Modeling of progressive delamination in a thin film driven by diffusion-induced stresses

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1. Introduction

Nowadays, Li-ion battery becomes more and more widely used due to its high gravimetric and volumetric energy density, high operating voltage as well as low self-discharge rate. Traditional Li-ion batteries employ carbonaceous anodes whose capacity is about 372 mAh/g (Dahn et al., 1995), which is incapable of fulfilling the increasing demands in high energy applications (Kim et al., 2006). A promising candidate for anodes is silicon which has much higher capacity of about 4000 mAh/g (Boukamp et al., 1981). However, Si experiences up to 300–400% volume expansion (Baggetto et al., 2008; Green et al., 2003; Kasavajjula et al., 2007). Such a large volume change may result in high stress and subsequent cracking and pulverization of Si electrode, finally leads to capacity fade during cycling (Kasavajjula et al., 2007).

There have been many experimental attempts that improve the structure stability and performance of electrodes with various structural configurations, such as nanowires (Chan et al., 2008), particles (Li et al., 1999) and thin films (Baggetto et al., 2008; Souquet and Duclot, 2002; Sethuraman et al., 2010; Li et al., 2011). It is found that nano-structures show better mechanical and cyclic stability. Considering both the capacity and durability, Xiao et al. (2011) fabricated square silicon islands on copper substrate. Delamination between the island and substrate was observed in charging when the island size is larger than a critical value, indicating that the interface effects play very important roles in electrode failure.

There are also many theoretical works addressing the diffusion induced stress (DIS) in electrodes. For example, Golmon et al. (2010) simulated the DIS caused by insertion of lithium ions into spherical silicon particles using a fully-coupled diffusion-elasticity model. Using cohesive model Bhandakkar and Gao (2010, 2011) simulated crack nucleation and predicted the critical size for strip and cylindrical electrode. Deshpande et al. (2010) evaluated the impact of surface strain energy on DIS in nanowire structure. Zhao et al. (2011) developed a coupled diffusion-large plastic deformation theory for DIS in spherical particles. However, most works discussing DIS mainly focused on the behavior of a single particle or nanowire. The interaction between the active material and substrate are much less investigated.

Recently, Haftbaradaran et al. (2012) discussed the interfacial delamination in both two dimensional layered structure and axisymmetric structure by using energy release rate in couple with simple shear-lag stress analysis. The critical size of the electrode was predicted. However, the evolution process of the interface delamination was not studied. Our previous study (Zhang et al., 2012) provided the design insights of layered plate electrodes based on diffusion induced stress but also ignored the interfacial effects and delamination.
A circular active film deposited on substrate, as shown in Fig. 1, is going to be considered to study the interfacial effects and progressive delamination. This paper aims to: (1) develop a semi-analytical model for the progressive interface delamination induced by diffusion induced stresses using cohesive model; (2) simulate the analytical model for the progressive interface delamination induced by neglecting the diffusion from edge is expected to occur faster than that in radial direction, suggesting that the discrepancy of plate. This may affect not very much the further growth of delamination since the delaminated part can expand freely without edge restriction.

For an active plate which expands upon lithiation but shrinks upon delithiation, there may be two kinds of deformation. One is the radial extension/contraction which depends on average Li-ion concentration, and the other one is the bending that depends on the inhomogeneous distribution of Li-ions. As shown in Fig. 3, lithiation induces a protruding and radially extending deformation, while delithiation leads to a concave and radially contracting deformation. Because the deformation of the active layer is restricted by the substrate, the mismatch between the substrate and deforming plate will result in interfacial stress concentration near the edge of the circular plate.

As lithiation/delithiation goes on, the interfacial normal/shear stress becomes larger and larger and finally leads to interface damage. Delamination is thus initiated from the edge of the interface, as shown in Fig. 3. Corresponding to the radial extension/contraction and bending deformation upon lithiation/delithiation, there are also two delamination modes, i.e. sliding and opening.

\[ D \frac{\partial^2 c}{\partial z^2} = \frac{i_n}{r} \quad \text{for} \quad z = -h/2, \]
\[ D \frac{\partial^2 c}{\partial z^2} = 0 \quad \text{for} \quad z = h/2 \]

for galvanostatic charging, where \( F = 96485.3 \text{ C/mol} \) is Faraday’s constant and \( i_n \) is the surface current density which is positive for lithiation but negative for delithiation. The distribution of Li-ion concentration is provided by Crank (1979):

\[ c(z, t) = i_n h \left[ \frac{D t}{h^2} + \frac{3(z/h - 1/2)^2 - 1}{6} - \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \times \cos \left( \frac{n\pi}{h} \left( \frac{z}{h} - \frac{1}{2} \right) \right) \exp \left( -n^2 \pi^2 \frac{D t}{h^2} \right) \right]. \]

The concentrations along thickness at different time are plotted in Fig. 2. The boundary condition at \( z = h/2 \) in Eq. (3) has been assumed for both bonded and delaminated zones for several reasons. Mathematically, the assumption makes the problem much simpler to be solved. Physically, the ions migrate through electrolyte to the top free surface with a much shorter distance than to the delaminated surface. In addition, the assumed boundary condition may influence the distribution of ions mainly within the delaminated portion of plate. This may affect not very much the further growth of delamination since the delaminated part can expand freely without edge restriction.
In present work, the cohesive model is employed to characterize the constitutive behavior of the interface. During progressive growth of delamination, there may exist at most three zones in the interface, i.e. damage free zone, cohesive zone and debonding zone. Damage free zone is the region where the plate and substrate are perfectly bonded. Before loading, the whole interface is damage free. Cohesive zone is the region ahead of a propagating crack, where the cohesive failure in term of damage/plasticity takes place. Debonding zone forms due to delamination, where the plate and substrate separate completely. Distribution of the three zones is depicted in Fig. 3.

Fig. 4 depicts the cohesive law (Camacho and Ortiz, 1996) employed in this work, where the normal and shear cohesive failures are assumed to evolve uncorrelated. In the figure, $\sigma_{nc}$ and $\sigma_{tc}$ are the normal and shear cohesive strengths, respectively. Once either the interfacial normal or shear stress in damage free zone is beyond corresponding strength, it is regarded that damage/plasticity is induced and the region falls into the cohesive zone. After that, the dependence of stresses with respect to interfacial separations is governed by the triangular cohesive law, according to which the cohesive stresses degenerate linearly with the interfacial separation in cohesive zone as described by:

\[
\sigma_n = \begin{cases} 
\sigma_{nc}(1 - \delta_n/\delta_{nc}) & \delta_n \leq \delta_{nc}, \\
0 & \delta_n > \delta_{nc},
\end{cases}
\] (5a)

\[
\sigma_t = \begin{cases} 
\sigma_{tc}(1 - \delta_t/\delta_{tc}) & 0 < \delta_t \leq \delta_{tc}, \\
-\sigma_{tc}(1 + \delta_t/\delta_{tc}) & -\delta_{tc} \leq \delta_t < 0, \\
0 & |\delta_t| > \delta_{tc},
\end{cases}
\] (5b)

where $\delta_n$ and $\delta_t$ are the interfacial opening and sliding displacements, $\delta_{nc}$ and $\delta_{tc}$ are corresponding displacement limits.

Once either opening or sliding displacement is beyond the limits, it is considered that the interface delaminates completely and both interfacial stresses are reduced to zero at the new crack surfaces. The crack criterion is thereby written as $\text{Max}(|\delta_n|/\delta_{nc},|\delta_t|/\delta_{tc}) - 1$. The area embraced by the triangles in Fig. 4 is the dissipated...

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**Fig. 3a.** The protruding deformation caused by lithiation and the corresponding edge crack.

**Fig. 3b.** The concave deformation caused by delithiation and the corresponding edge crack.

**Fig. 4a.** The triangular traction-separation law of normal stress. Here, the fracture energy of the material, $\Gamma = \sigma_{nc}\delta_{nc}/2$.

**Fig. 4b.** The triangular traction-separation law of shear stress. Here, the fracture energy of the material, $\Gamma = \sigma_{tc}\delta_{tc}/2$. 
fracture energy $\Gamma = \sigma_{\text{lc}} h_b c_2 = \sigma_{\text{lc}} h_b c_2$ which represents the interfacial bonding toughness.

3. Governing equations and numerical solutions

In order to solve the delamination problem described in the previous section, the thin film electrode during lithiation/delithiation is decomposed into the active layer with distributed vertical and horizontal loads, $p(r)$ and $q(r)$, and the substrate with distributed surface loads, $p(r)$ and $q(r)$. Fig. 5. Then, the unknown distributed loads, which are equal to interfacial normal stress $p(r) = \sigma_1(r)$ and the interfacial shear stress $q(r) = \sigma_2(r)$, can be solved by enforcing the interface displacement continuity within the damage-free zone and the cohesive law within the cohesive zone and debonding zone.

The active layer is modeled using the thin plate theory because the layer is customarily prepared very thin in experiments, e.g. around 100 nm (Li et al., 2011; Xiao et al., 2011). For the axisymmetric plate, the radial displacement $u_r$ and deflection $w_0$ of the mid-plane are functions of $r$ only. In analogy to the solution for the circular plate under temperature loading (Mastrojannis et al., 1987), the deflection due to Li-ion concentration gradient satisfies:

$$\nabla^4 w(r) = \frac{p(r)}{E_r} + \frac{1}{2I_r} \frac{1}{r^2} \frac{d}{dr} [a q(r)] - \frac{1}{I} \frac{1}{1 - v_p} \nabla^2 M_r,$$

(6)

with boundary conditions

$$w_r(r) = \text{finite}, \quad \frac{dw_r(r)}{dr} = 0 \quad \text{for} \quad r = 0, 0 \leq r \leq R.$$

(7)

The mid-plane radial displacement $u_r(r)$ is expressed as:

$$\frac{d^2 u_r}{r^2} + \frac{1}{r} \frac{du_r}{dr} u_r = -\frac{h q(r)}{12I} + \frac{1}{3} \frac{1}{r^2} \frac{d}{dr} \frac{\Omega c_{\text{ave}}}{c_{\text{ave}}} dr,$$

(9)

with boundary conditions:

$$u_r(r) = 0 \quad \text{for} \quad r = 0,$$

(10)

$$N_r(r) = 0 \quad \text{for} \quad r = R.$$

(11)

where $N_r$ is the radial force resultant, $\Omega$ the partial molar volume, $c_{\text{ave}} = \frac{1}{2} j_{\text{ave}}(z)$ the average concentration. The Eq. (9) is generally valid, in which the last term disappears for the present assumption of one-dimensional diffusion. The specific expressions of $M_r$, $M_r$, $Q$ and $N_r$ are provided in Appendix A.

The solutions of Eqs. (6)-(11) with the assumption of one-dimensional diffusion $(M_r$ and $c_{\text{ave}}$) are independent of $r$ are:

$$w_p(r) = r^2 \left\{ -\int_0^r \frac{h q(r) (r')^2}{12I} dr' + \int_0^r \frac{h q(r) (r')^2}{12I} dr' + \frac{1}{2I_r} \frac{1}{r^2} \frac{d}{dr} [a q(r)] \right\}$$

$$- \frac{1}{2I} \int_0^r \frac{p(r) (r')^2}{12I} dr' + \frac{1}{2I} \int_0^r \frac{p(r) (r')^2}{12I} dr' + \frac{1}{2I_r} \frac{1}{r^2} \frac{d}{dr} [a q(r)]$$

$$+ \frac{h}{24I} \int_0^r \frac{q(r) (r')^2}{12I} dr' + \frac{h}{24I} \int_0^r \frac{q(r) (r')^2}{12I} dr' + \frac{h}{24I} \int_0^r \frac{q(r) (r')^2}{12I} dr' + \frac{1}{2I_r} \frac{1}{r^2} \frac{d}{dr} [a q(r)]$$

$$+ \int_0^r \frac{q(r) (r')^2}{12I} dr' + \int_0^r \frac{q(r) (r')^2}{12I} dr' + \frac{1}{2I_r} \frac{1}{r^2} \frac{d}{dr} [a q(r)]$$

(12)

$$u_p(r) = \frac{\Omega c_{\text{ave}} r}{3} + \frac{hr^2}{24I} \int_0^r \frac{q(r) (r')^2}{12I} dr'$$

(13)

where $j = (1 - v_p)/(1 + v_p)$. Both $r$ and $\rho$ are radial coordinate varying from 0 to $R$. The unknown constant $l_0$ which represents the rigid displacement of plate can be derived from the global self-balance condition:

$$\int_0^r \frac{p(r) dr}{r} = 0.$$

(14)

It is clearly shown that both $u_r$ and $w_p$ are functions of $r$ only and can be obtained once the Li-ion concentration $c(z)$ and interfacial stresses $p(r)$ and $q(r)$ are known.

The semi-infinite substrate is considered as a homogeneous and isotropic material with Young’s modulus $E_s$ and Poisson’s ratio $\nu_s$. It subjects to the distributed surfaces loads applied by the plate, the boundary conditions are therefore:

$$\sigma_{zz}(r, h/2) = p(r) = \sigma_{zz}(r, h/2) = q(r) \quad 0 \leq r \leq R,$$

$$\sigma_{zz}(r, h/2) = \sigma_{zz}(r, h/2) = 0 \quad R < r < \infty.$$

(15)

Following the solution given by Mastrojannis et al. (1987), the vertical displacement of the surface is:

$$w_s(r) = -\frac{2(1 - \nu_s^2)}{E_s} \int_0^r \frac{q(r) p(r) \rho}{\rho} \int_0^r \frac{q(r) \rho}{\rho} d\rho dr$$

$$+ \left( \frac{1 + \nu_s}{1 - \nu_s} \right) \int_0^r \frac{q(r) \rho}{\rho} d\rho dr$$

$$+ \frac{4(1 - \nu_s^2)}{E_s} \int_0^r \frac{q(r) p(r) \rho}{\rho} d\rho dr$$

$$+ \left( \frac{1 + \nu_s}{1 - \nu_s} \right) \int_0^r \frac{q(r) \rho}{\rho} d\rho dr,$$

(16)

and the radial displacement of surface:

$$u_s(r) = -\frac{2(1 - \nu_s^2)}{E_s} \int_0^r \frac{q(r) p(r)}{\rho} \int_0^r \frac{J_1(r') \rho J_1(r') d\rho dr}{\rho}$$

$$+ \left( \frac{1 + \nu_s}{1 - \nu_s} \right) \int_0^r \frac{q(r) p(r)}{\rho} d\rho dr$$

$$+ \frac{4(1 - \nu_s^2)}{E_s} \int_0^r \frac{q(r) p(r)}{\rho} d\rho dr$$

$$+ \left( \frac{1 + \nu_s}{1 - \nu_s} \right) \int_0^r \frac{q(r) \rho}{\rho} d\rho dr,$$

(17)

where $J_1$ is the Bessel function of the first kind of $i$ th order, $k = \sqrt{4\rho/(r + \rho)^2}$, $K$ and $E$ are the complete elliptic integrals of the first and second kind. And the relationship between Bessel function and complete elliptic integrals has been used:

$$\int_0^r \frac{J_1(r') \rho J_1(r') d\rho dr}{\rho} = \frac{2}{\pi} \frac{K(k)}{r + \rho},$$

(18)

$$\int_0^\infty \frac{J_1(r') \rho J_1(r') d\rho dr}{\rho} = \frac{2}{2\pi} \frac{K(k)}{r + \rho}.$$

(19)
Eqs. (12), (13), (16) and (17) provide the expressions of radial and vertical displacements for both the plate and substrate. They are now ready for the use of interfacial conditions.

In the damage free zone defined by \(0 < r < R - l_c - l_d\) where \(R\) is the plate radius and \(l_c\) the length of cohesive zone and \(l_d\) the length of debonding zone (refer to Fig. 3), the plate and semi-infinite substrate are perfectly bonded. Both vertical and radial displacements are continuous across the interface. The interfacial continuity is written as:

\[
w_p = w_s, \quad u_p = u_s. \quad (20a, b)
\]

Substituting Eqs. (12), (13), (16) and (17) into Eq. (20a,b) leads to two integral equations as follows

\[
\begin{align*}
\int_0^R F_p(r, \rho, R, h, E_s, E_p, v_p, v_p)g_p(\rho)\,d\rho + \int_0^R F_q(r, \rho, R, h, E_s, E_p, v_p, v_p)q(\rho)\,d\rho - L_0 &= f_c(t, r, h, E_p, v_p, \Omega, D), \\
\int_0^R G_p(r, \rho, E_s, v_t)p(\rho)\,d\rho + \int_0^R G_q(r, \rho, R, h, E_s, E_p, v_p, v_p)q(\rho)\,d\rho &= g_c(t, r, h, i, \Omega),
\end{align*}
\]

where the integral kernels \(F_p, G_p, F_q\) and \(G_q\) depend upon location, elastic properties of the plate and substrate, as well as radius of the plate, but do not depend upon charging/discharging time. \(f_c\) and \(g_c\) are items related to Li-ion concentration \(c\), depending upon location, the properties of the active plate, charging/discharging velocity, as well as charging/discharging time. For simplicity, the detailed expressions of these six variables are provided in Appendix B.

In the cohesive zone defined by \(R - l_c - l_d < r < R\), the stresses are continuous but the displacements are not due to cohesive opening/sliding separation. Therefore, the interface displacement condition is:

\[
w_p + \delta_n = w_s, \quad u_p + \delta_t = u_s. \quad (22a, b)
\]

By substituting Eqs. (12), (13), (16) and (17) into Eqs. (22a,b) and using the cohesive laws, Eqs. (5a,b), we have

\[
\begin{align*}
\int_0^R f_p(r, \rho, R, h, E_s, E_p, v_p, v_p)g_p(\rho)\,d\rho + \frac{2\Gamma}{3\sigma_{nc}} q(\rho) &= f_c(t, r, h, E_p, v_p, \Omega, i, \delta_n), \\
\int_0^R g_p(r, \rho, E_s, v_t)g_p(\rho)\,d\rho + \frac{2\Gamma}{\sigma_{nc}} q(\rho) &= g_c(t, r, h, i, \Omega) + \frac{2\Gamma}{3\sigma_{nc}},
\end{align*}
\]

where the relationship of the interfacial bonding strengths \(\sigma_{nc} = \sqrt{3\sigma_{nc}}\) has been assumed.

In the debonding zone defined by \(R - l_d < r < R\), the plate and substrate separate completely. The displacements are no longer continuous. For the stresses, if the crack is open, i.e. \(\delta_n > 0\), both normal and shear stresses are equal to zero. If the crack is closed, i.e. \(\delta_n = 0\), the normal stress is still continuous, and the shear stress is determined by friction. The boundary conditions are therefore written as:

\[
p(r) = 0, \quad q(r) = 0, \quad \text{if} \quad \delta_n > 0 \quad (24a, b)
\]

and

\[
q = \text{sgn}(\delta_t)\mu p, \quad w_s = w_p \quad \text{if} \quad \delta_n = 0, \quad (25a, b)
\]

where \(\mu\) is the friction coefficient of the interface. Substituting Eqs. (12), (13), (16) and (17) into Eq. (25b) leads to

\[
\begin{align*}
\int_0^R f_p(r, \rho, R, h, E_s, E_p, v_p, v_p)\bar{p}(\rho)\,d\rho + \mu \int_0^R f_q(r, \rho, R, h, E_s, E_p, v_p, v_p)\bar{q}(\rho)\,d\rho - L_0 &= f_c(t, r, h, E_p, v_p, \Omega, i, D), \quad \text{if} \quad \delta_n = 0, \quad (26)
\end{align*}
\]

Now we have obtained the governing equations given by Eqs. (14), (21a,b), (23a,b), (24a,b), (25a) and (26) for the unknown interfacial normal stress \(p\) and shear stress \(q\), as well as the integral constant \(L_0\).

To simplify the equations, normalization is employed as:

\[
\begin{align*}
\bar{r} &= r/R, \quad \bar{p} = p/R, \quad \bar{q} &= q/R, \quad \bar{\rho} = \rho/R, \quad \bar{h} = h/R, \quad \bar{\Omega} = \Omega/R, \quad \bar{L}_0 = L_0/R, \quad \bar{t} = t/R, \quad \bar{\rho} = \rho/R, \quad \bar{q} = q/R, \quad \bar{h} = h/R, \quad \bar{\Omega} = \Omega/R, \quad \bar{\mu} = \mu/R.
\end{align*}
\]

Applying the normalization to the governing equations, we have

\[
\begin{align*}
\int_0^1 f_p(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{p}(\bar{\rho})\,d\bar{\rho} + \int_0^1 f_q(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{q}(\bar{\rho})\,d\bar{\rho} &= f_c(\bar{r}, \bar{t}, E_p, v_p, \bar{\Omega}, i, D), \\
\int_0^1 g_p(\bar{r}, \bar{\rho}, E_s, v_t)\bar{p}(\bar{\rho})\,d\bar{\rho} + \int_0^1 g_q(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{q}(\bar{\rho})\,d\bar{\rho} &= g_c(\bar{r}, \bar{t}, h, i, \Omega) + \frac{1}{\sqrt{3R}}, \quad (27a, b)
\end{align*}
\]

for \(\bar{r}\) in damage free zone \(0 < \bar{r} < 1 - l_c - l_d\), and

\[
\begin{align*}
\int_0^1 f_p(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{p}(\bar{\rho})\,d\bar{\rho} + \int_0^1 f_q(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{q}(\bar{\rho})\,d\bar{\rho} &= f_c(\bar{r}, \bar{t}, \bar{R}, \bar{\bar{h}}, E_s, E_p, v_p, v_p)\bar{p}(\bar{\rho})\,d\bar{\rho} - \bar{L}_0 \\
- \bar{\bar{L}}_0 &= \bar{f}_c(\bar{r}, \bar{t}, \bar{R}, \bar{\bar{h}}), \\
\int_0^1 g_p(\bar{r}, \bar{\rho}, E_s, v_t)\bar{p}(\bar{\rho})\,d\bar{\rho} + \int_0^1 g_q(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{q}(\bar{\rho})\,d\bar{\rho} &= \frac{1}{3R}\bar{\bar{g}}(\bar{r}, \bar{t}) + \text{sgn}(\delta_n)\frac{1}{R}, \quad (28a, b)
\end{align*}
\]

for \(\bar{r}\) in cohesive zone \(1 - l_c - l_d < \bar{r} < 1 - l_c\), and

\[
\begin{align*}
\bar{q} &= \text{sgn}(\delta_t)\mu \bar{p}, \quad \text{if} \quad \delta_n > 0, \quad (29a, b)
\end{align*}
\]

\[
\begin{align*}
\bar{q} &= \text{sgn}(\delta_t)\mu \bar{p}, \quad \text{if} \quad \delta_n = 0, \quad (30a)
\end{align*}
\]

and

\[
\begin{align*}
\int_0^1 f_p(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{p}(\bar{\rho})\,d\bar{\rho} + \mu \int_0^1 f_q(\bar{r}, \bar{\rho}, \bar{R}, \bar{h}, E_s, E_p, v_p, v_p)\bar{q}(\bar{\rho})\,d\bar{\rho} - \bar{L}_0 &= \bar{f}_c(\bar{r}, \bar{t}, \bar{R}, \bar{h}), \quad \text{if} \quad \delta_n = 0, \quad (30b)
\end{align*}
\]

for \(\bar{r}\) in debonding zone \(1 - l_d < \bar{r} < 1\). And the global self-balance condition is

\[
\int_0^1 \bar{p}(\bar{\rho})\,d\bar{\rho} = 0. \quad (31)
\]
The explicit expressions for the coefficients in the dimensionless governing equations given above are listed in Appendix B.

From the dimensionless governing equations, one can figure out the key influence parameters which dominate the interface stresses and delamination. When the whole interface is damage-free where \( l_1 = l_2 = 0 \), the Eqs. (27a,b) and (31) govern the problems. It can be concluded that the interfacial stresses \( p \) and \( q \) at a given charging time \( t \) depend on five parameters, i.e. \( L/R = h/R \), \( E \), \( v_i \) and \( v_p \), and \( h = l_0 h \Omega /F \). If the material system is given, \( E \), \( v_i \) and \( v_p \) would be fixed. Therefore, there are only two influence parameters determining the stress distributions, i.e. \( h \) and \( l_0 h \Omega /F \).

Once the cohesive zone forms, according to Eqs. (28a,b), \( h \) and \( R \) are separated as two independent influence parameters. In addition, the cohesive strength \( \sigma_c \) is introduced to be among the influence parameters. Therefore, the interfacial stress and the growth of delamination depend upon seven parameters, i.e. \( h \), \( R \), \( l_0 \), \( \sigma_c \), \( E \), \( v_i \) and \( v_p \). If the materials are given, three parameters, i.e. \( h \), \( R \) and \( l_0 \), together govern the interfacial stresses and delamination process.

It can be found from the dimensionless governing Eqs. (27a)–(31) that the interfacial stresses are linear functions of dimensionless parameter \( l = l_0 h \Omega /F \). In the expression, \( l_0 h \Omega /F \) is the velocity ratio of charging to diffusion describing the Li-ion concentration gradient on the charging boundary. Taking \( h \) into account, \( l_0 h \Omega /F \) represents the concentration inhomogeneity along plate thickness. And \( \Omega \) is the partial molar volume representing the volume expansion induced by Li-ion intercalation. Therefore, \( l = l_0 h \Omega /F \) describes the diffusion induced deformation inhomogeneity along plate thickness. It is a very important parameter which describes how the charging/discharging velocity, characteristic dimension of system and material properties influence the diffusion induced deformation inhomogeneity in a combined way. A similar dimensionless parameter has been emphasized by Cheng and Verbrugge (2009) for the diffusion induced stress in a spherical particle. It has to be mentioned that the dimensionless parameter \( l = l_0 h \Omega /F \) is relevant only to the constant current charging condition examined here. For more general cases where lithiation and delithiation involve the interfacial (electrochemical) kinetics the electrochemical Biot number introduced by Cheng and Verbrugge (2010) will play a role in the problem.

The linear governing Eqs. (27a)–(31) were obtained based upon the triangular cohesive law, which is the mathematically simplest among cohesive laws that describe the descending behavior of traction-displacement relation for interface decohesion. The approach developed could be incorporated with other types of cohesive relations such as further simpler Dugdale–Barenblatt rectangular cohesive law or more complicated nonlinear exponential law. The rectangular cohesive law is expected to be more relevant to the strong interface with ductile substrate. However, it is believed that the use of different cohesive laws may only influence the stress distribution in the cohesive zone, and would predict the similar delamination behavior as long as the fracture energy and strength are the same.

In order to obtain the final solutions of interfacial stresses \( p(r) \) and \( q(r) \), numerical method is employed to solve the governing equations provided by Eqs. (27a)–(31). As shown in Fig. 6, the plate radius \( R \) is divided into \( \psi \) segments. Writing the dimensionless radius as \( \tilde{r} = \tilde{r}_i = (2i - 1)/2\psi \) which denotes the midpoint of the \( i \)th line segment, the interface is thereby partitioned into three zones: damage free zone \((1 \leq i \leq \phi)\), cohesive zone \((\phi + 1 \leq i \leq \xi)\) and deloboning zone \((\xi + 1 \leq i \leq \psi)\).

And then, the dimensionless governing Eqs. (27a)–(31) are discretized into system of linear equations as follows (see details in Appendix C):

\[
\begin{align*}
\sum_{j=1}^{\psi} \mathbf{p}_i (\tilde{r}_j, \tilde{r}_j) & \mathbf{p}(\tilde{r}) + \mathbf{F}_j (\tilde{r}_j, \tilde{r}_j) \mathbf{q}(\tilde{r}) - \bar{L}_0 = i \bar{f}_c (\tilde{r}_i, \tilde{r}) & \text{for } 1 \leq i \leq \phi, \\
\sum_{j=1}^{\psi} \mathbf{G}_i (\tilde{r}_j, \tilde{r}_j) & \mathbf{p}(\tilde{r}) + \mathbf{q}_j (\tilde{r}_j, \tilde{r}_j) \mathbf{q}(\tilde{r}) - \bar{G}_c (\tilde{r}_i, \tilde{r}) = 0 & \text{for } \phi + 1 \leq i \leq \xi, \\
\mathbf{p}(\tilde{r}) &= \mathbf{q}(\tilde{r}) = 0, & \text{if } \delta_n > 0, \text{ for } \xi + 1 \leq i \leq \psi.
\end{align*}
\]

If \( \delta_n = 0 \), \( \mathbf{q}(\tilde{r}) = \text{sgn}(\delta_n) \mu \mathbf{p}(\tilde{r}) \) and \( \mathbf{p}(\tilde{r}) \) at discrete point \( \tilde{r} \) at \( i \leq \psi \) can be obtained by solving the 2 \( \psi \) + 1 linear algebraic equations provided by Eqs. (32a)–(36).

For a given charging/discharging time, repeatedly solving the Eqs. (32a)–(36) is required in order to determine the lengths of the cohesive zone and debonding zone, \( l_1 \) and \( l_2 \). In the first iteration, initial trial values of segment number \( \phi \) and \( \xi \) are assumed, and the interfacial stresses \( p(\tilde{r}) \) and \( q(\tilde{r}) \) are evaluated by solving the system of linear Eqs. (32a)–(36). If the interfacial stress is larger than cohesive strength, corresponding segments fall into the cohesive zone. And if the interface separation is beyond the maximum cohesive opening/sliding displacement, corresponding segments fall into the debonding zone. Accordingly, the number \( \phi \) and \( \xi \) are adjusted and the second iteration starts. The iteration will stop when no more segments become the cohesive zone and debonding zone, in other words, the segment number \( \phi \) and \( \xi \) no longer change.

The plots of delammiantion length against time in Fig. 7 illustrate the numerical convergence with the number of line segments \( \psi \) and the difference between curves with \( \psi > 100 \) is invisible. In the succeeding section to obtain the results in order to ensure the convergence and high accuracy.

The only assumption of the present semi-analytical solution is the thin plate theory which is known to be accurate enough for the plates with the diameter-to-thickness ratio \( 2R/h > 5 \). Given
the numerical scheme used above is accurate enough, the present solution is believed to be very accurate. For thicker active layers where the present semi-analytical solution is not valid, one could use the finite element method coupled with cohesive model to solve the problem.

4. Results and discussion

4.1. Evolutions of cohesive zone and debonding zone

Firstly, let us examine the progressive delamination of the interface induced by lithiation/delithiation. As discussed in preceding section, the delamination process is governed by three parameters, i.e. \( h, R \) and \( i \), for a given material system where debonding strength \( \sigma_u = 2 \times 10^{-4} \), the elastic modulus ratio \( E = 0.2 \), Poisson ratios \( \nu_h = \nu_p = 0.3 \). Moreover, the friction coefficient \( \mu = 0 \) is assumed. Therefore, the delamination will be discussed with respect to the variations of \( h, R \) and \( i \).

Fig. 8 illustrates the evolutions of cohesive zone and debonding zone with respect to charging time for different \( i \). In the figure, \( l_c \) represents the length of cohesive zone and \( l_d \) of debonding zone. It is seen that the cohesive zone nucleates very early and develops very easily. This is because the free edge is the stress concentration site where very high interfacial stresses can be induced by small amount of intercalation of Li-ions, making the concentrated stress at the edge of interface beyond the cohesive bonding strength and causing the cohesive zone to nucleate and advance.

As lithiation continuously goes on, the cohesive zone advances from the circumferential edge towards the center and finally covers the whole interface. After that, there is a short time for the whole interface to be held at cohesive state. And then, once the elastic energy cannot be relaxed with cohesive separation, crack is induced from the edge of the plate. This makes part of area in the cohesive zone to be free crack surface, as shown in the figure with rising of \( l_d \) in response to the decrease of \( l_c \).

In Fig. 8, it is found that cohesive zone extends forward in an accelerating manner while debonding zone advances in a slowing down manner. For the former, creation of new cohesive zone is to reduce the expansion mismatch by providing larger interfacial displacements to have the elastic energy relaxed. As cohesive zone expands from the circumferential edge towards the center, because the circumference is larger in the outer region, \( l_c \) must increase in an accelerating way to induce same area of new cohesive zone in unit time. And for the debonding zone, the advancing speed is determined by energy release rate which depends on the size of remaining interface. Therefore, \( l_d \) increases in a slowing down manner because the remaining interface is smaller and smaller.

Fig. 8 also shows the effects of parameter \( i \) on damage evolution. It is found that smaller \( i \) leads to slower damage initiation and smaller crack speed, indicating the smaller \( i \) is preferred in application of real batteries. As discussed before, \( i = \frac{h \Omega}{FD} \) represents the lithiation induced expansion inhomogeneity along plate thickness \( h \). Reduction of \( i \) can be realized by reducing the surface current density \( i_0 \) and partial molar volume \( \Omega \). The former explains why fast charging is not preferred in real applications, e.g. charging to our mobile phones. And the second tells why graphite whose lithiation induced volume variation is only 1/30 of that of silicon is more mechanically stable in batteries.

Fig. 9 illustrates the evolution of cohesive zone and debonding zone with respect to dimensionless charging time \( t \) for different plate thickness. In the figure, the dimensionless radius \( R \) and parameter \( i \) are kept constant while the plate thickness \( h \) varies. Although the varying \( h \) is involved in both \( i = \frac{i_0 h \Omega}{FD} \) and \( \dot{t} = \frac{dt}{h^2} \), the product of \( \dot{t} = \frac{i_0 h \Omega}{FD} \) represents the dimensionless average Li-ion concentration in the active plate. Therefore, the time coordinate can be regarded as the scale of average concentration.
In Fig. 9, the accelerating propagation of cohesive zone and slowing down advancing of debonding zone are again illustrated. Besides these, it is found that damages including cohesive failure and debonding occur later in the plates with smaller \( R \). It means that reducing \( h \) could help the plates to store more Li-ion in unit volume before damage initiates. This modification can be realized in two ways according to the expression of \( h = h_0 \sigma_c / 2 \Gamma \). The first one is reducing the plate thickness \( h \). This operation reduces the radial repulsion force in plate, and thereby reduces the interfacial shear stress. And the second way is to promote the interface fracture energy \( \Gamma \) by improving the bonding quality.

It is also found that varying \( h \) impacts more remarkably on the development of cohesive failure but less significant on debonding. This is because formation of same area of debonding zone releases much more energy. The evolution of \( t_h \) is thus less affected.

Fig. 10 illustrates the influence of plate radius on the evolution of cohesive zone and debonding zone. The most significant finding in this figure is that there exists a length limit of cohesive zone. If the plate radius is smaller than the length limit, debonding would evolve quite gently. However, once the plate radius is larger than the length limit, the first debonding will be very violent, in a suddenly jumping way.

For illustration, plates with four radii are simulated in Fig. 10. Among them, \( R = 10 \) and 25 are the cases where the plate radius is smaller than the said length limit. Evolutions of cohesive zone and debonding zone in these two plates are quite similar as those studied in previous cases. Firstly, cohesive zone initiates and covers whole interface. And then, part of interface in the cohesive zone cracks into free surface, leading gradual growth of debonding zone. However, in the case of \( R = 100 \), the length of cohesive zone stops at about \( L_\sigma_c/2 \Gamma = 57 \) although the dimensionless radius of the plate is 100. And, right after this moment, both cohesive zone and debonding zone extend forward very quick by the length of \( L_\sigma_c/2 \Gamma = 43 \) and the damage free zone is eliminated. This is probably because a high elastic energy in the large disk has built up just before delamination initiation, once the debonding starts a long delamination length is required to relax the high elastic energy in a unit time. It can be seen in the figure that \( t_h \) rises up in a nearly vertical manner for the plate with radius \( R = 100 \) at crack initiation. Therefore, Fig. 10 tells that the active plate must be prepared very small in radius to avoid abrupt destruction.

It is seen from Fig. 10 that the time to delamination initiation is significantly postponed as the radius \( R \) gets smaller. This suggests that a critical radius seems to exist for the island thin film electrode in which delamination does not occur any more. We run the model with a Si disk with thickness \( h = 100 \) nm on Cu substrate to search for the possible critical size. The material mechanical parameters are adopted as: \( E_s = 200 \) GPa, \( E_p = 40 \) GPa (Haftbaradaran et al., 2012), \( v_s = v_p = 0.3 \), \( \sigma_{\text{crit}} = 40 \) MPa (Xiao et al., 2011), \( \sigma_{\text{crit}} = 3 \sigma_{\text{crit}} \), \( \Gamma = 1 \sim 3 \) J/m² (Bhandakkar and Gao, 2010; Haftbaradaran et al., 2012; Yan et al., 2011; Yang, 2011). The partial molar volume is chosen as \( \Omega = 2 \times 10^{-3} \) m³/mol (Bhandakkar and Gao, 2010). The diffusivity of Li-ion in Si varies in a wide range (Johari et al., 2011; Balke et al., 2010) depending on both concentration and matrix crystallography. Due to the fact that Si is amorphous in most of the time during lithiation, \( D = 2 \times 10^{-14} \) m²/s is employed. The numerical results from our model show there exists indeed a critical size for such 100 nm Si thin film electrode, equal to 0.2–0.6 \( \mu m \) for \( \Gamma = 1 \sim 3 \) J/m². This predicted critical size is one order of magnitude smaller than the island size of the Si patterns which remain on the substrate after charging/discharging cycles (Xiao et al., 2011). The discrepancy is believed because the present model ignores plasticity and stress-assisted diffusion in electrodes, which have been shown to have significant influence on the diffusion induced stress and to bring the DIS down (Bower et al., 2011; Zhao et al., 2011; Cui et al., 2012; Gao et al., 2013). Hence the present work can be used as a conservative estimate for delamination.

Fig. 11 illustrates delamination maps in \( l \sim R \) plane and \( l \sim h \) plane, which show the damage-free plus cohesive region and the cohesive plus debonding region at the time moment \( t = 1000 \). The vertical dash line shows the boundary where the thin plate...
theory is valid. The horizontal dash line is the charge limit when the ionic concentration at surface reaches the stoichiometric limit of Li$_{4.4}$Si under galvanostatic charging operation. The damage-free region is not included in the maps since it is invisibly small. This is consistent with the Fig. 8 where the very early initiation for cohesive damage was observed due to high stress concentration near the free edge. In the figure the boundary separating the damage-free plus cohesive region and the cohesive plus debonding region indicates that charging velocity has to be brought down for a thicker and wider active plate in order to avoid delamination. Furthermore, the maps tell that it is possible to select appropriately thickness and radius of active plate, and charging velocity to avoid delamination during a given charging duration.

4.2. Evolutions of interfacial stresses and separation displacements

In this section, in order to provide supplementary evidences for the evolutions of progressive delamination and also to provide the insights of interface stress distribution, evolutions of the interfacial stresses and displacements will be examined. According to previous discussions, there are three stages in lithiation/delithiation: (1) the whole interface is damage free; (2) damage free zone and cohesive zone coexist; and (3) cohesive zone and debonding zone coexist. The interfacial stresses in these three stages will be investigated separately.

Fig. 12 provides the stress profile in damage free stage with different aspect ratio $R/h$. Because the stresses in the inner region denoted by $t < 0.8$ are nearly zero, only the stresses in the outer region are plotted. The negative value of $i$ means a delithiation process in which the active plate contracts in radial direction and bends concavely as shown in Fig. 3a. Therefore, in Fig. 12, the shear stresses are all positive and the normal stresses are tensile at the edge but compressive in the region inwards. It is found that all stresses are very high near the edge. Therefore, damage would initiate from the edge towards the plate center in lithiation/delithiation.

As discussed before, $R/h$ and $i$ are the two governing parameters in damage free stage. Fig. 12 illustrates the impacts of the former. Comparing the two plates with different ratio $R/h$, the stresses are distributed more uniformly in the plate with smaller ratio.

Fig. 13 illustrates the impacts of the dimensionless parameter $i$ on the stresses. In the figure, both lithiation and delithiation are investigated. Because both operations start from stress free state, the stresses obtained are symmetric for lithiation and delithiation. This figure shows that larger dimensionless parameter $i$ induces larger stress concentration. Therefore, charging at a moderate speed is preferable.

The damage free stage is very short in the whole charging duration. The next two stages are more important. As discussed before, once damage initiates, the stresses and displacements are controlled by $h$, $R$ and $i$. Therefore, the evolutions of interfacial stresses in stages 2 and 3 will be discussed according to these three parameters.

Fig. 14 provides the profiles of the interfacial stresses at a moment when damage free zone and cohesive zone coexist. The shear stress is almost zero in the region away from the edge. As the position moving outwards, the shear stress rises up quickly in front of the cohesive zone. When the stress reaches the cohesive strength which could also be considered as the yielding stress, the region falls into cohesive zone and the stress starts to decrease with the interfacial separation as governed by the cohesive law. And as the position moving outwards from center, the normal stress is compressive. Across the boundary between damage-free zone and cohesive zone the interfacial compressive normal stress will jump down because the gradient of shear stress is discontinuous. Once entering the shear cohesive zone, the compressive normal stress starts to decrease and finally changes to tensile and reaches the normal cohesive strength.
This figure proofs that the distribution of cohesive zone that the interfacial delamination is dominated by shear stress because the length of shear cohesive zone is much larger than that of normal cohesive zone. Secondly, this figure again reveals the impacts of dimensionless plate thickness \( \frac{i}{h} \) that reducing \( \frac{i}{h} \) could help to improve the stability of the electrode during lithiation/delithiation, as has been presented in Fig. 9. It can be seen in Fig. 14 that the length of cohesive zone \( l_c \) is much smaller in the plate with smaller \( \frac{i}{h} \) at the same charging time.

Fig. 15 illustrates the impact of plate radius \( R \) when damage free zone and cohesive zone coexist. In order to compare the lengths of \( l_c \) in plates with different radius \( R \), two horizontal coordinate axes are employed. The two axes start both from the right edge and extend inwards. The figure shows that the radius has very limited impacts on the distributions of stresses and cohesive zones at the present stage. It seems that the stresses depend only on how far the point is away from the edge, but not depend on how large the plate is. The reason may be attributed to the formation of cohesive zone which alternates the profile of local shear stress to a quite simple form determined by cohesive relation. Therefore, it can be explained in Fig. 10 that \( l_c \) grows along almost the same routine for plates with different radius.

Fig. 16 shows the impacts of different dimensionless parameter \( i \) in this stage. This figure illustrates that larger dimensionless parameter \( i \) is not preferred because it leads to much faster growth of cohesive zone. This figure can be used as supplementary proof of Fig. 8.

Fig. 17(a) illustrates the interfacial stresses when cohesive zone and debonding zone coexist. And Fig. 17(b) is provided to distinguish the debonding zone. In Fig. 17(b), the horizontally aligned dotted line represents the maximum interfacial sliding displacement allowed by the cohesive law. The debonding zone is therefore the region where the interfacial sliding displacements are beyond the value given by the line.

In debonding zone, both shear and normal stresses vanish. And in the cohesive zone which is from the very center to crack tip, the shear stresses decrease from the cohesive shear strength to zero and the normal stresses are tensile at the crack tip but compressive in the inner region. Because the interfacial opening displacements are all almost zero, it can be concluded that the delamination is induced completely by shear stress.

Fig. 17(a) also shows the impacts of dimensionless plate thickness \( h \). Because the product of dimensionless parameter \( i \) and charging time \( t \) is equal to \( i, \Omega t/h \) which is just the dimensionless average concentration independent on \( h \), the stresses corresponding to different \( h \) are discussed under the condition that the average Li-ion concentration is the same. According to the figure, it is found that reducing \( h \) could promote the length of uncracked zone. This is in consistent with the discussions for Fig. 9.
5. Conclusions

In this paper, a semi-analytical method based on cohesive model has been developed to investigate the progressive growth of interface delamination in a thin film electrode driven by Li-ion diffusion. The solution of the active layer was obtained with employing elastic thin plate theory. And the substrate was solved by considering it as an infinitely large body. The delamination of the interface between the active layer and substrate was described using cohesive model. And analytical governing equations were obtained by combining the plate and substrate using interface conditions. At last, the solutions were obtained by numerically solving the governing equations.

It is found that there are seven dimensionless variables governing the progressive delamination process of the interface. They are the plate thickness $h$, plate radius $R$, the elastic modulus ratio $E$, the Poisson’s ratio of $v_i$ and $v_p$, the cohesive strength $\sigma_c$ and the lithiation induced deformation inhomogeneity $i$. If materials are given, the seven governing parameters can be reduced to three, i.e. $h$, $R$ and $i$. When the interface is damage free, the interfacial stresses are determined by the aspect ratio $R/h$ and the parameter $i$.

During damage, it is found that the cohesive zone moves forward in acceleration and the debonding zone propagates in a slowing down manner. Reducing the dimensionless plate thickness $h$ down to be smaller than 1 could postpone the interfacial delamination and improve the electrode stability. This operation can be realized by reducing the plate thickness $h$ and strengthening the interface bonding. The dimensionless radius $R$ is found to have great impacts on the propagating speed of debonding zone at the beginning of cracking. Plates with smaller $R$ exhibits smaller debonding speed. And if $R$ is very large, the delamination would occur in a suddenly jumping way. Therefore, plates with smaller radius are more preferred in real batteries. And in all cases, increasing $i$ would result in negative effects, such as larger stresses and faster damages. Therefore, high rate charging is not preferred in the real operations of Li-ion batteries.

Plastic deformation and stress-assisted diffusion have been neglected in the developed model. Both have been shown to have a great influence on the DIS in Si electrodes. The model is not applicable to Si electrodes for quantitative prediction of delamination, and can be considered only as a very conservative estimate. In addition, neglecting the diffusion from edge causes inaccurate ionic concentration distribution near edge. Our ongoing analysis considering two-dimensional diffusion indicates the error for delamination growth is around 10%, and the detail will be reported elsewhere.

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Appendix A. Force and moment resultants in plates

In analogy to the thermo-elastic plate problem, the force and moment resultants in the plate can be expressed as follows:

$$N_r = \frac{12i}{h^2} \left( \frac{du_p}{dr} + \frac{v_p}{r} \frac{dp}{dr} \right) - \frac{N_c}{1 - v_p},$$  

(A.1)
\[ N_p = \frac{12I}{h^2} \left( \frac{u_p}{r} + \frac{u_p}{\tau} \right) - \frac{N_c}{1 - v_p}, \]  
(\text{A.2})

\[ M_r = - \left( \frac{d^2w_p}{dr^2} + \frac{u_p}{r} \frac{dw_p}{dr} \right) - \frac{M_c}{1 - v_p}, \]  
(\text{A.3})

\[ M_\theta = - \left( \frac{u_p}{r} \frac{d^2w_p}{dr^2} + \frac{1}{r} \frac{dw_p}{dr} \right) - \frac{M_c}{1 - v_p}, \]  
(\text{A.4})

\[ Q = - \frac{d}{dr}(\nabla^2 w_p) = \frac{h^2\rho(r)}{8R^2 (r^2 + \lambda^2 \rho^2)} \left( \frac{1}{2} \rho^2 - \rho^2 + 2 \rho^2 \ln(\rho^2) \right) \]  
(\text{A.5})

where \( N_c \) and \( M_c \) are the concentration induced force and moment resultants which are given by

\[ N_c = \frac{E_p \Omega_p}{3} \frac{h^2}{2} c(z) dz = \frac{E_p \Omega_p}{3} \frac{h^2}{2} c(z) dz, \quad M_c = \frac{E_p \Omega_p}{3} \frac{h^2}{2} c(z) dz, \]  
(\text{A.6})

**Appendix B. Coefficient functions in the governing equations**

\[ F_p(r, \rho, h, E_p, \nu_p, \nu_p) = - \frac{4(1 - \nu_p^2)}{E_p} \left[ \frac{K(k)}{\pi(r + \rho)} \right] \frac{\rho^2}{8R^2} \left[ \frac{1}{2} \rho^2 + 2 \rho^2 \ln(\rho^2) \right] \]  
(\text{B.1})

\[ F_\theta(r, \rho, h, E_p, \nu_p, \nu_p) = \frac{h^2 \rho}{8R^2} (r^2 + \lambda^2 \rho^2) \]  
(\text{B.2})

\[ C_p(r, \rho, E_p, \nu_p) = \left\{ \begin{array}{ll} \frac{(1 + \nu_p)(1 - 2\nu_p)}{E_p} & 0 < \rho < r, \\
0 & r < \rho < R, \end{array} \right. \]  
(\text{B.3})

\[ C_\theta(r, \rho, h, E_p, \nu_p, \nu_p) = \frac{(1 - \nu_p^2)}{E_p} (r + \rho) \left[ 2E(k) - (2 - K)K(k) \right] \]  
(\text{B.4})

\[ f_c(r, t, h, E_p, \Omega, \nu_h, D) = - \frac{r^2 E_p \Omega}{6(1 - \nu_p)} \int_{h/2}^{h/2} c(z) dz = - \frac{i_\Omega \rho h}{FD} \frac{r^2 E_p}{6(1 - \nu_p^2)} \int_{h/2}^{h/2} c(z) dz, \]  
(\text{B.5})

\[ g_c(r, t, h, \Omega, \nu_h) = \frac{i_\Omega \rho h}{E h}, \]  
(\text{B.6})

where \( \lambda = (1 - \nu_p^2)/(1 + \nu_p) \), \( E_p = E h^3/12 \left( 1 - \nu_p^2 \right) \).

**Appendix C. Derivation of the system of linear equations in numerical solution**

Numerical integration of the integrals in Eqs. (27)–(31) is made by using the first integral mean value theorem. Take \( \int_0^1 F_p d\rho \) in the equations as an example:

\[ \int_0^1 F_p d\rho \approx \frac{F_p(\rho) + \rho F_p(\rho)}{2}, \]  
(\text{C.1})

where, \( \eta_j = (j - 1)/\psi, \quad F_p(\rho, \rho) = \int_0^1 F_p(\rho, \rho) d\rho \) is evaluated by using MATLAB numerical integration. The midpoint of each discrete segment has been used to approximately evaluate the stress. Accuracy of this scheme using numerical integration available in the commercial package is believed to be equivalent with the direct use of Trapezoidal’s rule. The error induced by this approximation would be minimized by employing as fine as possible discretization. By doing numerical integration for all integrals involved, Eqs. (27a,b) can be rewritten as follows in the discrete form:

\[ \sum_{j=1}^{\psi} F_p(\rho_j) + \sum_{j=1}^{\psi} F_q(\rho_j) = T_0 = \tilde{t} c, \]  
(\text{C.2})

\[ \sum_{j=1}^{\psi} C_p(\rho_j) + \sum_{j=1}^{\psi} C_q(\rho_j) = \tilde{g}, \]  
(\text{C.3})

Finally, the system of linear Eqs. (32a)–(36) can be obtained by carrying out the same numerical integration.
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