

**BTP-1**

*Thesis submitted to the  
Indian Institute of Technology Kharagpur  
In partial fulfillment for the award of the degree*

*of*

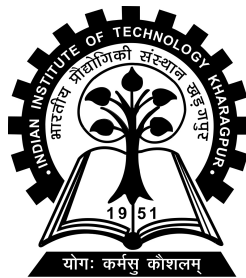
**Dual Degree (B.Tech + M.Tech)**

*by*

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Under the guidance of

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**MECHANICAL ENGINEERING**

**INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR**

**Autumn Semester, 2024-2025**

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# CERTIFICATE

This is to certify that the thesis entitled **BTP-1**, submitted by **Himanshu Sharma** to the Indian Institute of Technology Kharagpur, is a record of bona fide research work under my supervision and I consider it worthy of consideration for the award of the degree of **Dual Degree (B.Tech + M.Tech)** of the Institute.

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**Supervisor**

**Date:**

## DECLARATION

I certify that

- a. The work contained in the thesis is original and has been done by myself under the general supervision of my supervisor.
- b. The work has not been submitted to any other Institute for any degree or diploma.
- c. I have followed the guidelines provided by the Institute in writing the thesis.
- d. I have conformed to the norms and guidelines in the Ethical Code of Conduct of the Institute.
- e. Whenever I have used materials (data, theoretical analysis, and text) from other sources, I have given due credit to them by citing them in the text of the thesis and giving their details in the references.
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## ABSTRACT

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# Chapter 1

## Introduction

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# Chapter 2

## Problem Description

Consider a thin film of Silicon with height  $H$  and length  $L$ . All the loadings and geometry are considered to be independent of the third direction, hence the problem is formulated with plane strain assumption. There is an existing solid electrolyte interphase (SEI) layer on top of the Silicon film with a height of  $H_{\text{SEI}}$ . The origin is placed at the middle of bottom face of the Silicon film, as shown in figure 2.1. The bottom face of the Si thin film is considered to be rigidly fixed to a metallic substrate. The left and right faces are considered to have a roller type boundary condition for both Si and SEI. A uniform flux of Li-ions from the top surface of SEI is present.

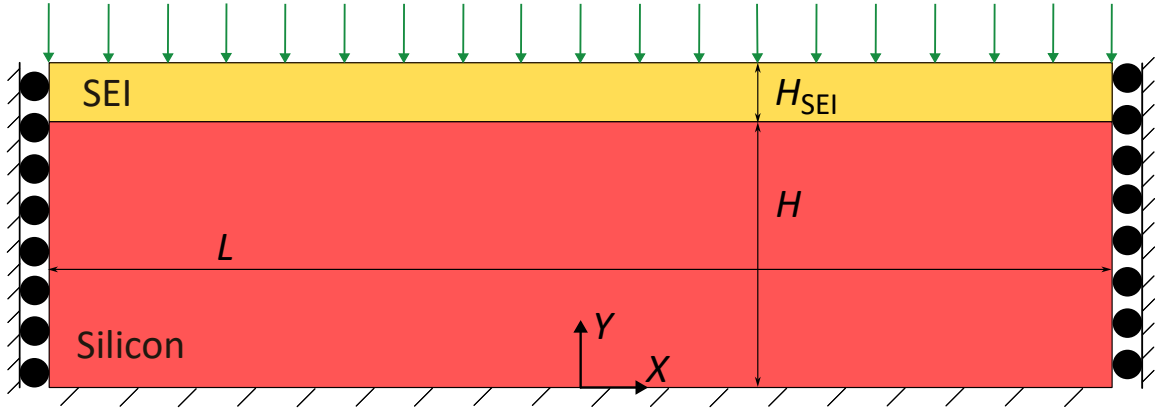


Figure 2.1: Schematic of the problem showing geometric parameters and boundary conditions.

SEI is considered to be completely permeable to Li-ions and thus doesn't undergo any deformation due to lithiation. In the Silicon thin film, the diffusion leads to a stress field. This is termed as diffusion induced stress (DIS) in the literature. The



stress field in turn affects the process of diffusion called stress enhanced diffusion (SED). This leads to two way coupled system of PDEs. Due to large deformation of the Si during lithiation, it is necessary to formulate the problem with finite deformation theory with an elasto-plastic constitutive behaviour. In the present study, both Si and SEI are considered to exhibit a viscoplastic nature. The constitutive law for elastic regime is taken to be isotropic and concentration dependent for Silicon film and constant for SEI. For Mechanical equilibrium, a quasi-static model is employed.

# Chapter 3

## Mathematical Formulation

### 3.1 Kinematics

Consider a certain particle, initially located at the coordinate  $\mathbf{X}$ . During deformation, this particle follows a path

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t). \quad (3.1)$$

Let  $\mathbf{u}(\mathbf{X}, t)$  be the displacement of the material particle located at  $\mathbf{X}$ . Then

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X}. \quad (3.2)$$

The total deformation gradient and Green-Lagrange strain are denoted by  $\mathbf{F}$  and  $\mathbf{E}$ , respectively. Therefore,

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_{\mathbf{X}} \mathbf{u} + \mathbf{I}, \quad (3.3)$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I}) \quad (3.4)$$

where  $\mathbf{I}$  is the second order isotropic tensor.

Let  $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\}$  be the orthonormal basis in the reference configuration. corresponding components of  $\mathbf{X}$  are denoted by  $X, Y$  and  $Z$  and that of  $\mathbf{u}$  by  $u, v$  and  $w$ . In the present study, plane strain deformation is assumed. Therefore, the components of  $\mathbf{F}$  are given by (Lai et al., 2009)

$$[\mathbf{F}] = \begin{bmatrix} 1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & 0 \\ \frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial Y} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix}. \quad (3.5)$$

Both Inelastic and elastic deformation gradients are considered to be finite (Bower et al., 2011). Hence, a multiplicative decomposition of  $\mathbf{F}$  into elastic and inelastic deformation is necessary. As shown in 3.1, the body is first considered to reach an intermediate stress free state and then it undergoes an elastic deformation to reach the current configuration. As derived by Lee (1969), the total deformation gradient

$$\mathbf{F} = \mathbf{F}^{\text{el}} \cdot \mathbf{F}^{\text{inel}} \quad (3.6)$$

$$\text{where, } \mathbf{F}^{\text{el}} = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_I} \text{ and } \mathbf{F}^{\text{inel}} = \frac{\partial \mathbf{x}_I}{\partial \mathbf{X}}$$

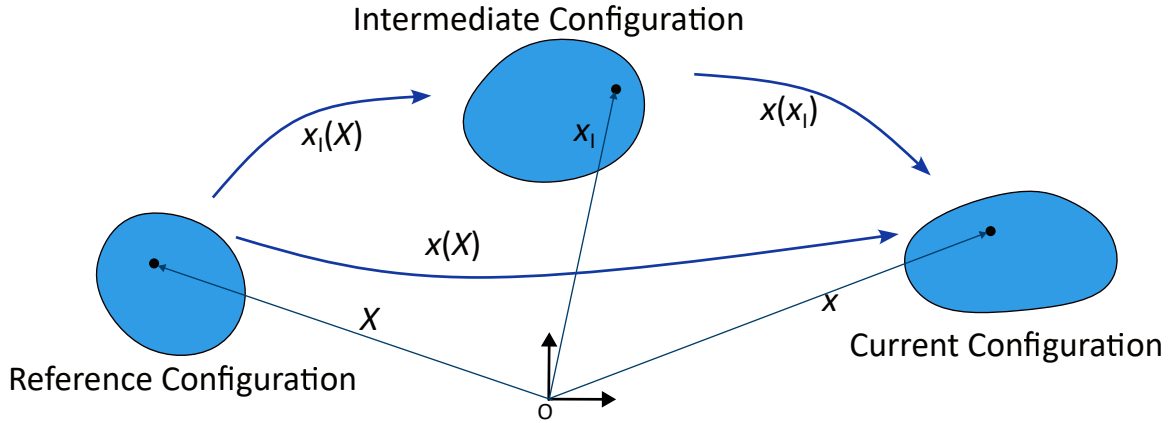


Figure 3.1: Decomposition of deformation gradient into elastic and inelastic part.

$\mathbf{F}^{\text{el}}$  and  $\mathbf{F}^{\text{inel}}$  denote the deformation gradients due to elastic deformation and inelastic deformation respectively.

The inelastic deformation gradient tensor,  $\mathbf{F}^{\text{inel}}$ , has contribution from two sources. It is further decomposed as

$$\mathbf{F}^{\text{inel}} = \mathbf{F}^{\text{c}} \cdot \mathbf{F}^{\text{p}}. \quad (3.7)$$

Where  $\mathbf{F}^{\text{c}}$  and  $\mathbf{F}^{\text{p}}$  are deformation gradients due to diffusion and plastic flow, respectively.

## 3.2 Viscoplastic Flow

A viscoplastic constitutive relation of the following form is considered:

$$\mathbf{D}^{\text{p}} = \frac{\partial G(\sigma_{\text{eff}})}{\partial \tau} \quad (3.8)$$

Where  $\mathbf{D}^P$  is the rate dependent plastic deformation tensor,  $G(\sigma_{\text{eff}})$  is the flow potential,  $\boldsymbol{\tau}$  is the deviatoric part of Cauchy stress tensor and  $\sigma_f$  is yield strength defined as

$$\sigma_f = \begin{cases} \sigma_{f,\text{si}} & \text{for Silicon } (-L/2 \leq X \leq L/2 \text{ and } 0 \leq Y \leq H) \\ \sigma_{f,\text{SEI}} & \text{for SEI layer } (-L/2 \leq X \leq L/2 \text{ and } 0 \leq Y \leq H + H_{\text{SEI}}) \end{cases}$$

Various studies (Bower et al., 2011; Cui et al., 2012) have adopted a power law of following form for flow potential

$$G(\sigma_{\text{eff}}) = \frac{\sigma_f \dot{d}_0}{m+1} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right)^{m+1} H \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (3.9)$$

$$\Rightarrow \mathbf{D}^P = \frac{3\boldsymbol{\tau} \dot{d}_0}{2\sigma_{\text{eff}}} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right)^m H \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right). \quad (3.10)$$

where  $\sigma_{\text{eff}}$  is the effective von Mises stress, defined in section 3.4,  $H$  is the unit step function,  $\sigma_f$  is the yield strength of Silicon,  $m$  is the stress exponent for plastic flow and  $\dot{d}_0$  is the strain rate for plastic flow. Considering an irrotational plastic flow (Gurtin and Anand, 2005*a,b*; Bhowmick and Chakraborty, 2023)

$$\mathbf{D}^P = \mathbf{F}^{\text{el}} \cdot \mathbf{F}^{\text{c}} \cdot \dot{\mathbf{F}}^P \cdot (\mathbf{F}^P)^{-1} \cdot (\mathbf{F}^{\text{c}})^{-1} \cdot (\mathbf{F}^{\text{el}})^{-1} \quad (3.11)$$

$$\Rightarrow \dot{\mathbf{F}}^P = (J)^{-1} \frac{3}{2} \frac{\mathbf{M}_0^{\text{el}} \cdot \mathbf{F}^P}{\sigma_{\text{eff}}} \dot{d}_0 \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right)^m H \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (3.12)$$

$$\text{where } \mathbf{M}_0^{\text{el}} = J(\mathbf{F}^{\text{el}})^{\text{T}} \cdot \boldsymbol{\tau} \cdot (\mathbf{F}^{\text{el}})^{-\text{T}} \quad (3.13)$$

$$\text{and } J = \det(\mathbf{F}). \quad (3.14)$$

$\mathbf{M}_0^{\text{el}}$  is the deviatoric part of Mandel stress (Mandel, 1971). The expression for Mandel stress is  $\mathbf{M}^{\text{el}} = J(\mathbf{F}^{\text{el}})^{\text{T}} \boldsymbol{\sigma} (\mathbf{F}^{\text{el}})^{-\text{T}}$ . Attributing to the assumption of plane strain,  $\mathbf{F}^P$  is considered to be of the following form:

$$[\mathbf{F}^P] = \begin{bmatrix} \lambda_{11} & \lambda_{12} & 0 \\ \lambda_{21} & \lambda_{22} & 0 \\ 0 & 0 & \lambda_{33} \end{bmatrix}. \quad (3.16)$$

Since,  $\det(\mathbf{F}^P) = 1$

$$\lambda_{33} = 1/(\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}). \quad (3.17)$$

### 3.3 Diffusion Induced Deformation

The compound formed between Lithium and Silicon is of the form  $\text{Li}_\chi\text{Si}$ . Let the stoichiometric concentration and maximum concentration of Lithium ions per atom of Silicon be denoted by  $\chi_0$  and  $\chi_{\max}$ . Defining a non-dimensional measure of the Li-ions concentration as  $\tilde{c} = (\chi - \chi_0)/\chi_{\max}$ . since,  $\chi_0$  is the stoichiometric ratio it signifies the stress free state of the particle and hence,  $\tilde{c}$  is a measure of the deviation of the particle from undeformed state. The deformation due to lithiation is quantified by an isotropic deformation gradient denoted by  $\mathbf{F}^c$  and given by

$$\mathbf{F}^c = (J^c)^{1/3} \mathbf{I} \quad (3.18)$$

where  $J^c = 1 + 3\eta\chi_{\max}\tilde{c}$  is the volumetric change experienced by the Silicon film upon insertion of Li-ions.  $\eta$  is a material parameter giving rate of change in volume w.r.t.  $\tilde{c}$ . It may be noted that as  $\tilde{c}$  approaches 1,  $\det(\mathbf{F}^c)$  approaches 4. Therefore the body undergoes a volumetric change of about 300% due to diffusion of Li-ions, justifying the use of large deformation analysis.

Since, SEI is permeable to lithiation  $\mathbf{F}^c$  will be considered only for Silicon. Therefore, for the purpose of modelling  $\tilde{c}$  is considered zero in SEI making  $\mathbf{F}^c$  equal to  $\mathbf{I}$ .

### 3.4 Mechanical Equilibrium

From equations 3.6 and 3.7,

$$\mathbf{F}^{\text{el}} = \mathbf{F} \cdot (\mathbf{F}^p \cdot \mathbf{F}^c)^{-1}. \quad (3.20)$$

The elastic Green-Lagrange strain  $\mathbf{E}^{\text{el}} = \frac{1}{2} [(\mathbf{F}^{\text{el}})^\top \cdot \mathbf{F}^{\text{el}} - \mathbf{I}]$ .

The constitutive relation for the elastic deformation is expressed in terms of the strain energy per unit volume in the intermediate configuration,  $\hat{w}(\mathbf{F}, \tilde{c})$ . Denoting the elasticity tensor of Silicon by  $\mathbb{C}$  and its components by  $C_{ijkl}$ ,

$$\hat{w}(\mathbf{F}, \tilde{c}) = \frac{1}{2} C_{ijkl} E_{ij}^{\text{el}} E_{kl}^{\text{el}}. \quad (3.22)$$

$\mathbb{C}$  is concentration dependent and assumed to be isotropic. Hence, its components can be expressed in terms of Lamé coefficients as

$$C_{ijkl}(\tilde{c}) = \lambda_{\text{mat}}(\tilde{c})\delta_{ij}\delta_{kl} + \mu_{\text{mat}}(\tilde{c})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \quad (3.23)$$

$$\implies \hat{w}(\mathbf{F}, \tilde{c}) = [\lambda_{\text{mat}}(\tilde{c})(\text{tr}(\mathbf{E}^{\text{el}}))^2 + 2\mu_{\text{mat}}(\tilde{c})\mathbf{E}^{\text{el}} : \mathbf{E}^{\text{el}}]. \quad (3.24)$$

The lamé parameters,  $\lambda_{\text{mat}}(\tilde{c})$  and  $\mu_{\text{mat}}(\tilde{c})$  are given by

$$\lambda_{\text{mat}}(\tilde{c}) = \frac{E_{\text{mat}}(\tilde{c})\nu_{\text{mat}}}{(1 + \nu_{\text{mat}})(1 - 2\nu_{\text{mat}})}, \quad \mu_{\text{mat}}(\tilde{c}) = \frac{E_{\text{mat}}(\tilde{c})}{2(1 + \nu_{\text{mat}})}.$$

The material properties  $E_{\text{mat}}(\tilde{c})$  and  $\nu_{\text{mat}}$  are defined domainwise as follows:

$$E_{\text{mat}}(\tilde{c}) = \begin{cases} E_{\text{si}}(1 + \eta_{\text{E}}\chi_{\text{max}}\tilde{c}) & \text{for Silicon} \\ E_{\text{SEI}} & \text{for SEI} \end{cases} \quad \text{and} \quad \nu_{\text{mat}} = \begin{cases} \nu_{\text{si}} & \text{for Silicon} \\ \nu_{\text{SEI}} & \text{for SEI} \end{cases}$$

The elastic second Piola-Kirchhoff stress is denoted by  $\mathbf{S}^{\text{el}}$ . Therefore,

$$\begin{aligned} \mathbf{S}^{\text{el}} &= \frac{\partial \hat{w}(\mathbf{F}, \tilde{c})}{\partial \mathbf{E}^{\text{el}}} \\ \implies \mathbf{S}^{\text{el}} &= \lambda_{\text{mat}}(\tilde{c})\text{tr}(\mathbf{E}^{\text{el}})\mathbf{I} + 2\mu_{\text{mat}}(\tilde{c})\mathbf{E}^{\text{el}}. \end{aligned} \quad (3.25)$$

Let  $\mathbf{S}$  denote the second Piola-Kirchhoff stress. Now, by pulling back  $\mathbf{S}^{\text{el}}$  from the intermediate configuration to the reference configuration (Gurtin et al., 2010) the second Piola-Kirchhoff stress is obtained as

$$\begin{aligned} \mathbf{S} &= J^{\text{inel}}(\mathbf{F}^{\text{inel}})^{-1} \cdot \mathbf{S}^{\text{el}} \cdot (\mathbf{F}^{\text{inel}})^{-\text{T}} = J^c(\mathbf{F}^{\text{p}} \cdot \mathbf{F}^{\text{c}})^{-1} \cdot \mathbf{S}^{\text{el}} \cdot (\mathbf{F}^{\text{p}} \cdot \mathbf{F}^{\text{c}})^{-\text{T}} \\ \implies \mathbf{S} &= (J^c)^{1/3}(\mathbf{F}^{\text{p}})^{-1} \cdot \mathbf{S}^{\text{el}} \cdot (\mathbf{F}^{\text{p}})^{-\text{T}}. \end{aligned} \quad (3.26)$$

And the first Piola-Kirchhoff stress is

$$\mathbf{P} = \mathbf{F} \cdot \mathbf{S}. \quad (3.27)$$

The Cauchy stress tensor,  $\boldsymbol{\sigma}$ , is given by  $\boldsymbol{\sigma} = (J)^{-1}\mathbf{F} \cdot \mathbf{S} \cdot \mathbf{F}^{\text{T}}$ . The deviatoric part of Cauchy stress is  $\boldsymbol{\tau} = \boldsymbol{\sigma} - (1/3)\text{tr}(\boldsymbol{\sigma})\mathbf{I}$ . The von Mises stress is  $\sigma_{\text{eff}} = \sqrt{\frac{3}{2}\tau_{ij}\tau_{ij}}$ .

In the absence of any body forces, the conservation of momentum leads to

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = 0. \quad (3.31)$$

### 3.5 Diffusion

Assuming flux to be negligible in the  $z$  direction, the conservation of mass is given by

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_X}{\partial X} + \frac{\partial j_Y}{\partial Y}\right). \quad (3.32)$$

Where  $\mathbf{j}$  is the flux vector and  $c$  is a dimensional measure of Li-ions concentration, defined as  $c = \tilde{c} \chi_{\max} / V_{\text{m}}^{\text{B}}$ . In the current configuration the flux is denoted by  $\hat{\mathbf{j}}(\mathbf{x}, t)$  and it is given by: (cite a paper which describes the following equation)

$$\hat{\mathbf{j}}(\mathbf{x}, t) = -\frac{1}{R_g T} \frac{D \chi_{\max} \tilde{c}}{V_{\text{m}}^{\text{B}}} \nabla_{\mathbf{x}} \mu \quad (3.34)$$

where  $R_g$  is the universal gas constant,  $T$  is the operating temperature,  $D$  is the diffusivity of  $\text{Li}_x\text{Si}$ ,  $V_{\text{m}}^{\text{B}}$  is the partial molar volume of Silicon and  $\mu$  is the chemical potential. Diffusivity, is related to the state of stress by the following equation:

$$D = D_0 \exp\left(\frac{\alpha S_{\text{h}}}{E_0}\right) = D_0 \exp\left(\alpha \frac{S_{11} + S_{33}}{2E_0}\right) \quad (3.35)$$

where  $E_0$  is defined in section 3.6.

In the reference configuration, the flux is  $\mathbf{j}(\mathbf{X}, t) = J(\mathbf{F})^{-1} \cdot \hat{\mathbf{j}}$  (how is the previous expression derived). Now,

$$\begin{aligned} (\nabla_{\mathbf{x}} \mu)_i &= \frac{\partial \mu}{\partial x_i} \\ &= \frac{\partial \mu}{\partial X_j} \frac{\partial X_j}{\partial x_i} \\ \implies \nabla_{\mathbf{x}} \mu &= \mathbf{F}^{-\text{T}} \cdot \nabla_{\mathbf{X}} \mu. \end{aligned} \quad (3.36)$$

From above equations, the flux,  $\mathbf{j}(\mathbf{X}, t)$ , in Lagrangian description is expressed as

$$\mathbf{j} = -\frac{1}{R_g T} \frac{D \chi_{\max} \tilde{c}}{V_m^b} (\mathbf{F})^{-1} \cdot (\mathbf{F})^{-\text{T}} \cdot \nabla_{\mathbf{X}} \mu. \quad (3.37)$$

The chemical potential  $\mu$  is composed of two parts:  $\mu = \mu_0 + \mu_{\text{s}}$ , where  $\mu_0$  and  $\mu_{\text{s}}$  are the stress-independent and stress-dependent part, respectively.  $\mu_0$  can be written as  $\mu_0 = R_g T \log(\gamma \tilde{c})$ , where  $\gamma$  is the activity coefficient and considered to be concentration dependent, given by the following equation:

$$\gamma = \frac{1}{1 - \tilde{c}} \exp\left(\frac{1}{R_g T} [2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]\right). \quad (3.39)$$

The stress-dependent part of the chemical potential is (Cui et al., 2012)

$$\mu_{\text{s}} = \frac{V_m^b}{\chi_{\max}} \left[ -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left( J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right]. \quad (3.40)$$

State of charge is a measure of the degree of lithiation. It is expressed as an average concentration over the domain as follows:

$$\begin{aligned}
\text{soc} &= \frac{1}{LH} \int_{-L/2}^{L/2} \int_0^H \tilde{c} dy dx \\
&= H^2 \frac{1}{LH} \int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x} \\
&= \frac{H}{L} \int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}
\end{aligned} \tag{3.41}$$

### 3.6 Non-dimensionalisation

$$\tilde{j}_X, \tilde{j}_Y, \tilde{J}_0, \tilde{\mathbf{j}} = \frac{HV_m^B}{(\chi_{\max} D_0)} (j_X, j_Y, J_0, \mathbf{j}) \tag{3.42}$$

$$\tilde{X}, \tilde{Y}, \tilde{u}, \tilde{v} = \frac{1}{H} (X, Y, u, v) \tag{3.43}$$

$$\tilde{t} = D_0 t / H^2 \tag{3.44}$$

$$\tilde{\mu}_{\text{si}}, \tilde{\lambda}_{\text{si}}, \tilde{E}_{\text{si}} = \frac{1}{E_0} (\mu_{\text{si}}, \lambda_{\text{si}}, E_{\text{si}}), \text{ where } E_0 = \frac{R_g T}{V_m^B} \tag{3.45}$$

$$\tilde{\mu}_0, \tilde{\mu}_1, \tilde{\mu}_2, \tilde{\mu}_3 = \frac{1}{R_g T} (\mu_0, \mu_1, \mu_2, \mu_3) \tag{3.46}$$

$$\tilde{D} = \frac{D}{D_0} \tag{3.47}$$

$$\dot{\tilde{d}}_0 = \frac{\dot{d}_0 H^2}{D_0} \tag{3.48}$$

$$\tilde{\mathbf{S}}^{\text{el}}, \tilde{\mathbf{S}}, \tilde{\mathbf{P}}, \tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\tau}}, \tilde{\mathbf{M}}_0^{\text{el}}, \tilde{\sigma}_{\text{eff}}, \tilde{\sigma}_{\text{f}} = \frac{1}{E_0} (\mathbf{S}^{\text{el}}, \mathbf{S}, \mathbf{P}, \boldsymbol{\sigma}, \boldsymbol{\tau}, \mathbf{M}_0^{\text{el}}, \sigma_{\text{eff}}, \sigma_{\text{f}}) \tag{3.49}$$

### 3.7 Boundary and Initial Conditions

The initial composition is taken to be  $\text{Li}_{\chi_0}\text{Si}$  which is a stress free state with  $\tilde{c}$  being zero.

$$\tilde{c}(\tilde{X}, \tilde{Y}, 0) = 0, \tag{3.50}$$

$$\tilde{u}(\tilde{X}, \tilde{Y}, 0) = 0, \tag{3.51}$$

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0. \tag{3.52}$$



The bottom face is considered to be fixed and the two side faces can exhibit motion in Y-direction only. Therefore,

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0, \quad (3.53)$$

$$\tilde{u}(-1/2, \tilde{Y}, \tilde{t}) = \tilde{u}(1/2, \tilde{Y}, \tilde{t}) = 0. \quad (3.54)$$

There is a flux from the top surface, which is considered to be of the following form:

$$\text{During Lithiation, } \tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})) \text{ and} \quad (3.55)$$

$$\text{During Delithiation, } \tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0\tilde{c}(\tilde{X}, 1, \tilde{t}). \quad (3.56)$$

Table 3.1: Values of material properties and operating parameters

Material property or parameter	Value
$D_0$ , Diffusivity of Silicon	$10^{-16} \text{ m}^2\text{s}^{-1}$
$E_{\text{si}}$ , Elastic modulus of pure silicon	90 GPa
$E_{\text{SEI}}$ , Elastic modulus of SEI layer	3-10 GPa
$\nu_{\text{si}}$ , Poisson's ratio of pure Silicon	0.22
$\nu_{\text{SEI}}$ , Poisson's ratio of SEI layer	0.30
$\sigma_{f,\text{si}}$ , Yield strength of pure Silicon	1.5Gpa
$\sigma_{f,\text{SEI}}$ , Yield strength of SEI layer	
$R_g$ , Universal gas constant	$8.314 \text{ JK}^{-1}\text{mol}^{-1}$
$T$ , Temperature	298.15 K
$H$ , Initial height of Silicon thin film	200 $\mu\text{m}$
$L$ , Initial length of Silicon thin film	20 $\mu\text{m}$
$H_{\text{SEI}}$ , Initial length of SEI layer	10 $\mu\text{m}$

# Appendix A

## Equations in Component Form

In the development of following equations only non-zero components of various tensors are mentioned.

Introducing  $\tilde{X}$ ,  $\tilde{Y}$ ,  $\tilde{u}$  and  $\tilde{v}$  in equation 3.5, the component of  $\mathbf{F}$  are

$$[\mathbf{F}] = \begin{bmatrix} 1 + \frac{\partial \tilde{u}}{\partial \tilde{X}} & \frac{\partial \tilde{u}}{\partial \tilde{Y}} & 0 \\ \frac{\partial \tilde{v}}{\partial \tilde{X}} & 1 + \frac{\partial \tilde{v}}{\partial \tilde{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix}. \quad (\text{A.1})$$

From 3.20

$$F_{11}^{\text{el}} = \frac{F_{11} \lambda_{22} - F_{12} \lambda_{21}}{Jc^{1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (\text{A.2a})$$

$$F_{21}^{\text{el}} = \frac{F_{21} \lambda_{22} - F_{22} \lambda_{21}}{Jc^{1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (\text{A.2b})$$

$$F_{12}^{\text{el}} = -\frac{F_{11} \lambda_{12} - F_{12} \lambda_{11}}{Jc^{1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (\text{A.2c})$$

$$F_{22}^{\text{el}} = -\frac{F_{21} \lambda_{12} - F_{22} \lambda_{11}}{Jc^{1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (\text{A.2d})$$

$$F_{33}^{\text{el}} = \frac{1}{Jc^{1/3} \lambda_{33}} \quad (\text{A.2e})$$

The components of  $\mathbf{E}^{\text{el}}$  are

$$E_{11}^{\text{el}} = \frac{F_{11}^{\text{el}^2}}{2} + \frac{F_{21}^{\text{el}^2}}{2} - \frac{1}{2} \quad (\text{A.3a})$$

$$E_{21}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (\text{A.3b})$$

$$E_{12}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (\text{A.3c})$$

$$E_{22}^{\text{el}} = \frac{F_{12}^{\text{el}^2}}{2} + \frac{F_{22}^{\text{el}^2}}{2} - \frac{1}{2} \quad (\text{A.3d})$$

$$E_{33}^{\text{el}} = \frac{F_{33}^{\text{el}^2}}{2} - \frac{1}{2} \quad (\text{A.3e})$$

Non-dimensionalizing lamé constants and using 3.25

$$\tilde{S}_{11}^{\text{el}} = J^c \left( 2 E_{11}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (\text{A.4a})$$

$$\tilde{S}_{21}^{\text{el}} = 2 E_{21}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (\text{A.4b})$$

$$\tilde{S}_{12}^{\text{el}} = 2 E_{12}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (\text{A.4c})$$

$$\tilde{S}_{22}^{\text{el}} = J^c \left( 2 E_{22}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (\text{A.4d})$$

$$\tilde{S}_{33}^{\text{el}} = J^c \left( 2 E_{33}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (\text{A.4e})$$

From 3.26 and 3.27

$$\tilde{S}_{11} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{22}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{12}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{22} - \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (\text{A.5a})$$

$$\tilde{S}_{21} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{21} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (\text{A.5b})$$

$$\tilde{S}_{12} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{22} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (\text{A.5c})$$

$$\tilde{S}_{22} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{21}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{11}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{21} - \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (\text{A.5d})$$

$$\tilde{S}_{33} = \frac{\tilde{S}_{33}^{\text{el}}}{J^{c^{2/3}} \lambda_{33}^2} \quad (\text{A.5e})$$

$$\tilde{P}_{11} = F_{11} \tilde{S}_{11} + F_{12} \tilde{S}_{21} \quad (\text{A.6a})$$

$$\tilde{P}_{21} = F_{21} \tilde{S}_{11} + F_{22} \tilde{S}_{21} \quad (\text{A.6b})$$

$$\tilde{P}_{12} = F_{11} \tilde{S}_{12} + F_{12} \tilde{S}_{22} \quad (\text{A.6c})$$

$$\tilde{P}_{22} = F_{21} \tilde{S}_{12} + F_{22} \tilde{S}_{22} \quad (\text{A.6d})$$

$$\tilde{P}_{33} = \tilde{S}_{33} \quad (\text{A.6e})$$

$$\tilde{\sigma}_{11} = \frac{F_{11} \tilde{P}_{11} + F_{12} \tilde{P}_{12}}{J} \quad (\text{A.7a})$$

$$\tilde{\sigma}_{21} = \frac{F_{11} \tilde{P}_{21} + F_{12} \tilde{P}_{22}}{J} \quad (\text{A.7b})$$

$$\tilde{\sigma}_{12} = \frac{F_{21} \tilde{P}_{11} + F_{22} \tilde{P}_{12}}{J} \quad (\text{A.7c})$$

$$\tilde{\sigma}_{22} = \frac{F_{21} \tilde{P}_{21} + F_{22} \tilde{P}_{22}}{J} \quad (\text{A.7d})$$

$$\tilde{\sigma}_{33} = \frac{\tilde{P}_{33}}{J} \quad (\text{A.7e})$$

$$\tilde{\tau}_{11} = \frac{2\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (\text{A.8a})$$

$$\tilde{\tau}_{21} = \tilde{\sigma}_{21} \quad (\text{A.8b})$$

$$\tilde{\tau}_{12} = \tilde{\sigma}_{12} \quad (\text{A.8c})$$

$$\tilde{\tau}_{22} = \frac{2\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (\text{A.8d})$$

$$\tilde{\tau}_{33} = \frac{2\tilde{\sigma}_{33}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} \quad (\text{A.8e})$$

$$\tilde{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2}(\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2 + \tilde{\tau}_{33}^2 + 2\tilde{\tau}_{12}^2)} \quad (\text{A.9})$$

Using 3.13

$$\tilde{M}_{11}^{el} = - \frac{J \left( F_{11}^{el} F_{12}^{el} \tilde{\tau}_{12} - F_{11}^{el} F_{22}^{el} \tilde{\tau}_{11} + F_{12}^{el} F_{21}^{el} \tilde{\tau}_{22} - F_{21}^{el} F_{22}^{el} \tilde{\tau}_{21} \right)}{F_{11}^{el} F_{22}^{el} - F_{12}^{el} F_{21}^{el}} \quad (\text{A.10a})$$

$$\tilde{M}_{21}^{el} = - \frac{J \left( F_{12}^{el^2} \tilde{\tau}_{12} - F_{22}^{el^2} \tilde{\tau}_{21} - F_{12}^{el} F_{22}^{el} \tilde{\tau}_{11} + F_{12}^{el} F_{22}^{el} \tilde{\tau}_{22} \right)}{F_{11}^{el} F_{22}^{el} - F_{12}^{el} F_{21}^{el}} \quad (\text{A.10b})$$

$$\tilde{M}_{12}^{el} = \frac{J \left( F_{11}^{el^2} \tilde{\tau}_{12} - F_{21}^{el^2} \tilde{\tau}_{21} - F_{11}^{el} F_{21}^{el} \tilde{\tau}_{11} + F_{11}^{el} F_{21}^{el} \tilde{\tau}_{22} \right)}{F_{11}^{el} F_{22}^{el} - F_{12}^{el} F_{21}^{el}} \quad (\text{A.10c})$$

$$\tilde{M}_{22}^{el} = \frac{J \left( F_{11}^{el} F_{12}^{el} \tilde{\tau}_{12} - F_{12}^{el} F_{21}^{el} \tilde{\tau}_{11} + F_{11}^{el} F_{22}^{el} \tilde{\tau}_{22} - F_{21}^{el} F_{22}^{el} \tilde{\tau}_{21} \right)}{F_{11}^{el} F_{22}^{el} - F_{12}^{el} F_{21}^{el}} \quad (\text{A.10d})$$

$$\tilde{M}_{33}^{el} = J \tilde{\tau}_{33} \quad (\text{A.10e})$$

These equations need editing if Fpdot\_mat.tex is changed

$$\dot{\tilde{F}}_{11}^p = \dot{d}_0 \left( \frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left( \frac{3 \tilde{M}_{11}^{el} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{el} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (\text{A.11a})$$

$$\dot{\tilde{F}}_{21}^p = \dot{d}_0 \left( \frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left( \frac{3 \tilde{M}_{21}^{el} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{el} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (\text{A.11b})$$

$$\dot{\tilde{F}}_{12}^p = \dot{d}_0 \left( \frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left( \frac{3 \tilde{M}_{11}^{el} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{el} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (\text{A.11c})$$

$$\dot{\tilde{F}}_{22}^p = \dot{d}_0 \left( \frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left( \frac{3 \tilde{M}_{21}^{el} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{el} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (\text{A.11d})$$

$$\dot{\tilde{F}}_{33}^p = \frac{3 \tilde{M}_{33}^{el} \dot{d}_0 \lambda_{33} \left( \frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m}{2 J \tilde{\sigma}_{\text{eff}}} \text{H} \left( \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (\text{A.11e})$$

$$\tilde{\mathbf{j}} = \frac{\mathbf{j}H}{\frac{\chi_{\max}}{V_m^B} D_0} = -\frac{1}{R_g T} \tilde{D} \tilde{c}(\mathbf{F})^{-1}(\mathbf{F})^{-\top} \nabla_{\mathbf{x}} \mu \quad (\text{A.12})$$

$$D = D_0 \exp\left(\frac{\alpha S_h}{E_0}\right) = D_0 \exp(\alpha \tilde{S}_h) = D_0 \exp\left(\alpha \frac{\tilde{S}_{11} + \tilde{S}_{33}}{2}\right) \quad (\text{A.13})$$

$$\tilde{\mu}_0 = \log(\gamma \tilde{c}) \quad (\text{A.14})$$

$$\tilde{\mu}_s = \frac{1}{R_g T} \mu_s \quad (\text{A.15})$$

$$\begin{aligned} &= \frac{V_m^b}{R_g T \chi_{\max}} \left[ -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left( J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{C}_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left( J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \end{aligned} \quad (\text{A.16})$$

$$\tilde{C}_{ijkl} \tilde{E}_{kl}^{\text{el}} = \tilde{P}_{ij}^{\text{el}} = \tilde{S}_{ij}^{\text{el}} / J^c \quad (\text{A.17})$$

$$\implies \tilde{C}_{ijkl} = \tilde{\lambda}_{si}(\tilde{c}) \delta_{ij} \delta_{kl} + \tilde{\mu}_{si}(\tilde{c}) (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (\text{A.18})$$

$$\begin{aligned} \tilde{\mu}_s &= \frac{1}{\chi_{\max}} \left[ -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{P}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left( -\frac{1}{3} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left( -\frac{1}{3} (2 \tilde{E}_{mn}^{\text{el}} + \delta_{mn}) + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ -\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \delta_{mn} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} \left[ -\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mm}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \\ &= \frac{1}{\chi_{\max}} (\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3) \end{aligned} \quad (\text{A.19})$$

$$\tilde{\mu}_1 = -\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{P}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{P}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (\text{A.20})$$

$$\tilde{\mu}_2 = -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} + \tilde{P}_{33}^{\text{el}}] \quad (\text{A.21})$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (\text{A.22})$$

$$\frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} = \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} + \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (\text{A.23})$$

$$\begin{aligned} \tilde{\mu}_3 &= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \delta_{il} \delta_{jk} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \\ &= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{kk}^{\text{el}} \tilde{E}_{ii}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \tilde{E}_{ji}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \\ &= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} (\text{tr}(\mathbf{E}^{\text{el}}))^2 + J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \\ &= \frac{1}{2} J^c [\tilde{\lambda}'_{si}(c) (\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}})^2 + 2\tilde{\mu}'_{si}(\tilde{c}) ((\tilde{E}_{11}^{\text{el}})^2 + (\tilde{E}_{22}^{\text{el}})^2 + (\tilde{E}_{33}^{\text{el}})^2 + 2(\tilde{E}_{12}^{\text{el}})^2)] \end{aligned} \quad (\text{A.24})$$

$$\begin{aligned} \tilde{\mathbf{j}} &= \mathbf{j} H V_m^b / (\chi_{\max} D_0) \\ &= -\frac{D}{D_0} H \tilde{\mathbf{c}} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^T \nabla_{\mathbf{x}} \tilde{\mu} \end{aligned} \quad (\text{A.25})$$

$$\begin{aligned} \tilde{j}_x &= \frac{-\bar{D} H \tilde{c}}{J^2} \left( \frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \\ &= \frac{-\bar{D} \tilde{c}}{J^2} \left( \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} \tilde{j}_y &= \frac{-\bar{D} H \tilde{c}}{J^2} \left( \frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \\ &= \frac{-\bar{D} \tilde{c}}{J^2} \left( \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{11} \tilde{F}_{12} + \tilde{F}_{21} \tilde{F}_{22}) \right) \end{aligned} \quad (\text{A.27})$$

Momentum Conservation equations in non-dimensional form:

$$\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (\text{A.28a})$$

$$\text{and, } \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0. \quad (\text{A.28b})$$

Mass conservation Equation in non-dimensional form:

$$\begin{aligned}
\frac{\partial c}{\partial t} &= -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y}\right) \\
\frac{\chi_{\max}}{V_{\text{m}}^{\text{B}}} \frac{D_0}{H^2} \frac{\partial \tilde{c}}{\partial t} &= -\left(\frac{1}{H} \frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{1}{H} \frac{\partial \tilde{j}_y}{\partial \tilde{Y}}\right) \frac{\chi_{\max}}{V_{\text{m}}^{\text{B}}} \frac{D_0}{H} \\
\Rightarrow \frac{\partial \tilde{c}}{\partial \tilde{t}} &= -\left(\frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{\partial \tilde{j}_y}{\partial \tilde{Y}}\right)
\end{aligned} \tag{A.29}$$



# Appendix B

## To do

- Add full stops at the end of equations
- Export equation with “,” from MATLAB
- numbering of inline equations
- where
- unwanted vertical space
- one section need explanation
- Add relevant citations
- Table of parameters
- Write about SEI as well
- explanation of BCs and IC
- figure
- Properties of SEI

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