Stress diffusion interactions in an elastoplastic medium in the presence of geometric discontinuity

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**ABSTRACT**

This paper aims to study the effect of stress-diffusion interactions and its effect on the localization of the plastic strain in an elastoplastic material using a fully coupled chemo-mechanical system. The transient coupled system is solved using a finite element formulation in an open-source finite element solver FEniCS. We investigate the role of geometric discontinuities in scenarios involving diffusing species, namely, a plate with a notch/hole/void and particle with a void/hole/core. We also study the effect of stress concentrations and plastic yielding on the diffusion-deformation.

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**1 Introduction**

Diffusive species migration, such as hydrogen in steel [1], lithium in Lithium-Ion batteries (LIBs) [2], chlorine in cement [3] to name a few, cause local expansion/contraction of the materials leading to the localized chemical strains in the material. If the appropriate deformation of the solid does not accommodate these localized chemical strains, stresses referred to as diffusion-induced stress (DIS) [4] are induced. In addition to this, the localized stresses act as a driving force for the species diffusion in the materials, which is commonly referred to as stress-induced diffusion (SID) [5]. Therefore, there is a strong coupling between the diffusion and mechanics of the material, i.e., diffusion of the species causes localized stresses, and the localized stresses also influence the diffusion of the species and vice-versa. The response of the stress-diffusion interactions can be investigated in two aspects as:

- one-way coupling: where the gradient of concentration affects the deformation field, but the localized stress state does not influence the evolution of concentration,
- two-way coupling: in addition to the influence of the gradient of local hydrostatic stress on concentration, the localized concentration also influences the localized stress state.

The presence of diffusion species, either as an external gas or resulting from electrochemical reactions leads to the severe degradation in the material properties and failure of the material [6–9]. Failure due to these multi-physical phenomenon (stress-diffusion interactions [10]) shares a major portion of material failures, viz., chloride diffusion in civil structures [3, 11, 12], hydrogen diffusion in steels [1, 13–19], aluminum [20] and NiTi alloys [21–23], bacteria diffusion in biofilms [24–26], Li diffusion in LIBs [8, 9, 27, 28].

A number of frameworks for diffusion induced deformation and fracture have been proposed assuming an elastic medium [28–36] and using a thermal analogy to model stress-diffusion interactions [31, 37, 38]. In the design of systems where these interactions are involved, the radius and the aspect ratio of the particle plays a crucial role in the concentration of diffusing species as well as the fracture behavior [27, 31]. Furthermore, the fully coupled stress-diffusion interactions and the higher-order terms in the chemical potential also affects the concentration and the stress profile [39]. The geometrical, as well as the material discontinuities present in the system, also play a critical role [38, 40]. However, the assumption of an elastic medium may lead to inaccuracies in failure calculations beyond the elastic regime.

Study of failure of metallic specimens containing stress concentrations such as notches and sharp cracks showed that failure happened with restriction of a plastic zone to very near the fracture surface [41–44]. The hydrogen diffusion induced localized plasticity models [45–50] were able to show increased dislocation mobility in the presence of hydrogen diffusion, causing embrittlement. In-situ studies by Sethuraman et. al. [51] have shown that the stress exceeds yield strength during large deformation of silicon electrodes due to lithium insertion accompanied by plastic deformation. The plastic deformation helps maintain good performance and capacity during cyclic operation by
reducing stress buildup [52]. Sethuraman et. al. [51] experimentally found the evolution of flow stress induced by lithiation and found a strong hysteresis which showed plastic deformation of the electrode. Motivated by these observations continuum theories [53–56] have shown diffusion induced stress due to elastic-plastic deformation of the electrode material.

However, the effect of the plasticity on the one way and fully coupled stress diffusion interaction in the presence of the geometric discontinuities are still unclear. In this work, we numerically investigate the role of plasticity in one-way and two-way coupled stress-diffusion interactions. The investigation is performed for the general case of the stress-diffusion interaction framework. Hence, we have performed studies on hydrogen diffusion in steel as well as lithium diffusion in graphite anode particle.

The article is structured as follows: Section 2 presents governing equations for the coupled stress-diffusion interaction in an elastoplastic medium and the numerical implementation details in an open-source finite element package FEniCS. Section 3 describes the boundary value problem. Section 4 presents the results and discussions pertaining to the chosen boundary value problem. The major conclusions are discussed in the last section.

2. Numerical formulation

In the present study we make use of a continuum model to describe the coupled diffusion deformation. We make an approximation that the diffusion in the medium and the flux description in a coupled stress-diffusion interaction framework. Hence, we have performed studies on hydrogen diffusion in steel as well as lithium diffusion in graphite anode particle.

The chemo-mechanical problem now simplifies to two independent variables: displacements and concentration. The boundary value problem for the coupled diffusion-deformation model in the absence of body force and the source term then becomes: find $u : \beta \subset \mathbb{R}^2$ and $c : \beta \subset \mathbb{R}^2$.

The diffusion of the species is governed by the mass conservation:

$$\frac{\partial c}{\partial t} + \nabla \cdot J = 0, \quad (1a)$$

and the mechanics of the elastoplastic domain is governed by the equilibrium equation:

$$\mathbf{V} \cdot \sigma = 0, \quad (1b)$$

subject to the following boundary conditions:

$$u = \bar{u} \quad \forall x \in \Gamma_u, \quad (1c)$$

$$c = \bar{c} \quad \forall x \in \Gamma_c, \quad (1d)$$

$$\sigma \cdot n = \bar{t} \quad \forall x \in \Gamma_t, \quad (1e)$$

$$J \cdot n = \bar{j} \quad \forall x \in \Gamma_j, \quad (1f)$$

where $\sigma$ is the Cauchy stress tensor and $J$ is the flux vector.

The thermal analogy from previous studies is used to find the influence of concentration on the stress field as:

$$\sigma = C \left( \varepsilon - [\varepsilon - c_0] \frac{\Omega}{3} I - \varepsilon^p \right), \quad (2)$$

and the flux $J$ is related to the concentration and stresses by:

$$J = -D \left( \nabla c - \frac{\Omega}{RT} c \nabla \sigma_h \right), \quad (3)$$

where $C$ is the constitutive matrix for a linear isotropic material, $\varepsilon$ is the total infinitesimal strain, $\varepsilon^p$ is the plastic strain, $c_0$ is the initial or the reference concentration, $\Omega$ is the partial molar volume, $D$ is the diffusion coefficient, $R$ is the universal gas constant, $T$ is the absolute temperature and $\sigma_h = \frac{1}{2} \sigma_n$ is the hydrostatic stress.

2.1. Continuum mechanics modeling

In case of a coupled chemo-mechanical system the total strain increment $\dot{\varepsilon}$ can be decomposed additively. Following a small strain assumption proposed by Zhao et. al., [55] the decomposition of the strain increment can be written as:

$$d\varepsilon = d\varepsilon^e + d\varepsilon^p + d\varepsilon^h$$

where $d\varepsilon^e, d\varepsilon^p, d\varepsilon^h$ are the increments in elastic strain, diffusional strain and plastic strain respectively. The strain-displacement relationship gives,

$$
\varepsilon_{ij} = \frac{1}{2} ( u_{i,j} + u_{j,i}) .
\quad (5)
$$

In case of diffusion induced stress there is an additional strain due to concentration. For an isotropic continuum-material this is written as a dilatational strain rate given by,

$$\dot{\varepsilon} = \varepsilon \frac{\Omega}{3} I$$

\quad (6)

Since the material is elastically isotropic,

$$\dot{\sigma} = C^e : \dot{\varepsilon} = C^e : (\dot{\varepsilon} - \dot{\varepsilon}_p - \dot{\varepsilon}_c)$$

\quad (7)

$$\dot{\varepsilon}^p = \frac{1 + \nu}{E} \sigma - \frac{\nu}{E} (\sigma_{kk}) I.$$ 

\quad (8)

The isotropic $J_{2e}$ flow rule gives the yield condition as,

$$f = \sigma_e - \sigma_y (\varepsilon^p) = 0$$

\quad (9)

where $\sigma_e = \sqrt{\frac{2}{3} \mathbf{S}} : \mathbf{S}$ is the equivalent stress, and $\sigma_y$ is the yield stress, $\mathbf{S}$ is the deviatoric stress. The associated flow rule gives the plastic strain rate as,
\[ \dot{\varepsilon} = \lambda \frac{\partial f}{\partial \sigma} = \frac{3}{2} \frac{S}{\sigma_c} \]  

(10)

where \( \lambda \) is the loading parameter is found using the consistency condition \( \dot{f} = 0 \).

The consistency condition is written as:

\[ j = \frac{3}{2} \frac{S : \dot{\sigma}}{\sigma_c} - \left( \frac{\partial \sigma_c}{\partial \sigma_c} \right) \frac{\partial \sigma}{\partial \sigma} = 0 \]  

(11)

From the plastic flow rule, we get

\[ \dot{\varepsilon}_p^0 = \frac{3}{2} \frac{S : \dot{\sigma}}{\sigma_c} = \lambda \]  

(12)

\[ \dot{\varepsilon}_p^0 = \frac{9}{4} \frac{S : \dot{\sigma}}{S} \frac{S}{\sigma_c} \]  

(13)

where \( \frac{\partial \sigma_c}{\partial \sigma_c} = H \) is the hardening constant for linear hardening.

For numerical simplicity in the context of this paper, we have implemented linear isotropic and kinematic hardening to study the evolution of plastic strain fields. For small range of plastic strains it is a reasonable assumption because the focus of this paper is mainly toward studying the influence of plastic strain in SID in the presence of geometric discontinuities. Appendix 5 contains the detailed derivation for the Kinematic hardening model used for numerical studies in this paper.

### 2.2. Weak form and finite element implementation

In this section, we develop the weak form and the corresponding discrete form for Eq. (1a) and (1b). Let \( \mathcal{U} \) and \( \mathcal{C} \) are the displacement and the concentration trial spaces and \( \mathcal{V} \) and \( \mathcal{P} \) are the displacement and the concentration test spaces:

\[ \mathcal{U} := \{ u(x) \in [c^0(\Omega)]^d : u \in [\mathcal{W}(\Omega)]^d \subseteq [H^1(\Omega)]^d \} \]

\[ u = \bar{u} \quad \text{on} \quad \Gamma_u \}

\[ \mathcal{C} := \{ c(x) \in [c^0(\Omega)]^d : c \in [\mathcal{W}(\Omega)]^d \subseteq [H^1(\Omega)]^d \} \]

\[ c = \bar{c} \quad \text{on} \quad \Gamma_c \}

\[ \mathcal{V} := \{ v(x) \in [c^0(\Omega)]^d : v \in [\mathcal{W}(\Omega)]^d \subseteq [H^1(\Omega)]^d \}

\[ v = 0 \quad \text{on} \quad \Gamma_v \}

\[ \mathcal{P} := \{ p(x) \in [c^0(\Omega)]^d : p \in [\mathcal{W}(\Omega)]^d \subseteq [H^1(\Omega)]^d \}

\[ p = 0 \quad \text{on} \quad \Gamma_p \}

where the space \( \mathcal{W}(\Omega) \) includes linear displacement fields and concentration field. Upon applying the standard Galerkin procedure, the corresponding weak formulation of Eq. (1a) and (1b) is to find \( u \in \mathcal{U} \) and \( c \in \mathcal{C} \) such that \( \forall v \in \mathcal{V} \) and \( \forall p \in \mathcal{P} \):

\[ a(u, v) = \ell(v), \]  

(14a)

\[ b(c, p) = \ell(p) \]  

(14b)

where

\[ a(u, v, c) = \int_{\Omega} \sigma(u, c) : \varepsilon(v) \ d\Omega, \]  

(15a)

\[ \ell(v) = \int_{\Gamma_v} \dot{\varepsilon} \cdot \varepsilon \ d\Gamma, \]  

(15b)

\[ b(c, p, \sigma_h) = \int_{\Omega} \frac{\partial c}{\partial \sigma} p \ d\Omega + \int_{\Omega} (\nabla p)^T \nabla \sigma_c \ d\Omega \]  

(15c)

\[ - \int_{\Omega} (\nabla p)^T c \nabla \sigma_h \ d\Omega, \]  

(15d)

For the temporal discretization, we partition the time interval of interest \( \tau \) into \( n_{\text{step}} \) sub-intervals and focus on typical time slab \([t_i, t_{i+1}]\). To approximate the time derivative of the concentration \( c \), we apply the backward Euler time integration scheme as:
\[ \frac{\partial c}{\partial t} = \epsilon_{t+1} - \epsilon_i \]  
\quad (16)

where \( \Delta t = t_{i+1} - t_i > 0 \) is the time increment. FEniCS [57] is an open source finite element package which translates the weak form of the coupled differential equations into the corresponding finite element solution. The total residual form \( F \) used in the FEniCS is given as,

\[ F = a(u, v) - \ell(v) + b(c, p) - \ell(p). \]  
\quad (17)

The Newton-Raphson scheme in the FEniCS can be called by, \( \text{solve}(F=-0, w, bcs) \), where \( w \) is the solution space and \( bcs \) are the boundary conditions. Algorithm 1 shows the solution procedure followed in the numerical analysis.

**Algorithm 1. Solution algorithm**

initialize displacement, concentration fields at time \( t_i \), \( c_i \)

while \( t_{i+1} < t_{end} \) do

Converged displacement, concentration fields, at time \( t_i \), \( c_i \)

Update strain rates \( \dot{\epsilon}_i, \dot{\epsilon}_c \) using backward Euler scheme

if Yield condition satisfied, \( f \geq 0 \) then

Update plastic strain rate \( \dot{\epsilon}_p \)

end

Update corresponding stress rate, \( \dot{\sigma}_i \) and stress field, \( \sigma_i \)

using backward Euler scheme.

Solve for \( F = 0 \) using Newton raphson scheme for displacement and concentration fields, at time \( t_{i+1} \), \( c_{i+1} \)

Update solution for \( t_i \) to solution at \( t_{i+1} \)

end

**Table 1. Material parameters for Li in graphite system [39].**

| Property                | Value          |
|-------------------------|----------------|
| Young’s modulus (\( E \)) | 19.25 GPa      |
| Poisson’s ratio (\( \nu \)) | 0.3            |
| Diffusivity (\( D \))     | \( 3.9 \times 10^{-14} \text{ m}^2/\text{s} \) |
| Temperature (\( T \))      | 300 K          |
| Partial molar volume (\( \Omega \)) | \( 4.17 \times 10^{-6} \text{ m}^3/\text{mol} \) |

**Table 2. Properties of the steel specimen used for analytical and numerical comparison [49].**

| Property                | Value          |
|-------------------------|----------------|
| Young’s modulus (\( E \)) | 210 GPa        |
| Poisson’s ratio (\( \nu \)) | 0.3            |
| Diffusivity (\( D \))     | \( 1.27 \times 10^{-9} \text{ m}^2/\text{s} \) |
| Temperature (\( T \))      | 300 K          |
| Partial molar volume (\( \Omega \)) | \( 1.96 \times 10^{-6} \text{ m}^3/\text{mol} \) |

3. **Problem definition**

We analyze two boundary value problems in this study:

- a plane strain domain with a circular hole of radius \( r \) as shown in Figure 1a. The effects of plasticity and singularity on stress-diffusion interactions is investigated. The radius of the hole \( r \) has been varied in order to vary the singularity level on the boundary of the hole. The initial or the reference concentration, \( c_0 \) is assumed to be zero. The initial and the boundary conditions for the system are \( \forall t > 0 \),

\[ u_x(-L/2,y,t) = 0, \quad u_y(-L/2,0,t) = 0, \quad u_x(L/2,y,t) = \bar{u}(t), \quad c(-L/2,y,t) = 1. \]

- a plane strain domain with a circular hole of radius \( r_o \) and inner radius \( r_i \), see Figure 1b. The initial concentration \( c_0 \) is assumed to be zero and outer boundary is subjected to constant flux \( f \).

The material parameters used in the simulation is tabulated in Table 1, which corresponds to the Li in the graphite system [39].

4. **Results and discussions**

In this section, the results pertaining to the interactions between stress and concentration will be presented. We analyze problems with increasing complexities. First, we start with (Section 4.1) the analysis of the two-dimensional

\[ \begin{align*}
\text{Figure 2. Plate with circular hole: (a) hydrostatic stress, } \sigma_h \text{ and (b) normalized concentration as a function of angle about the center, } \pi &= 3.14. \end{align*} \]
Figure 3. Plate with a circular hole: normalized concentration along the line (a) $\beta = 0$ and (b) $\beta = \pi/2$.

Figure 4. Plate with circular hole: (a) hydrostatic stress, $\sigma_h$, and (b) normalized concentration as a function of angle about the center, $\pi = 3.14$.

Figure 5. Plate with a circular hole: normalized concentration along the line (a) $\beta = 0$ and (b) $\beta = \pi/2$. 
diffusion in pure elastic medium and validation with the analytical solution. Then we validate the current implementation (one-way coupled elastoplastic simulation) with the commercial available finite element package Abaqus [58] and analyzed the effect of two-way coupling. The effect of plastic yielding on the stress-diffusion interaction will be discussed in the Section 4.2. The effect of one-way and two-way coupling for the particle model with and without the plasticity for applied external flux is investigated in the Section 4.3.

4.1. Implementation validation with the analytical model and the effect of plasticity

The implemented model is validated with the analytical solution available for the pure diffusion. From the analytical solution for a circular hole of radius $a$ in an infinite body under plane deformation and tensile forces $p$, the hydrostatic stresses in polar coordinates $(r, \beta)$ are given by [49]:

$$
\sigma_h(r, \beta) = \left(1 + \nu\right)p \left(\frac{2R^2}{r^2} \cos 2\beta - 1\right),
$$

and the concentration is given by:

$$
C(r, \beta) = C_0 e^{-\frac{2(1+\nu) \beta p}{3} \cos 2\beta + C_0 Q} \left[ -LambertW\left(Ge^{-\frac{2(1+\nu) \beta p}{3} \cos 2\beta + C_0 Q}}\right) \right]
$$

**Table 3.** Diffusion as the thermal analogy.

| Heat equation | Mass diffusion equation |
|---------------|------------------------|
| $\rho C_p \frac{dT}{dt} + \nabla \cdot \mathbf{Q} + \rho g = 0$ | $\frac{D}{\theta} \nabla \cdot \mathbf{J} + \theta \mathbf{Q} = 0$ |
| Degree of freedom: $T$ | Degree of freedom: $c$ |
| Heat flux: $\mathbf{Q}$ | Diffusion flux: $\mathbf{J}$ |
| Heat source: $\rho g$ | Diffusive source: $\mathbf{Q}$ |
| Density: $\rho c_p$ | 1 Unit |

**Figure 6.** Plate with a circular hole: Plastic strain along the line (a) $\beta = 0$, (b) $\beta = \pi/4$ and (c) $\beta = \pi/2$. 

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where \( k = \frac{V_H}{RT}, \quad Q = \frac{2a\sqrt{\frac{1}{C_0}}}{{(1-C_0/C_2)}^{3/2}} \), \( \text{LambertW}(x) \) is the Lambert function.

### 4.1.1. Diffusion in the pure elastic medium

In order to validate the FEniCS implemented model, a rectangular domain with a circular hole with aspect ratio \((L/r) = 10 \& 20\), where \(L\) is the length of the domain and \(r\) is the radius of the hole, is considered. The initial and the boundary conditions for the system are \(\forall t > 0\),

\[
\sigma_x(-L/2, y, t) = -p, \quad \sigma_x(L/2, y, t) = p, \\
c(x, y, t = 0) = C_0 \quad (\text{outside the hole}),
\]

where \(p\) is the uni-axial tensile load of 100 MPa magnitude. The boundary of the domain is assumed insulated such that species can not leave the system. The effect of plasticity is neglected and material is assumed to be perfectly elastic for comparison. The material properties of the specimen is tabulated in Table 2.

Figure 2 compares the numerical solution for the concentration and the hydrostatic stress with the analytical model as a function of angle about the center. The implemented FEniCS numerical results show decent match with the analytical solution as the aspect ratio of the problem domain increases. The state of stress changes from compressive to tensile as the angle increases as shown in Figure 2a. The maximum hydrostatic stress is at \(\beta = \pi/2\) and the minimum hydrostatic stress is at \(\beta = 0\). The distribution of the concentration species follows the distribution of the hydrostatic stress. The tensile sites are capable of holding more diffusing species than the compressive sites and hence the concentration at the tensile sites is more, which is evident from Figure 2b.

Figure 3 compares the concentration of species along the line at \(\beta = 0\) and \(\beta = \pi/2\). The concentration level shows a decent match with the analytical model for both along the line at \(\beta = 0\) and \(\beta = \pi/2\). Moreover, the concentration increases as the distance from the compressed region increases as shown in Figure 3a and decreases as the distance from the tensile region increases as shown in Figure 3b. Hence singularity level at the localized sites plays a critical role on the concentration build up.

### 4.1.2. Effect of plastic yielding on the concentration

Let us assume a plane strain plate with an elastoplastic medium is subjected to the same boundary conditions as presented in the Section 4.1.1. Figure 4 shows the hydrostatic stress and the concentration around the hole. The plastic yielding reduces the magnitude of the hydrostatic stress at the compressive as well as the tensile states as shown in Figure 4a.

The distribution of the concentration species follows from the distribution of the hydrostatic stress which has a

![Figure 7. Plate with a hole: normalized concentration with respect to normalized time at points A and B for one-way coupled system.](image)

![Figure 8. Plate with a hole: evolution of normalized hydrostatic stress, \(\sigma_h\) with respect to the normalized time at point (a) A (b) B for for one-way coupled system in an elastoplastic medium.](image)
lower magnitude than the pure elastic medium at the tensile as well as the compressive sites. The reduced magnitude of tensile stress pulls lesser concentration of diffusing species from the surroundings and the reduced magnitude of compressive stress pushes through lesser concentration of species to the surrounding and hence the species concentration is less at the tensile sites and more at the compressive sites in an elastoplastic medium than a purely elastic medium as shown in Figure 4b. Figure 5 shows the distribution of the concentration along line $\beta = 0$ and $\beta = \pi/2$ with and without plasticity effect. The concentration level increases as the distance from the singular region increases for elastic as well as elastoplastic medium as shown in Figure 4b. Figure 5 shows the distribution of the concentration along line $\beta = 0$ and $\beta = \pi/2$ with and without plasticity effect. The concentration level increases as the distance from the singular region increases but the magnitude of the concentration level is less for the elastoplastic medium as region $\beta = \pi/2$ is in tensile state of stress as shown in Figure 5b.

The introduction of the diffusing species in or out of the media affects the magnitude and evolution of the plastic yielding at tensile and compressive region respectively. Figure 6 shows the equivalent plastic strain at normalized time 0.7 along $\beta = 0$, $\pi/4$ and $\pi/2$. The line along $\beta = 0$ starts with the compressive zone which implies a reduction of concentration of diffusive species which reduces the stress concentration and hence shows lesser plastic yielding. The line along $\beta = 0$ starts with the compressive zone which implies an accumulation of concentration of diffusive species which increases the tensile stress and hence shows higher plastic yielding. Away from the singularity the effect of plastic yielding decreases with distance.
Before analyzing the problem in detail, we have verified our elastoplastic FEniCS implementation against Abaqus results with one-way coupling. In Abaqus, we have used coupled-thermal analysis (in elastoplastic medium) which is the one-way coupled analysis in our context. The thermal and the diffusion equation are analogous to each other. The analogy is given in Table 3. The thermal strain due to temperature gradient in case of coupled-thermal analysis is analogous to the chemical strain developed due to the concentration gradient in case of coupled-diffusion analysis. However in case of thermal analysis the stress field does not influence the temperature distribution which is the same as the one-way coupled system in mass diffusion where the stress field does not influence the concentration distribution.

**Figure 7** shows the concentration at points A and B with respect to the normalized time for one-way coupled problem. The point A is nearer than the point B from the left boundary and hence the concentration is higher at point A at any point of time. However, both points reach steady state concentration level at the end of the simulation which is consistent with the work of Natarajan et al. [40]. This is due to the fact that the effect of stresses is not considered in one-way coupling. Our implementation results show excellent agreement with the Abaqus results, see Figure 7. **Figure 8** also compares the hydrostatic stress evolution at points A and B with respect to the normalized time in an elastoplastic medium. The implemented model is able to capture tensile to compressive state at point A and compressive to tensile state at point B which is also evident from the Abaqus results.

In order to illustrate the effect of plasticity on the stress-diffusion interactions, we compare the results of pure elastic and elastoplastic material and two-way coupled model. **Figure 9** shows the hydrostatic stress evolution at different points as a function of normalized time for pure elastic as well as elastoplastic material. The state of stress at a point A is initially tensile but changes to compressive due to continuous pulling and concentration evolution in the domain. Moreover, the state of stress changes from compressive to tensile at point B. The plastic yielding significantly reduces the stress level in the tensile site (point B) and makes it less
compressive in the compressive site (point A). The level of concentration in the domain depends on the gradient of concentration as well as the localized state of stress. Tensile sites are able to hold more concentration whereas compressed sites tries to push the concentration to nearby sites. Figure 10a shows the concentration evolution at the point A. Initially the state of stress at this point is tensile and gradient of concentration is also present, the concentration of species increases with respect to time. But as the state of stress changes from tensile to compressive (at normalized time 0.3 please refer Figure 9a), the point A is no longer able to take/hold the concentration of the species and hence magnitude of concentration of the species starts decreasing. However in an elastoplastic medium the compressive stress is reduced due to plastic yielding which reflects on the higher concentration compared to pure-elastic medium. In contrast at point B, the level of concentration increases monotonically as shown in Figure 10b. The initial increase in the concentration level is due to the gradient of the concentration and later gradient of hydrostatic term predominates which is responsible for the increase of concentration level. Once again, however we notice that the tensile stress reduction due to plastic yielding reduces concentration of the diffusing species at point B in an elastoplastic medium. Hence it can be concluded that the plastic yielding in the system plays a critical role in determining the steady state behavior.

Figures 11 and 12 shows the plastic strain evolution for one-way and two-way coupled system at different normalized times. In the two-way coupled system, there is a local stress relaxation (analogous to expansion due to temperature rise [40]) and therefore, it leads to a lower stress concentration around the singularity. The equivalent plastic strain due to tension around the hole is lesser in case of two-way coupled system than the one-way coupled system, see Figures 11 and 12. This provides evidence of the reduced tensile stress concentration and the concentration of the species due to the relaxation effect in case of two-way coupled system. Figure 13 compares the concentration contour of one-way and two-way coupled system at different normalized time. The asymmetry of the concentration in the case of one-way coupling is only due to the hole present in the
system, see Figure 13a, c and e. Whereas the asymmetry of the concentration in the case of two-way coupling is due to both hole and the stresses, see Figure 13b, d and f. In the case of two-way coupling, the location of the concentration build up is not the same as compared to the one way coupling. Although the point A is nearer to the point B from the left edge, the concentration build up is more at the point B. This observation is opposite to our earlier observation in one-way coupling. The main reason behind the different build up profile is due to stress induced diffusion effect in the case of two-way coupling. Hence in studying the stress diffusion interactions consideration of the effect of stresses on the singularities is mandatory. The effect is more dominant if there is a high stress gradient present in the domain as in case of stress singularities due to discontinuities.

4.3. Analysis of boundary value problem b

In the recent times, hollow nano-anode structures have attracted attention because of their extra space to
Figure 14. Hydrostatic stress at outer radius (a) without void (b) with void.

Figure 15. Hydrostatic stress at inner radius (a) without void (b) with void.

Figure 16. Concentration at outer radius (a) without void (b) with void.
Figure 17. Concentration at inner radius (a) without void (b) with void.

Figure 18. Hydrostatic stress along radius (a) without void (b) with void.

Figure 19. Plastic strain at outer and inner radius (a) without void (b) with void.
accommodate the volume expansion/contraction due to charge and discharge and hence increases the cyclic performance (Figure 1b). We attempt to understand the influence of a void in a particle on the chemo-mechanical behavior for elastoplastic material.

Due to the incoming flux (charging operation) on the boundary, the outer surface of the particle undergoes compression and the inner surface of the particle undergoes tension, see Figures 14 and 15. From our earlier observation, these stresses consequently affect the diffusion process for the two-way coupled system. At the outer radius (compressive region) the two-way coupled system shows lesser concentration of diffusive species as compared to the one-way coupled system whereas at the inner radius (tensile region) the two-way coupled system shows higher concentration as compared to the one-way coupled system, as shown in Figures 16 and 17.

The stress in elastoplastic medium is lowered than in pure elastic medium due to plastic yielding. The plastic yielding lowers the tensile stress at the inner radius (tensile region) and hence causes an outflux leading to a decrease in concentration compared to pure elastic media, see Figure 17. The inverse effect occurs at the outer radius (compressive region), where a reduction in compressive stress due to plastic yielding causes an influx of diffusing species leading to an increase in concentration, see Figure 16.

When comparing the concentration in one-way coupled model with and without plasticity as shown in Figures 16 and 17, we see negligible difference because the stress field does not influence the diffusion process in that case. We
also note that the compressive stress (at the outer radius) in case of two-way coupled system is more than the one-way coupled system and the tensile stress (at the inner radius) is less in case of two-way coupled system is more than the one-way coupled system, as shown in Figures 14 and 15. This is due to the stress-relaxation effect caused by flux of diffusing species out of the compressive region and into the tensile region respectively as discussed in the previous section. The plastic yielding reduces the overall singularity in stress due to compression and tension in both one-way and two-way coupled systems. However, due to the stress-relaxation effect in two-way coupled system, we see (in Figure 19) higher plastic yielding at the outer radius and lower plastic yielding at the inner radius for two-way coupled system when compared to one-way coupled system. From the concentration, contour plots as shown in Figures 20–23, concentration is lesser at the outer radius and more at the inner radius in case of the two-way coupled system when compared to one-way system which further illustrates the stress-relaxation effect in two-way system. Along with this, Figure 18 gives us a qualitative understanding about the effect of induced stress on diffusion. We observe that due to a high gradient in concentration at the outer radius, the hydrostatic stress and its gradient is also high. As we move closer to the center the concentration gradient reduces, leading to a smaller/no gradient in the hydrostatic stress. This is similar to effect observed by Swaminathan et al. [39].

In order to illustrate the influence of discontinuities, we introduce a void in the particle model. We observe that introduction of the void in the coupled diffusion-deformation process increases the compressive stress at the outer radius (see Figure 14) and the tensile stress at the inner radius, see Figure 15. This consequently reflects on the plastic yielding and affects the diffusion process and vice versa, see Figure 19. At the outer radius (compressive region) the two-way coupled system shows a reduction in the concentration due to an increase in the compressive stress (see, Figure 16). At the inner radius (tensile region) the two-way coupled system shows an increase in concentration due to an increase in the compressive stress (see Figure 17). The effect of discontinuity on the concentration is negligible in one-way coupled model as expected because the stress does not influence the diffusion process. The concentration contour plots (see, Figures 20–23) further provide evidence to illustrate this effect.

5. Concluding remarks

In this paper, the effect of stress diffusion interactions in an elastoplastic material with/without discontinuity using a coupled chemo-mechanics system has been investigated. Moreover, the effect of the fully coupled system over the one-way coupled system is studied systematically for the general framework of the species diffusion in the solid. The buildup of concentration in the one-way coupling system depends only on the distance from the source, whereas the concentration build up in two-way coupling depends not only on the distance but also on the local stress state. The current study also reveals that the stress state in the domain is the determining factor in the study of the chemo-mechanics system and can change the buildup point of concentration (depends on the tensile and compressive site). The plastic yielding at the tensile sites reduces the local diffusion species and same affect is in reverse for the compressive sites. Moreover, the discontinuities in the domain severely affects the stress-diffusion interactions through stress singularities.

Further, the model can be extended to study hydrogen diffusion in steels as well as Li-ion diffusion in LIBs, which may show more complex constitutive models for plastic behavior or complicated geometries. The model can particularly be useful in predicting the fracture behavior in scenarios involving coupled-diffusion in elastoplastic solids. This can help in understanding the degradation due to hydrogen embrittlement or battery failure to enable better and safer designs.

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Compliance with ethical standards

The authors declare that they have no conflict of interest.

Data availability

No data was used to carry out this work.
Appendix A. Incremental equations for numerical scheme

In this appendix we see the numerical procedure for coupled deformation-diffusion using a Kinematic hardening model. Kinematic hardening model uses a back stress, $\beta_y$, which results in a dependence on loading in the hardening model.

The yield condition in case of Kinematic hardening can be rewritten as:

$$ f = \frac{1}{2}(S_{ij} - \beta_y)(S_{ij} - \beta_y) - \frac{1}{3} \beta_y^2 $$

(20)

where $S_{ij} = \sigma_{ij} - \frac{1}{3}\delta_{ij}\sigma$ is the deviatoric stress. We aim at modeling the back stress, $\beta_y$. We use a linear hardening model governed by:

$$ \dot{\beta}_y = h \dot{\epsilon}_p $$

(21)

where $h$ is the hardening constant. Using the associated flow rule,

$$ \dot{\beta}_y = h \dot{\epsilon}^a $$

(22)

Making use of the consistency condition,

$$ \dot{\beta}_y = h \dot{\epsilon}^a $$

(23)

where $h$ is the hardening constant. Using the associated flow rule,

$$ \dot{\beta}_y = h \dot{\epsilon}^a $$

(24)

The increment of the consistency condition,

$$ \dot{\beta}_y = h \dot{\epsilon}_p $$

(25)

In order to eliminate the rate of stress, we use again Hooke's law,

$$ \dot{\beta}_y = h \dot{\epsilon}_p $$

(26)

Solving first two equations,

$$ \dot{\beta}_y = h \dot{\epsilon}_p $$

(27)

We use the value of stress from the previous time step and approximate the rate of stress using Eqs. (21), (28), (29), and (30) to find the current stress states using Eq. (32) as detailed in procedure (see, Algorithm 1). For small time increments the numerical solution is accurate and the computational time is reasonable.