slab reduces due to corrosion, in Figure 3(d) we plot the virial stress, σ_{11} (a measure of mechanical stress) as a function of simulation time for a case with corrosion turned on (red line) and compare it against a case without corrosion (green line). As pits nucleate we observe that the load carrying capacity of the slab is reduced drastically and crack precursors are formed.

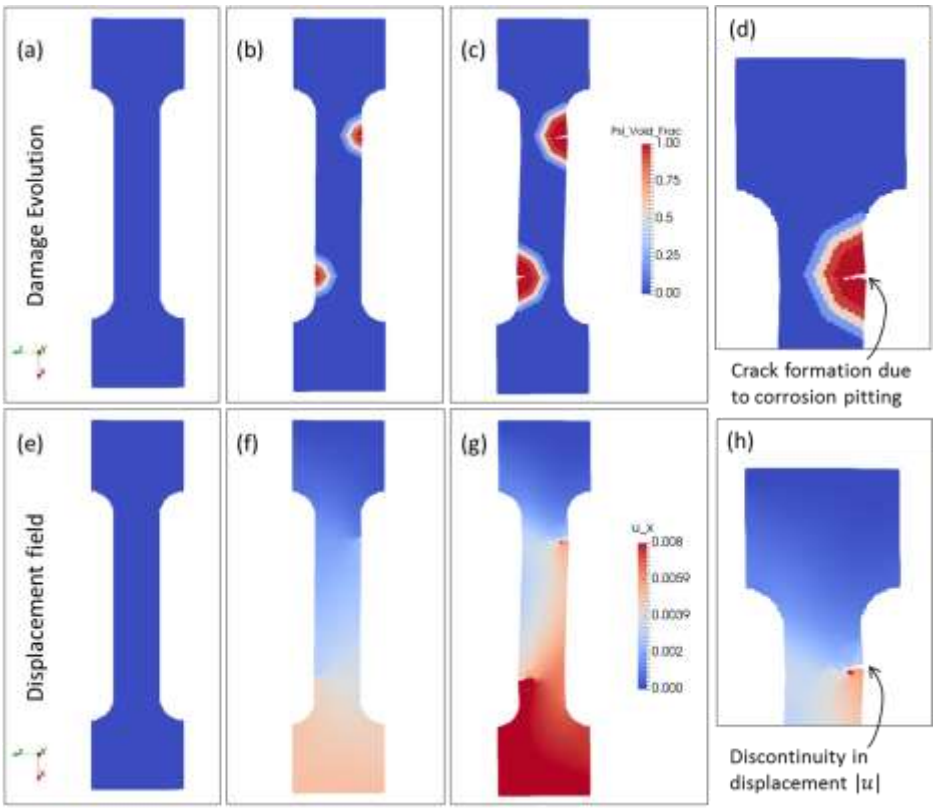

Figure 2: Corrosion pit initiation and growth simulation. Top: (a)-(d) damage evolution, Bottom: (e)-(f) show the corresponding displacement magnitude $|\mathbf{u}(\mathbf{x})|$. Sub-figure (d) and (h) are close-up view of incipient corrosion crack in snapshots (c) and (g). For visualization purposes the deformations are magnified using a factor of ~100.

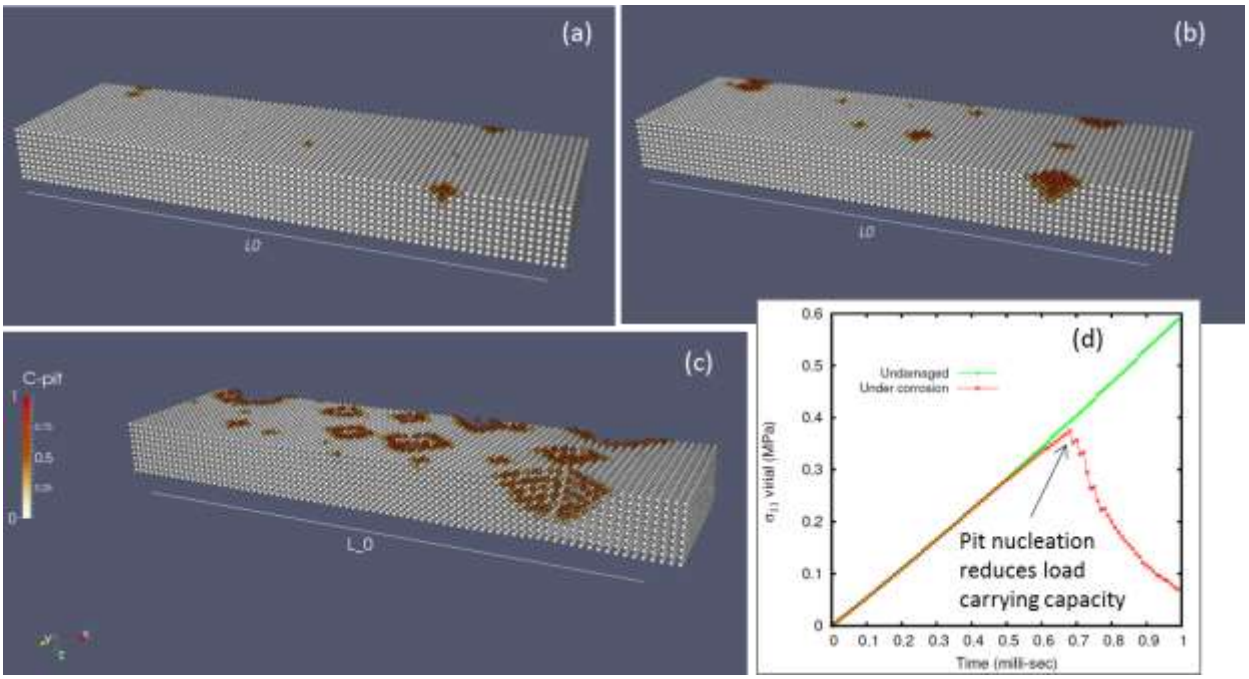

Figure 3: Temporal snapshots of pit nucleation in a slab subject to tensile load: (a)-(c) Snapshots as simulation proceeds, (d) comparison of virial stress (σ_{11}) evolution in corroding (red curve) vs non-corroding slab (green curve). A length marker (L_0) is placed to mark the initial dimension of the slab.

Crack Growth in a Pre-Corroded Plate

Next we investigate a scenario in which a pre-corroded plate is subject to tensile load, as shown in Figure 4(a). The corrosion field in the pre-corroded region weakens the material, leading to pit initiated crack formation, as shown in Figure 4 (b). At initial stages of crack formation a bifurcating crack path develops, due to the internal forces in the. Subsequently, crack grows as a function of simulation time, to reach the damaged state of Figure 4(c), where PD bonds between material regions are fully broken to yield a clear crack surface. Subfigure (d) shows the discontinuity in the displacement field across crack faces emanating from corrosion pit.

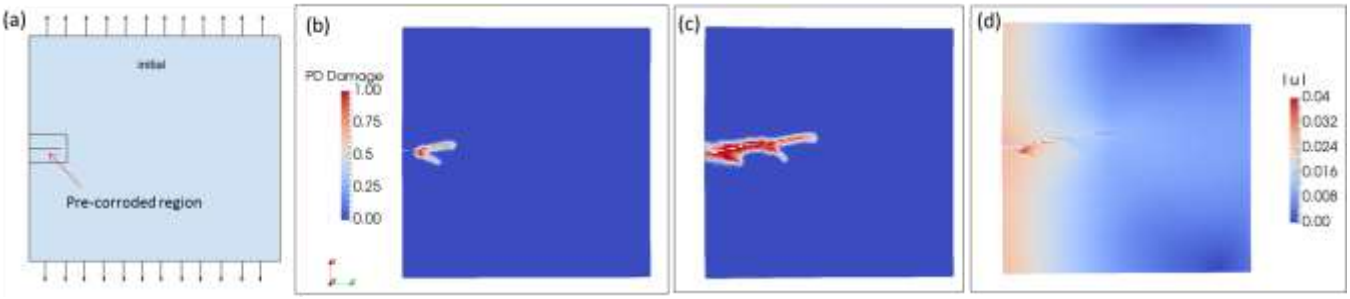

Figure 4: Corrosion crack propagation in a pre-corroded plate (a) schematic of the set-up, (b)-(c) temporal snapshots of % of bonds broken due to damage evolution, (d) displacement $|u|$ at snapshot corresponding to figure (c), illustrating the crack faces formed.

The simulations discussed above illustrate the capability of the developed PD meshless approach for capturing pitting corrosion damage physics, crack nucleation and growth mechanics.

PD approach for corrosion problems in general is at its infancy, as such we focused here on development and proof-of-concept demonstration using phenomenological damage parameters. While the examples reported in this paper are simplistic, they demonstrate the potential use of meshless PD approach for capturing the synergy of corrosion crack propagation in solids, under combined influence of corrosion and external loads. Further development of the PD models is needed to capture additional physics such as that of corrosion fatigue, H-embrittlement and more complex loading scenarios [17]. The PD model presented in this work has multiple damage/degradation variables, which need to be calibrated for a specific material/environment system to enable experimentally relevant comparisons. A full-discussion on the necessary model extensions is an active area of research [17] and is a subject of future publications.

CONCLUSIONS

A micro-chemically sensitive peridynamics framework for meshless simulation of corrosion damage and crack propagation is presented. The underlying approach extends the PD treatment of solid continua to include mechanistic effects of corrosion damage. In order to measure the extent of corrosion within each PD material particle, additional field variables in the form of corrosion degradation fields are introduced. The weakening of the material due to corrosion is formulated in terms of loss of stiffness and ability to stretch, using special degradation functions, per each bond interaction. Custom code was developed to numerically solve the mechanistic PD model equations. Multiple test cases were simulated to ascertain the phenomenological behavior of the PD material model and demonstrate its capabilities. Simulations are able to capture pit nucleation, pit growth, coalescence of pits, crack initiation from corrosion pit, crack growth under external loads. The developed PD approach is well suited for modeling crack propagation and failure, without the need to re-mesh the domain or the need for complicated crack path algorithms like that of XFEM or cohesive element method.

The PD approach is readily extendable to multiple chemical species resulting from corrosion of alloys, as well as more complex EAC phenomena (e.g., SCC, CF, H-embrittlement) and synergetic damage aspects due to nature of applied load [16, 17]. Such aspects are beyond the scope of this paper and will be discussed in future publications. Extension of PD framework for the EAC phenomena is an area of on-going research [17]. Ongoing research efforts include model calibration and identification of material/environment specific degradation parameters.

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