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# Stress induced by diffusion and local chemical reaction in spherical composition-gradient electrodes

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**Abstract** Composition-gradient electrodes with their excellent electrochemical performance and mechanical durability are superior to homogeneous ones. In this work, taking into account the local solid reaction and composition-gradient electrode, a generalized diffusion–deformation–reaction model with  $E$ ,  $D$ , and  $\Omega$ -dependent  $r$  under potentiostatic operation is developed. Then, some numerical simulations are performed to obtain the evolutions of concentration, radial stress, and tangential stress. The influences of Thiele number and reaction order on the concentration and stresses are also discussed. Finally, some comparisons between composition-gradient electrodes and homogeneous ones are made to show that the composition-gradient electrode is more helpful to improve the mechanical durability of Li-ion batteries than the homogeneous one.

## 1 Introduction

Lithium-ion batteries (LIBs) have attracted considerable interest due to their high energy density and long cycle lifetime [1–3]. During charging or discharging of LIBs, the lithium-ion diffusion/migration is usually accompanied by the chemical reaction, volume deformation of the electrode [4] and the stress generation, which is called diffusion-induced stress (DIS) [5]. Large deformation can lead to electrode cracks, fracture and even failure, which are the main reasons of a larger capacity loss of LIBs. Therefore, it is necessary to investigate the mechanisms of the lithium-ion concentration distribution and the spatiotemporal evolutions of the stress in the electrode to improve the capacity and cycle lifetime of lithium-ion batteries.

Prussin [5] first deduced the diffusion-induced stress by adopting a method similar to the thermal stress. Lee et al. found the analytical solution of diffusion-induced stress of a hollow cylinder [6] and a thin plate [7] under constant stress on the surface. Cheng and Verbrugge [8] gave analytical expressions for the evolution of stress and strain energy in a spherical electrode partially under the potentiostatic and galvanostatic operation. Subsequently, a crack initiation criterion was proposed to guide the development of electrode material for LIBs with enhanced mechanical durability [9]. Hao and Fang [10] considered the effects of surface/interface stress and developed a diffusion-induced stress model of core-shell spherical electrodes in lithium-ion batteries. Wang et al. [11] imitated the two-phase lithiation process of film and hollow core-shell electrodes to understand that the lithium-ion insertion or extraction leads to volume change and huge stress. Peng et al. [12] gave the stress analysis of a cylindrical composition-gradient electrode in the generalized plane strain condition. Zhang et al. [13] presented a theoretical model to discuss the effect of concentration-dependent elastic modulus on Li-ion

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diffusion and DIS in spherical composition-gradient electrodes. The diffusion-induced stress was considered in all these above-mentioned studies. However, the electrochemical reaction was not taken into account.

It is well known that the chemical reactions in Li-ion batteries can capture and alter the distribution of Li-ions in the electrode during charging or discharging. Yang [14] developed a diffusion–local solid reaction model to analyze the distribution of lithium-ion concentration. Zhang et al. [15] investigated the effect of reversible electrochemical reaction on lithium-ion diffusion and DIS in a cylindrical electrode of Li-ion batteries. Li et al. [16] proposed a mathematical model to discuss the effects of reversible reaction on Li-ion diffusion and DIS in a spherical composition-gradient electrode. Ji et al. [17] developed a new coupling model of the reversible electrochemical reaction, lithium diffusion and bending and revealed that the backward reaction can be ignored for potentiostatic charging. Suo and Yang [18] pointed out that diffusion and local chemical reaction had a vital influence on the expansion of the electrode. Although the chemical reaction was investigated in these works, the electrode material was regarded to be homogeneous, not a composition-gradient material, and the effect of stress on the diffusion–reaction was neglected for the sake of simplicity.

Recently, more and more composition-gradient electrodes have been reported due to their excellent electrochemical properties [19,20]. The objectives of this work are to investigate the diffusion-induced stresses with the local solid reaction and composition gradient in spherical electrode particles under potentiostatic operation. The present paper is organized as follows: first, a generalized diffusion–deformation–reaction model with diffusion coefficient  $D$ , elastic modulus  $E$  and partial molar volume  $\Omega$ -dependent radius under potentiostatic operation is developed. Then, some numerical calculations are carried out to discuss the evolutions of concentration, radial stress and tangential stress. In the meanwhile, the influences of the Thiele number and the reaction order on the concentration and stress are also investigated. Finally, some comparisons between composition-gradient electrodes and homogeneous ones are analyzed.

## 2 Model formulation

### 2.1 Mechanical equations

For simplicity, the electrode is assumed to be isotropic and the characteristic time for the deformation of the electrode is much smaller than that for the diffusion; thus, the equilibrium equation [21] describing the deformation of the electrode can be expressed as

$$\sigma_{ij,i} + f_j = 0, \quad (1)$$

where  $\sigma_{ij}$  are the components of the stress tensor,  $f_j$  is the components of body force and the comma represents the derivative with respect to the spatial variables.

Similar to the thermal stress, the stress–strain relationship [22] including diffusion is written as

$$\sigma_{ij} = \frac{E}{1+\nu} \varepsilon_{ij} + \frac{E\nu}{(1+\nu)(1-2\nu)} \varepsilon_{kk} \delta_{ij} - \frac{Ec\Omega}{3(1+\nu)} \delta_{ij}, \quad (2)$$

where  $\varepsilon_{ij}$  are the components of the strain tensor,  $\nu$  is the Poisson's ratio of the material,  $c$  is the concentration of lithium ions, and  $\delta_{ij}$  is the Kronecker symbol. In particular, Young's modulus  $E$  and the partial molar volume  $\Omega$  are regarded as a function of the spatial variable for the composition-gradient electrodes.

On the basis of the linear elasticity theory and small deformation hypothesis, the relationship of the strain tensor  $\varepsilon_{ij}$  and the displacement  $u_i$  is

$$\varepsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}). \quad (3)$$

Substituting Eqs. (2) and (3) into Eq. (1), the mechanical equilibrium equation can be rewritten as

$$(\lambda + G)u_{i,ji} + Gu_{j,ii} + \lambda_{,j}u_{i,i} + G_{,i}(u_{i,j} + u_{j,i}) - \frac{1}{3} [(3\lambda + 2G)\Omega c \delta_{ij}]_{,i} + f_j = 0, \quad (4)$$

where  $\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}$  and  $G = \frac{E}{2(1+\nu)}$ .

## 2.2 Diffusion–reaction equation

The chemical potential affected by the stress,  $\mu$ , in an ideal solid solution is [23]

$$\mu = \mu_0 + R_g \theta \ln c - \Omega \sigma^h, \quad (5)$$

where  $\mu_0$  is the chemical potential in a given standard state,  $R_g$  is the universal gas constant,  $\theta$  is the absolute temperature, and  $\sigma^h = \sigma_{ii}/3$  is the hydrostatic stress.

The relationship [24] between the chemical potential and the diffusion flux  $J_i$  is

$$J_i = -cM\mu_{,i} = -D \left[ c_{,i} - \frac{c}{R_g \theta} (\Omega \sigma^h)_{,i} \right], \quad (6)$$

where  $M$  is the mobility of Li-ions in the solid, and  $D = MR_g \theta$  is the diffusion coefficient of lithium in an unstressed state solid, which is supposed to be a function of the spatial variable for the composition-gradient electrodes.

Suppose that a local solid reaction in Li-ion batteries occurs as follows:



According to the results reported by Yang [14], the diffusion–reaction equation of lithium ions in the electrode is expressed as

$$\frac{\partial c}{\partial t} + J_{i,i} + kc^a = 0, \quad (8)$$

where  $a$ ,  $b$  and  $h$  are stoichiometric numbers of local solid reaction in lithium-ion batteries, and  $k$  is the chemical reaction rate coefficient.  $Li$ ,  $B$  and  $F$  are lithium ions, host atoms and reaction product, respectively.

According to Eqs. (6) and (8), one obtains

$$\frac{\partial c}{\partial t} = D_{,i} \left( c_{,i} - \frac{c}{R_g \theta} (\Omega \sigma^h)_{,i} \right) + D \left[ c_{,ii} - \frac{c_{,i}}{R_g \theta} (\Omega \sigma^h)_{,i} - \frac{c}{R_g \theta} (\Omega \sigma^h)_{,ii} \right] - kc^a. \quad (9)$$

## 2.3 Spherical composition-gradient electrode particle

As shown in Fig. 1, a spherical composition-gradient electrode particle is investigated. Due to the heterogeneous distribution of material compositions, elastic modulus, diffusion coefficient and partial molar volume of the spherical composition-gradient electrode material are supposed to be a linear function of  $r$  as in [12]

$$\begin{aligned} E &= (0.5 + r/r_0) E_0, \\ D &= (1.5 - r/r_0) D_0, \\ \Omega &= (1.2 - 0.4r/r_0) \Omega_0, \end{aligned} \quad (10)$$

where  $E_0$ ,  $D_0$  and  $\Omega_0$  are elastic modulus, diffusion coefficient and partial molar volume of the homogeneous electrode.

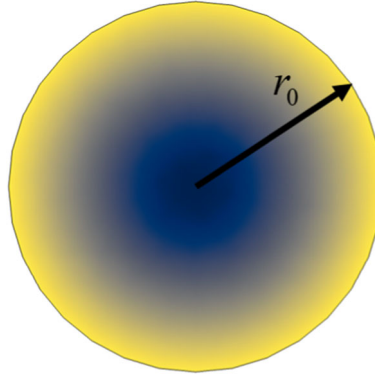
For the spherical electrode, Eq. (4) neglecting the body force will change to

$$(\lambda + 2G) \frac{\partial^2 u}{\partial r^2} + \left[ \frac{d}{dr} (\lambda + 2G) + \frac{2\lambda + 4G}{r} \right] \frac{\partial u}{\partial r} + \left( 2 \frac{d\lambda}{dr} - \frac{2\lambda + 4G}{r} \right) \frac{u}{r} = \frac{1}{3} \frac{\partial}{\partial r} [(3\lambda + 2G) \Omega c]. \quad (11)$$

Suppose the lithium-ion diffusion is along the radial direction. Equation (9) for the spherical composition-gradient electrode particle will reduce to

$$\frac{\partial c}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 D \frac{\partial c}{\partial r} - \frac{r^2 D c}{R_g \theta} \left( \frac{\partial \sigma^h}{\partial r} \Omega + \frac{d\Omega}{dr} \sigma^h \right) \right] - kc^a, \quad (12)$$

where  $\sigma^h = (\sigma_r + 2\sigma_\theta)/3$  is the hydrostatic stress.  $\sigma_r$  and  $\sigma_\theta$  are the radial stress and tangential stress, respectively.



**Fig. 1** Schematic of a spherical composition-gradient electrode particle

Suppose the initial concentration in the electrode to be zero. For the potentiostatic charging, the concentration at the surface of the electrode particle is  $c_0$ . Due to the symmetry of the spherical electrode, the displacement at the center of the particle is zero. In addition, the surface of the particle is assumed to be stress-free and the diffusion flux  $J$  is zero at the center of the spherical electrode. Thus, the initial and boundary conditions are written as

$$c|_{t=0} = 0, \quad (13)$$

$$u|_{r=0} = 0, \quad \sigma_r|_{r=r_0} = 0, \quad J|_{r=0} = 0, \quad c|_{r=r_0} = c_0. \quad (14)$$

For simplification, the following dimensionless variables are introduced:

$$C = \frac{c}{c_0}, \quad T = \frac{D_0 t}{r_0^2}, \quad R = \frac{r}{r_0}, \quad U = \frac{u}{r_0}, \quad \bar{\sigma}^h = \frac{\sigma^h}{E_0}, \quad \bar{\sigma}_r = \frac{\sigma_r}{E_0}, \quad \bar{D} = \frac{D}{D_0}, \quad \bar{E} = \frac{E}{E_0}, \quad \bar{\Omega} = \frac{\Omega}{\Omega_0}. \quad (15)$$

Combining Eqs. (11), (12), and (15), the dimensionless reaction–diffusion–deformation equations with  $E$ ,  $D$  and  $\Omega$ -dependent  $r$  can be obtained as follows:

$$\frac{\partial C}{\partial T} = \frac{1}{R^2} \frac{\partial}{\partial R} \left[ R^2 \bar{D} \frac{\partial C}{\partial R} - q R^2 \bar{D} C \left( \frac{\partial \bar{\sigma}^h}{\partial R} \bar{\Omega} + \frac{d\bar{\Omega}}{dR} \bar{\sigma}^h \right) \right] - K C^a, \quad (16)$$

$$\alpha \bar{E} \frac{\partial^2 U}{\partial R^2} + \alpha \left( \frac{d\bar{E}}{dR} + \frac{2\bar{E}}{R} \right) \frac{\partial U}{\partial R} + 2 \left( \beta \frac{d\bar{E}}{dR} - \frac{\alpha \bar{E}}{R} \right) \frac{U}{R} = \gamma \frac{\partial}{\partial R} (\bar{E} \bar{\Omega} C), \quad (17)$$

where  $q = \frac{\Omega_0 E_0}{R_g \theta}$ ,  $\alpha = \frac{1-\nu}{1+\nu}$ ,  $\beta = \frac{\nu}{1+\nu}$ ,  $\gamma = \frac{\Omega_0 c_0}{3}$ , and  $K = \frac{kr_0^2}{D_0} c_0^{a-1}$ , which is a dimensionless coefficient called as the Thiele number [25]. It is noted that the Thiele number  $K$  describes the characteristic of the diffusion/reaction dynamics and also includes the reaction order  $a$ . Larger  $K$  means quick chemical reaction and slow diffusion and vice versa.

In a similar way, the dimensionless initial and boundary conditions become:

$$C|_{T=0} = 0, \quad (18)$$

$$U|_{R=0} = 0, \quad \bar{\sigma}_r|_{R=1} = 0, \quad \left[ \frac{\partial C}{\partial R} - q C \frac{\partial}{\partial R} (\bar{\Omega} \bar{\sigma}^h) \right] \Big|_{R=0} = 0, \quad C|_{R=1} = 1. \quad (19)$$

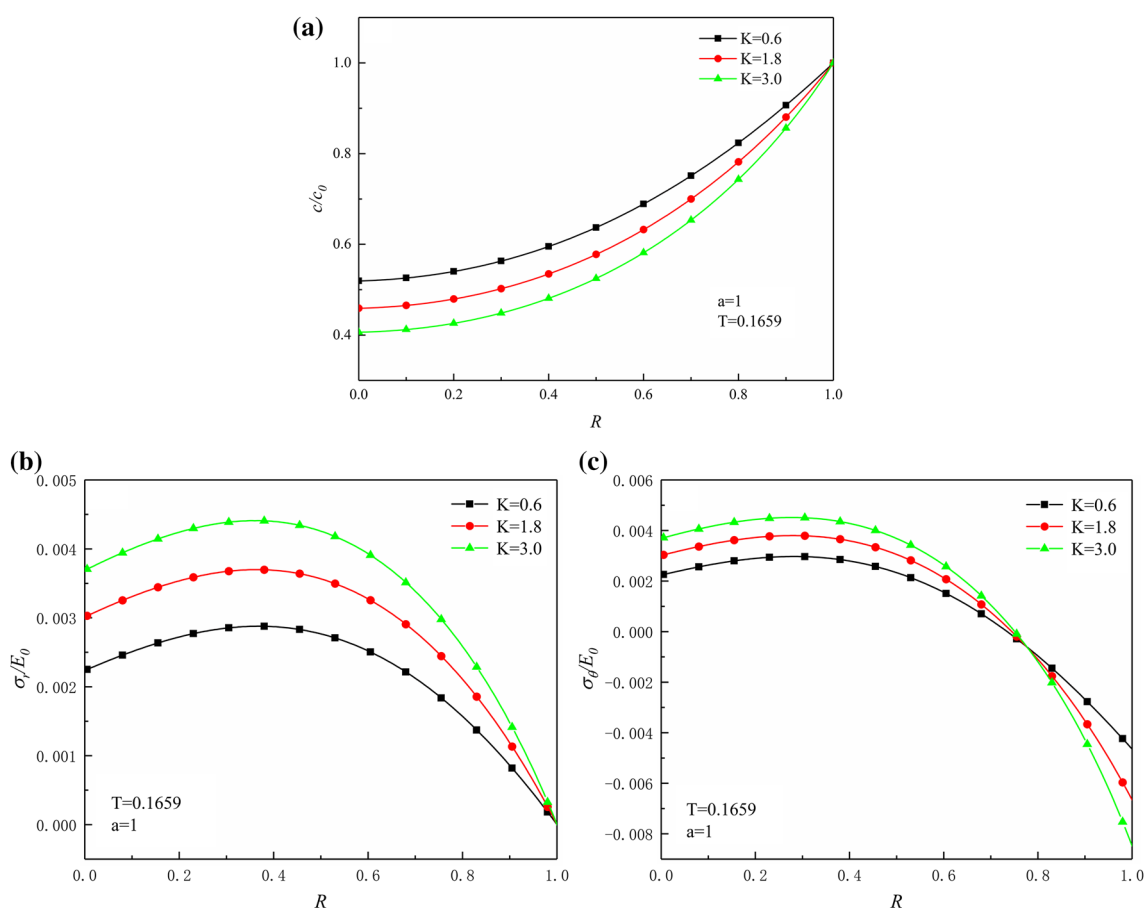
### 3 Numerical results and discussion

In order to discuss the evolutions of the concentration and stresses in the spherical gradient electrode particle, the electrode is assumed to be  $\text{Li}_{1.2}(\text{Mn}_{0.62}\text{Ni}_{0.38})_{0.8}\text{O}_2$  and the corresponding parameters used in the calculation are listed in Table 1. In the following, some numerical results will be given.

Figure 2 shows the spatial distribution of lithium-ion concentration and stresses in the spherical composition-gradient electrode particle during the process of potentiostatic charging for different Thiele numbers  $K$  at  $T = 0.1659$  and  $a = 1$ . It is seen from Fig. 2a that for all Thiele numbers  $K$ , the lithium-ion

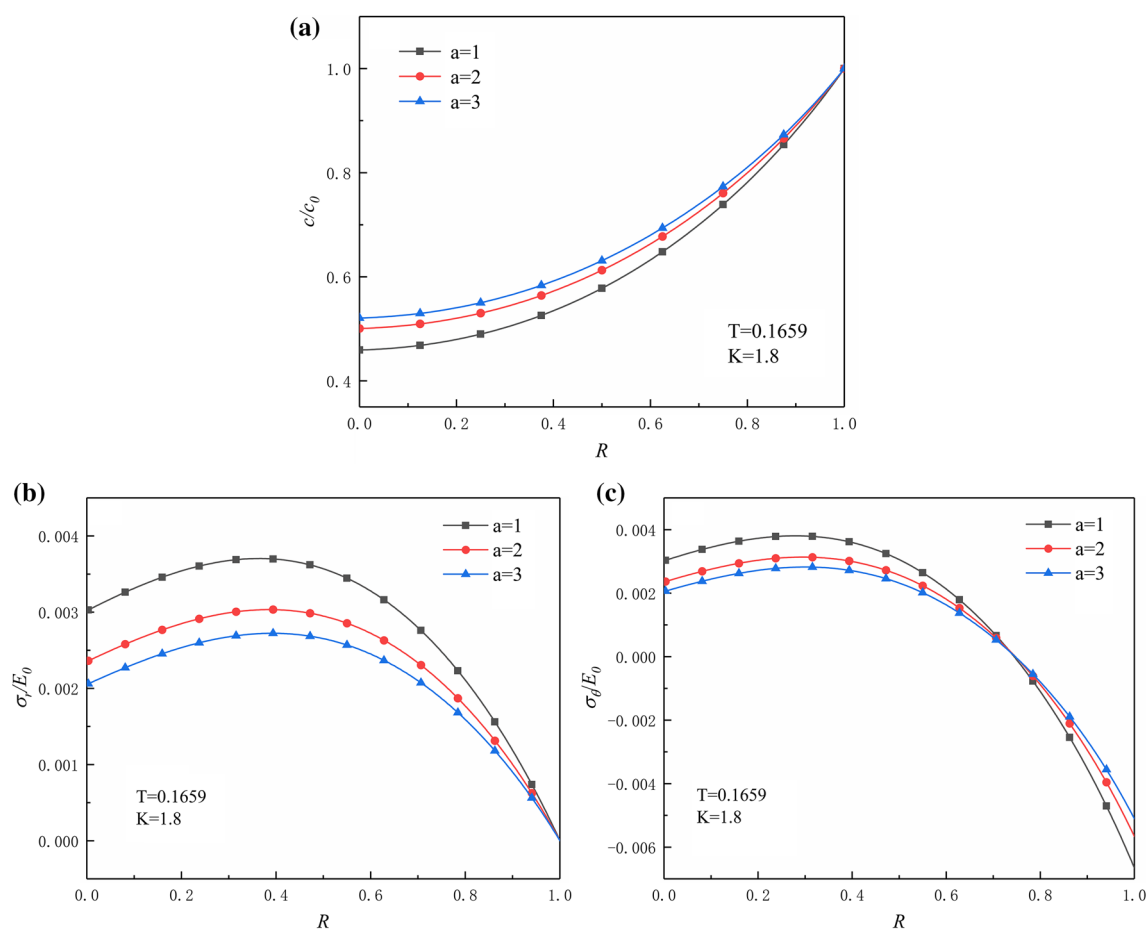
**Table 1** Parameters used in numerical simulation

| Parameter  | Value                       | Units                     |
|------------|-----------------------------|---------------------------|
| $E_0$      | 190 [12]                    | GPa                       |
| $\nu$      | 0.3 [12]                    | –                         |
| $\Omega_0$ | $3.497 \times 10^{-6}$ [12] | $\text{m}^3/\text{mol}$   |
| $D_0$      | $7.08 \times 10^{-15}$ [12] | $\text{m}^2/\text{s}$     |
| $c_0$      | $2.3 \times 10^4$ [12]      | $\text{mol}/\text{m}^3$   |
| $R_g$      | 8.314                       | $\text{J}/(\text{mol K})$ |
| $\theta$   | 293.15                      | K                         |

**Fig. 2** Spatial distributions of **a** Li-ion concentration, **b** radial stress, and **c** tangential stress for different Thiele numbers  $K$  at  $T = 0.1659$  and  $a = 1$ 

concentration gradually decreases as the distance from the surface increases. At a fixed spatial position and for the same diffusion–reaction time, the increasing Thiele number causes a decrease in lithium-ion concentration. This is because the larger Thiele number means that more lithium ions attend the chemical reaction according to Eq. (16), and thus, fewer lithium-ion concentrations diffuse into the electrode.

Figure 2b depicts the spatial distribution of radial stress under the potentiostatic operation for different Thiele numbers  $K$  at  $T = 0.1659$  and  $a = 1$ . It is found that the radial stress in the electrode, as expected, is tensile. With the decrease in the distance to the traction-free surface, the magnitude of radial stress increases first, reaches the maximum, and then decreases gradually. Such a trend is due to the linear increase in elastic modulus from the center to the surface, which is consistent with the results reported by [12,13]. For the same spatial position and the same diffusion–reaction time, a larger Thiele number  $K$  can cause an increase in the radial stress. Lithium ions diffuse from the surface to the center, which leads to a smaller concentration near the center than near the surface. Moreover, an inhomogeneous  $E(r)$  in Eq. (10) means that the elastic modulus



**Fig. 3** Spatial distributions of **a** Li-ion concentration, **b** radial stress, and **c** tangential stress for different chemical reaction orders  $a$  at  $T = 0.1659$  and  $K = 1.8$

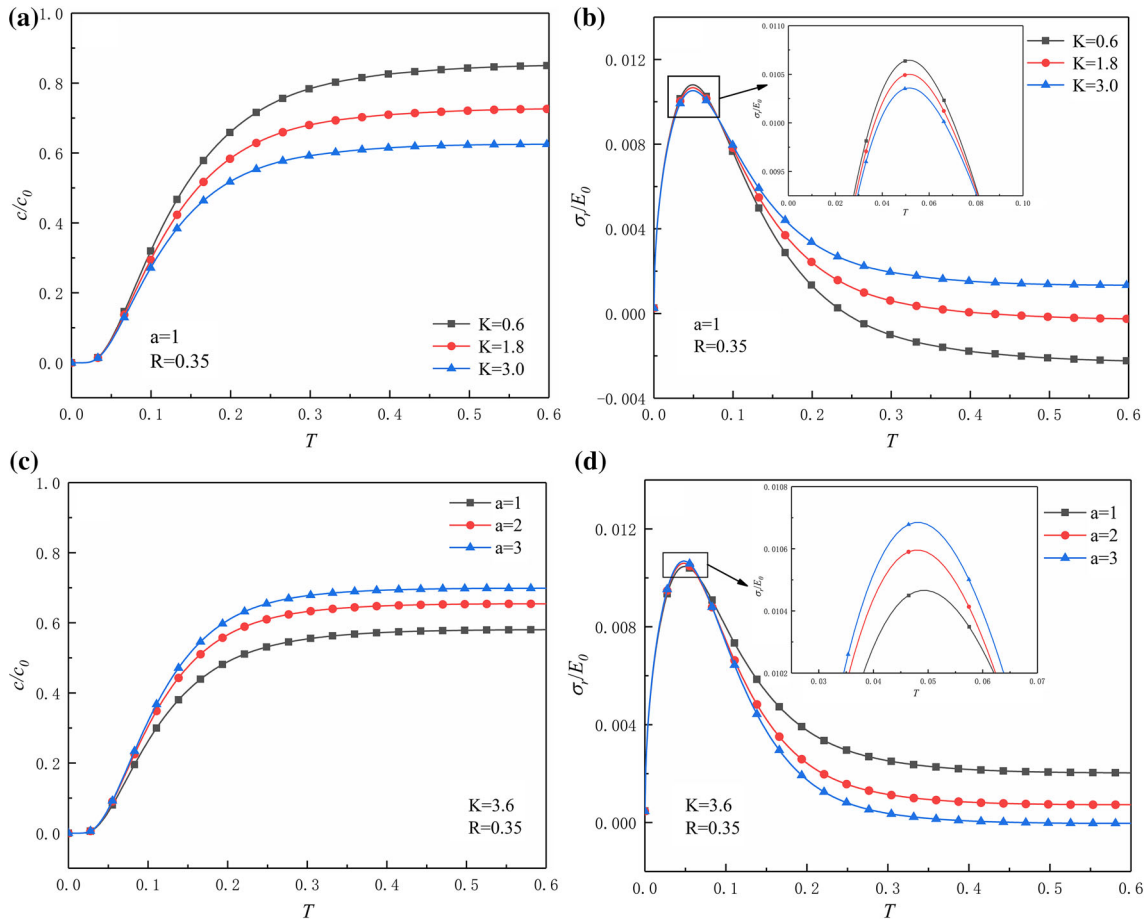
near the center is smaller than near the surface. Based on Eq. (2) and the above reasons, the stress near the center is larger than that near the surface.

The spatial distribution of tangential stress under potentiostatic charging for different Thiele numbers  $K$  is plotted in Fig. 2c. The stress is from tensile near the center to compressive at the surface for all Thiele numbers used in the calculation. The tangential stress also shows a trend of increasing first and then decreasing along the radial direction owing to the linear increase in elastic modulus from the center to the surface. At the same spatial position and the same dimensionless time, a larger Thiele number  $K$  causes a greater magnitude of tangential stress.

Figure 3 shows the spatial distribution of lithium-ion concentration, radial stress, and tangential stress in the spherical composition-gradient electrode particle during the potentiostatic charging for different chemical reaction orders  $a$  at  $T = 0.1659$  and for  $K = 1.8$ .

As seen from Fig. 3a, the lithium-ion concentration gradually decreases as the distance to the surface of the sphere increases. At the same spatial position and for the same reaction–diffusion time and the same  $K$ , the lithium concentration increases with increasing reaction order  $a$ , because the smaller reaction order  $a$  means more consumption of lithium in the local solid reaction and then leads to fewer lithium-ion concentration diffusion into the electrode.

Figure 3b illustrates the spatial distribution of radial stress for different chemical reaction orders  $a$ . The electrode is in the tensile state. It is found that the radial stress at the center increases initially and then decreases along the radial direction owing to the elastic modulus inhomogeneous distribution. At  $T = 0.1659$  and the same spatial position, the larger the reaction order, the smaller the radial stress, which shows that the reaction order has an influence on the radial stress of the electrode.



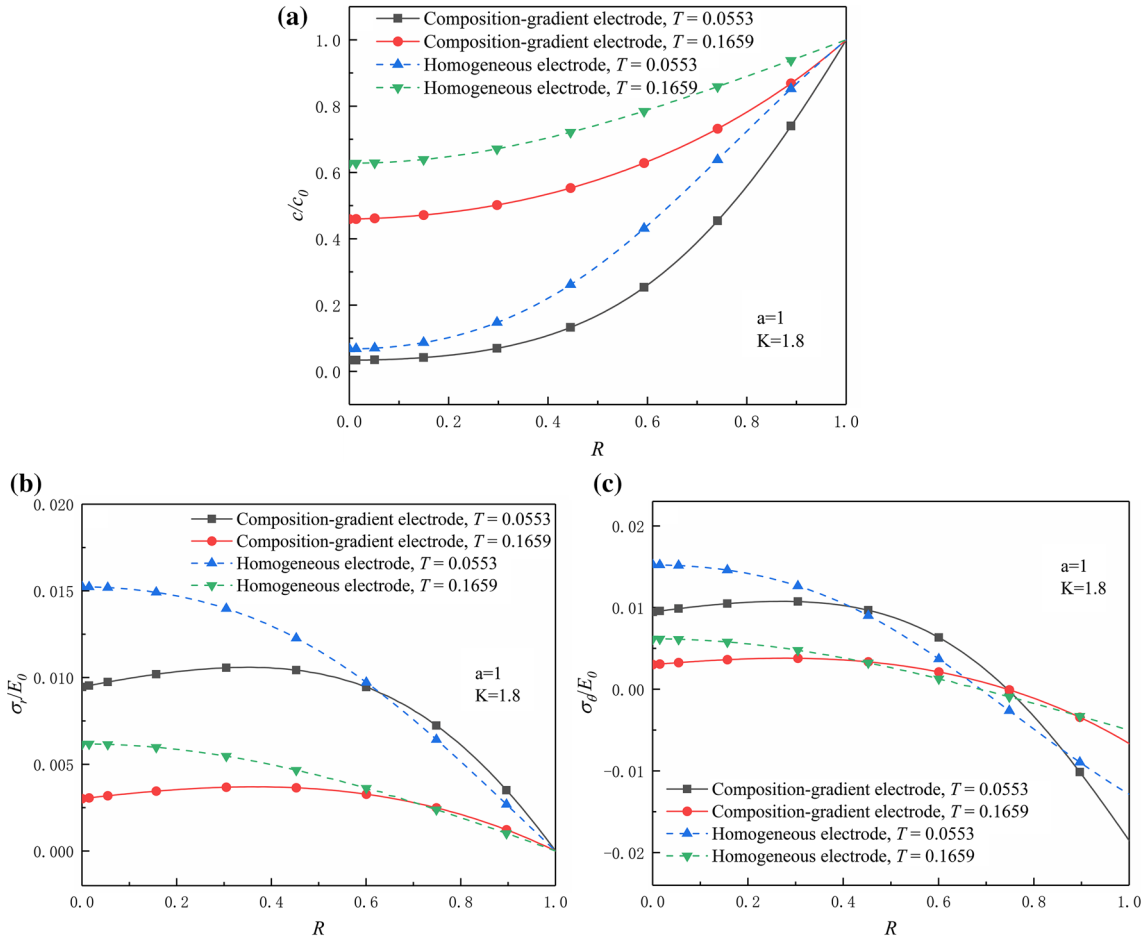
**Fig. 4** Temporal evolution of **a** Li-ion concentration and **b** radial stress for different Thiele numbers  $K$  at  $R = 0.35$  and  $a = 1$ ; temporal evolution of **c** Li-ion concentration and **d** radial stress for different chemical reaction orders  $a$  at  $R = 0.35$  and  $K = 3.6$

Figure 3c depicts the spatial distribution of tangential stress with different chemical reaction orders  $a$  at  $T = 0.1659$  and for  $K = 1.8$ . The tangential stress near the center lies in tension, while it becomes compressive at the surface. Moreover, the crossover from tensile to compressive occurs at about  $R = 0.75$ , and the maximum magnitude of tangential stress is at the surface. The tangential stress distribution has a similar variation trend as the radial stress. At the same spatial position and reaction–diffusion time, increasing the reaction order leads to fewer consumption of lithium and then causes a decrease in tangential stress.

It is well known that the initiation of cracks in an insertion electrode is related to the maximum radial tensile stress [26,27]. As seen from Figs. 2 and 3, the maximum radial stress occurs at about  $R = 0.35$ . Therefore, the temporal evolution of the lithium-ion concentration and the radial stress at  $R = 0.35$  are discussed in the following.

Figure 4a depicts the temporal evolutions of Li-ion concentration for different Thiele numbers  $K$  at  $R = 0.35$  and  $a = 1$ . For all Thiele numbers employed in this paper, the Li-ion concentration increases gradually as the dimensionless time elapses, and it will reach a steady state when the dimensionless time is long enough. In addition, the smaller the Thiele number, the higher the concentration at a certain dimensionless time.

The temporal evolutions of radial stress for different Thiele numbers  $K$  at  $R = 0.35$  and  $a = 1$  are plotted in Fig. 4b. When the diffusion–reaction time is shorter, the Thiele number  $K$  has little influence on the distribution of the radial stress. The radial stress will increase with increasing  $K$  for the longer diffusion–reaction times. For all Thiele numbers, the radial stress gradually increases up to the peak at  $T = 0.053$  and then decreases with increasing lithiation time. This evolution of the radial stress is similar to that in [18]. At the beginning of the lithiation, the radial stress is zero. With increasing diffusion–reaction time, the smaller concentration and relative larger deformation at  $R = 0.35$  cause the tensile radial stress to rise. When the time continues to



**Fig. 5** Comparisons of the spatial distributions of **a** Li-ion concentration, **b** radial stress, and **c** tangential stress in composition-gradient electrode and homogeneous one at  $T = 0.0533$  and  $T = 0.1659$  for  $a = 1$ ,  $K = 1.8$

increase, the concentration at  $R = 0.35$  will become larger and larger, while the deformation rate is smaller, which will result in the decrease in the radial stress, even change from positive to negative, and up to the steady for longer diffusion–reaction times.

Figure 4c describes the temporal evolutions of Li-ion concentration for different chemical reaction orders at  $R = 0.35$  and  $K = 3.6$ . For all the chemical reaction order used in this calculation, the lithium-ion concentration increases gradually with the dimensionless time and approaches the steady for the long enough time. For the same time, the increasing chemical reaction order causes an increase in lithium-ion concentration. The influence of chemical reaction order on the concentration is opposite to that of Thiele number.

Figure 4d exhibits the temporal evolutions of radial stress for different chemical reaction orders at  $R = 0.35$  and  $K = 3.6$ . For all the reaction order  $a$ , the radial stress increases first, reaches the maximum, and then decreases as the lithiation time goes on. Such trend is similar to that in Fig. 4b. For shorter diffusion–reaction times, the reaction order has little effect on the radial stress, which is also similar to the effect of Thiele number on it. However, the radial stress will decrease with the increase in the reaction order  $a$  for the longer diffusion–reaction times, which is opposite to the variation of the radial stress with Thiele number  $K$ .

The comparisons of the concentration, radial stress, and tangential stress in the composition-gradient electrode and homogeneous one at  $T = 0.0533$  and  $T = 0.1659$  for  $a = 1$ ,  $K = 1.8$  are made in Fig. 5. For the composition-gradient electrode, the diffusion coefficient  $D$ , elastic modulus  $E$  and partial molar volume  $\Omega$  are all the linear functions of  $r$  as shown in Eq. (10). For the homogeneous electrode,  $D$ ,  $E$  and  $\Omega$  are constant.

As seen from Fig. 5a, at the same spatial position and the same dimensionless time, the concentration in composition-gradient electrodes is lower than that in homogeneous electrodes, which is due to the smaller diffusion coefficient in composition-gradient electrode. In Figs. 5b, c, at the same dimensionless time, the



maximum radial stress and maximum tangential tensile stress in the composition-gradient electrodes are smaller than those in homogeneous electrodes, which coincides with the results of [12, 13]. These mean that the composition-gradient electrode is preferable to improve the mechanical durability of Li-ion batteries.

#### 4 Conclusions

In this work, taking into account the chemical reaction and gradient material, a generalized stress–diffusion–reaction coupling model is developed under potentiostatic operation. Then, some numerical calculations for a spherical electrode are simulated, and the results show that (1) the Thiele number  $K$  and the reaction order  $a$  have a significant influence on the distribution of the lithium-ion concentration for a longer lithiation time; (2) a smaller  $K$  and larger  $a$  contribute to improving the charge efficiency and reducing the maximum stresses in the gradient electrode; and (3) composition-gradient electrodes are preferable over homogeneous electrodes to improve the mechanical durability of Li-ion batteries.

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