

BTP-1

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September 26, 2024

0.1 Introduction

introduction

Chapter 1

Mathematical Formulation

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The geometry considered is a thin film of Silicon in the domain $-L/2 \leq X \leq L/2$ and $0 \leq Y \leq H$. Consider a certain particle, initially located at the coordinate \mathbf{X} . During deformation, this particle follows a path

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t) \quad (1.1)$$

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

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X} \quad (1.2)$$

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

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_{\mathbf{X}} \mathbf{u} + \mathbf{I} \quad (1.3)$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^T \cdot \mathbf{F} - \mathbf{I}) \quad (1.4)$$

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. Denoting the corresponding components of \mathbf{X} by X, Y and Z and that of \mathbf{u} by u, v and w , and assuming plane strain deformation the components of \mathbf{F} are given by:

$$[\mathbf{F}] = \begin{bmatrix} 1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & 0 \\ \frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial Y} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix} \quad (1.5)$$

Both Inelastic and elastic deformation gradients are considered to be finite. Hence, a multiplicative decomposition of \mathbf{F} into elastic and inelastic deformation is necessary. The body is first considered to reach an intermediate stress-free state and then it undergoes elastic deformation to reach the current configuration (Lee 1969).

$$\mathbf{F} = \mathbf{F}^{\text{el}} \cdot \mathbf{F}^{\text{inel}} \quad (1.6)$$

$$\text{in indicial notation, } F_{ij} = F_{ik}^{\text{el}} F_{kj}^{\text{inel}} \quad (1.7)$$

where \mathbf{F}^{el} and \mathbf{F}^{inel} are the deformation gradients due to elastic deformation and inelastic deformation respectively.

The inelastic deformation gradient tensor, \mathbf{F}^{inel} , has contribution from two sources - deformation due to concentration gradient, \mathbf{F}^{c} , and viscoplastic deformation, \mathbf{F}^{p} .

$$\mathbf{F}^{\text{inel}} = \mathbf{F}^{\text{c}} \cdot \mathbf{F}^{\text{p}} \quad (1.8)$$

1.1 Viscoplastic Deformation

A viscoplastic constitutive relation of the following form is considered.

$$\mathbf{D}^{\text{p}} = \frac{\partial G(\sigma_{\text{eff}})}{\partial \boldsymbol{\tau}} \quad (1.9)$$

Where \mathbf{D}^{p} is the rate dependent plastic deformation tensor, $G(\sigma_{\text{eff}})$ is the flow potential, σ_{eff} is the von Mises stress and $\boldsymbol{\tau}$ is the deviatoric part of Cauchy stress tensor. citation

$$G(\sigma_{\text{eff}}) = \frac{\sigma_{\text{f}} \dot{d}_0}{m+1} \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right)^{m+1} \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right) \quad (1.10)$$

$$\Rightarrow \mathbf{D}^{\text{p}} = \frac{3\boldsymbol{\tau} \dot{d}_0}{2\sigma_{\text{eff}}} \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right)^m \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right) \quad (1.11)$$

where, H is the unit step function, σ_{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.

$$\mathbf{D}^{\text{p}} = \mathbf{F}^{\text{el}} \mathbf{F}^{\text{c}} \dot{\mathbf{F}}^{\text{p}} (\mathbf{F}^{\text{p}})^{-1} (\mathbf{F}^{\text{c}})^{-1} (\mathbf{F}^{\text{el}})^{-1} \quad (1.12)$$

$$\Rightarrow \dot{\mathbf{F}}^{\text{p}} = (J)^{-1} \frac{3 \mathbf{M}_0^{\text{el}} \mathbf{F}^{\text{p}}}{2 \sigma_{\text{eff}}} \dot{d}_0 \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right)^m \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_{\text{f}}} - 1 \right) \quad (1.13)$$

$$\text{where, } \mathbf{M}_0^{\text{el}} = J(\mathbf{F}^{\text{el}})^{\text{T}} \boldsymbol{\tau} (\mathbf{F}^{\text{el}})^{-\text{T}} \quad (1.14)$$

$$J = \det(\mathbf{F}) \quad (1.15)$$

\mathbf{M}_0^{el} is the deviatoric part of Mandel stress (). The expression for Mandel stress is $\mathbf{M}^{\text{el}} = J(\mathbf{F}^{\text{el}})^{\text{T}} \boldsymbol{\sigma} (F^{\text{el}})^{-\text{T}}$. \mathbf{F}^{p} is assumed to be of the following form:

$$[\mathbf{F}^{\text{p}}] = \begin{bmatrix} \lambda_{11} & \lambda_{12} & 0 \\ \lambda_{21} & \lambda_{22} & 0 \\ 0 & 0 & \lambda_{33} \end{bmatrix} \quad (1.16)$$

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

$$\lambda_{33} = 1/(\lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21}) \quad (1.17)$$

1.2 Deformation due to concentration gradient

The compound formed between Lithium and Silicon is of the form Li_χSi . Let the stoichiometric concentration and maximum concentration of Silicon atoms per atom of Lithium be denoted by χ_0 and χ_{max} . Defining a non-dimensional measure of the Li-ions concentration as $\tilde{c} = (\chi - \chi_0)/\chi_{\text{max}}$. since, χ_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.

$$\mathbf{F}^{\text{c}} = (J^{\text{c}})^{1/3} \mathbf{I} \quad (1.18)$$

$$\text{where } J^{\text{c}} = 1 + 3\eta\chi_{\text{max}}\tilde{c} \quad (1.19)$$

η 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, $\det(\mathbf{F}^{\text{c}})$ 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.

1.3 Momentum Conservation

From equations 1.6 and 1.8, \mathbf{F}^{el} can be expressed as,

$$\mathbf{F}^{\text{el}} = \mathbf{F} \cdot (\mathbf{F}^{\text{p}} \cdot \mathbf{F}^{\text{c}})^{-1} \quad (1.20)$$

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

The strain energy per unit volume in the reference configuration, $W(\mathbf{F}, \tilde{c})$, is expressed as $W(\mathbf{F}, \tilde{c}) = J^{\text{inel}} \bar{w}(\mathbf{F}, \tilde{c})$, where $\bar{w}(\mathbf{F}, \tilde{c})$ is the strain energy per unit volume in the

intermediate configuration and $J^{\text{inel}} = \det(\mathbf{F}^{\text{inel}}) = J^c$.

$$W(\mathbf{F}, \tilde{c}) = \frac{J^c}{2} \frac{E(\tilde{c})}{1 + \nu} \left(\frac{\nu}{1 - 2\nu} (\text{tr} \mathbf{E}^{\text{el}})^2 + \text{tr}(\mathbf{E}^{\text{el}} \cdot \mathbf{E}^{\text{el}}) \right). \quad (1.21)$$

The elastic modulus of Silicon is concentration dependent with $E(\tilde{c}) = E_{\text{si}}(1 + \eta_{\text{E}} \chi_{\text{max}} \tilde{c})$. The elastic second Piola-Kirchhoff stress is denoted by \mathbf{S}^{el} . Differentiating W w.r.t \mathbf{E}^{el} gives,

$$\mathbf{S}^{\text{el}} = J^c [2\mu_{\text{si}}(\tilde{c}) \mathbf{E}^{\text{el}} + \lambda_{\text{si}}(\tilde{c}) \text{tr}(\mathbf{E}^{\text{el}}) \mathbf{I}] \quad (1.22)$$

Let \mathbf{P} and \mathbf{S} denote the first and second Piola-Kirchhoff stress, respectively. Thus

$$\mathbf{S} = (\mathbf{F}^c)^{-1} \cdot (\mathbf{F}^{\text{p}})^{-1} \cdot \mathbf{S}^{\text{el}} \cdot (\mathbf{F}^{\text{p}})^{-\text{T}} \cdot (\mathbf{F}^c)^{-\text{T}} \quad (1.23)$$

$$\mathbf{P} = \mathbf{F} \cdot \mathbf{S} \quad (1.24)$$

The Cauchy stress tensor, $\boldsymbol{\sigma}$ is given by $\boldsymbol{\sigma} = (J)^{-1} \mathbf{P} \cdot \mathbf{F}^{\text{T}}$. And, the deviatoric part of Cauchy is $\boldsymbol{\tau} = \boldsymbol{\sigma} - (1/3) \text{tr}(\boldsymbol{\sigma}) \mathbf{I}$. The von Mises stress is $\sigma_{\text{eff}} = \sqrt{\frac{3}{2}(\tau_{11}^2 + \tau_{22}^2 + \tau_{33}^2 + 2\tau_{12}^2)}$.

Conservation of momentum leads to

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = 0. \quad (1.25)$$

1.4 Mass Conservation

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

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_X}{\partial X} + \frac{\partial j_Y}{\partial Y} \right). \quad (1.26)$$

Where, \mathbf{j} is the flux vector and c is a dimensional measure of Li-ions concentration, defined as $c = \chi_{\text{max}}/V_{\text{m}}^{\text{B}} \tilde{c}$.

1.5 Non-Dimensionalization

$$\tilde{j}_X, \tilde{j}_Y, \tilde{J}_0, \tilde{\mathbf{j}} = \frac{HV_m^B}{(\chi_{\max} D_0)} (j_X, j_Y, J_0, \mathbf{j}) \quad (1.27)$$

$$\tilde{X}, \tilde{Y}, \tilde{u}, \tilde{v} = \frac{1}{H} (X, Y, u, v) \quad (1.28)$$

$$\tilde{t} = D_0 t / H^2 \quad (1.29)$$

$$\tilde{\mu}_{\text{si}}, \tilde{\lambda}_{\text{si}}, \tilde{E}_{\text{si}} = \frac{1}{E_0} (\mu_{\text{si}}, \lambda_{\text{si}}, E_{\text{si}}), \text{ where } E_0 = \frac{R_g T}{V_m^B} \quad (1.30)$$

$$\tilde{\mu}_0, \tilde{\mu}_1, \tilde{\mu}_2, \tilde{\mu}_3 = \frac{1}{R_g T} (\mu_0, \mu_1, \mu_2, \mu_3) \quad (1.31)$$

$$\tilde{D} = \frac{D}{D_0} \quad (1.32)$$

$$\tilde{d}_0 = \frac{\dot{d}_0 H^2}{D_0} \quad (1.33)$$

$$\tilde{\mathbf{S}}^{\text{el}}, \tilde{\mathbf{S}}, \tilde{\mathbf{P}}, \tilde{\boldsymbol{\sigma}}, \tilde{\boldsymbol{\tau}}, \tilde{\mathbf{M}}_0^{\text{el}}, \tilde{\sigma}_{\text{eff}}, \tilde{\sigma}_{\text{f}} = \frac{1}{E_0} (\mathbf{S}^{\text{el}}, \mathbf{S}, \mathbf{P}, \boldsymbol{\sigma}, \boldsymbol{\tau}, \mathbf{M}_0^{\text{el}}, \sigma_{\text{eff}}, \sigma_{\text{f}}) \quad (1.34)$$

1.6 Definition of the state of charge

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

$$\text{soc} = \frac{\int_{-L/2}^{L/2} \int_0^H \tilde{c} dy dx}{LH} \quad (1.35)$$

$$= H^2 \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{LH} \quad (1.36)$$

$$= H \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{L} \quad (1.37)$$

1.7 Non-Dimensional Equations in Component Form

$$[\mathbf{F}] = \begin{bmatrix} 1 + \frac{\partial \tilde{u}}{\partial \tilde{X}} & \frac{\partial \tilde{u}}{\partial \tilde{Y}} & 0 \\ \frac{\partial \tilde{v}}{\partial \tilde{X}} & 1 + \frac{\partial \tilde{v}}{\partial \tilde{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix} \quad (1.38)$$

$$F_{11}^{\text{el}} = \frac{F_{11} \lambda_{22} - F_{12} \lambda_{21}}{J^{c1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (1.39)$$

$$F_{21}^{\text{el}} = \frac{F_{21} \lambda_{22} - F_{22} \lambda_{21}}{J^{c1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (1.40)$$

$$F_{12}^{\text{el}} = -\frac{F_{11} \lambda_{12} - F_{12} \lambda_{11}}{J^{c1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (1.41)$$

$$F_{22}^{\text{el}} = -\frac{F_{21} \lambda_{12} - F_{22} \lambda_{11}}{J^{c1/3} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (1.42)$$

$$F_{33}^{\text{el}} = \frac{1}{J^{c1/3} \lambda_{33}} \quad (1.43)$$

$$E_{11}^{\text{el}} = \frac{F_{11}^{\text{el}2}}{2} + \frac{F_{21}^{\text{el}2}}{2} - \frac{1}{2} \quad (1.44)$$

$$E_{21}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (1.45)$$

$$E_{12}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (1.46)$$

$$E_{22}^{\text{el}} = \frac{F_{12}^{\text{el}2}}{2} + \frac{F_{22}^{\text{el}2}}{2} - \frac{1}{2} \quad (1.47)$$

$$E_{33}^{\text{el}} = \frac{F_{33}^{\text{el}2}}{2} - \frac{1}{2} \quad (1.48)$$

$$\tilde{S}_{11}^{\text{el}} = J^c \left(2 E_{11}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (1.49)$$

$$\tilde{S}_{21}^{\text{el}} = 2 E_{21}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (1.50)$$

$$\tilde{S}_{12}^{\text{el}} = 2 E_{12}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (1.51)$$

$$\tilde{S}_{22}^{\text{el}} = J^c \left(2 E_{22}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (1.52)$$

$$\tilde{S}_{33}^{\text{el}} = J^c \left(2 E_{33}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (1.53)$$

$$\tilde{S}_{11} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{22}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{12}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{22} - \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (1.54)$$

$$\tilde{S}_{21} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{21} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (1.55)$$

$$\tilde{S}_{12} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{22} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (1.56)$$

$$\tilde{S}_{22} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{21}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{11}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{21} - \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (1.57)$$

$$\tilde{S}_{33} = \frac{\tilde{S}_{33}^{\text{el}}}{J^{c^{2/3}} \lambda_{33}^2} \quad (1.58)$$

$$\tilde{P}_{11} = F_{11} \tilde{S}_{11} + F_{12} \tilde{S}_{21} \quad (1.59)$$

$$\tilde{P}_{21} = F_{21} \tilde{S}_{11} + F_{22} \tilde{S}_{21} \quad (1.60)$$

$$\tilde{P}_{12} = F_{11} \tilde{S}_{12} + F_{12} \tilde{S}_{22} \quad (1.61)$$

$$\tilde{P}_{22} = F_{21} \tilde{S}_{12} + F_{22} \tilde{S}_{22} \quad (1.62)$$

$$\tilde{P}_{33} = \tilde{S}_{33} \quad (1.63)$$

$$\tilde{\sigma}_{11} = \frac{F_{11} \tilde{P}_{11} + F_{12} \tilde{P}_{12}}{J} \quad (1.64)$$

$$\tilde{\sigma}_{21} = \frac{F_{11} \tilde{P}_{21} + F_{12} \tilde{P}_{22}}{J} \quad (1.65)$$

$$\tilde{\sigma}_{12} = \frac{F_{21} \tilde{P}_{11} + F_{22} \tilde{P}_{12}}{J} \quad (1.66)$$

$$\tilde{\sigma}_{22} = \frac{F_{21} \tilde{P}_{21} + F_{22} \tilde{P}_{22}}{J} \quad (1.67)$$

$$\tilde{\sigma}_{33} = \frac{\tilde{P}_{33}}{J} \quad (1.68)$$

$$\tilde{\tau}_{11} = \frac{2\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (1.69)$$

$$\tilde{\tau}_{21} = \tilde{\sigma}_{21} \quad (1.70)$$

$$\tilde{\tau}_{12} = \tilde{\sigma}_{12} \quad (1.71)$$

$$\tilde{\tau}_{22} = \frac{2\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (1.72)$$

$$\tilde{\tau}_{33} = \frac{2\tilde{\sigma}_{33}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} \quad (1.73)$$

$$\tilde{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2}(\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2 + \tilde{\tau}_{33}^2 + 2\tilde{\tau}_{12}^2)} \quad (1.74)$$

$$\tilde{M}_{11}^{\text{el}} = - \frac{J \left(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (1.75)$$

$$\tilde{M}_{21}^{\text{el}} = - \frac{J \left(F_{12}^{\text{el}^2} \tilde{\tau}_{12} - F_{22}^{\text{el}^2} \tilde{\tau}_{21} - F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (1.76)$$

$$\tilde{M}_{12}^{\text{el}} = \frac{J \left(F_{11}^{\text{el}^2} \tilde{\tau}_{12} - F_{21}^{\text{el}^2} \tilde{\tau}_{21} - F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (1.77)$$

$$\tilde{M}_{22}^{\text{el}} = \frac{J \left(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (1.78)$$

$$\tilde{M}_{33}^{\text{el}} = J \tilde{\tau}_{33} \quad (1.79)$$

Viscoplastic rates: These equations need editing if Fpdot.mat.tex is changed

$$\dot{\tilde{F}}_{11}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.80)$$

$$\dot{\tilde{F}}_{21}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.81)$$

$$\dot{\tilde{F}}_{12}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.82)$$

$$\dot{\tilde{F}}_{22}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.83)$$

$$\dot{\tilde{F}}_{33}^{\text{p}} = \frac{3 \tilde{M}_{33}^{\text{el}} \dot{d}_0 \lambda_{33} \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m}{2 J \tilde{\sigma}_{\text{eff}}} \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.84)$$

Viscoplastic rate equations in non-dimensional form:

$$\frac{d\lambda_{11}}{dt} = \frac{1}{t_{\text{ref}}} \frac{d\lambda_{11}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}}\lambda_{11} + \tilde{M}_{12}^{\text{el}}\lambda_{21}) \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.85)$$

$$\frac{d\lambda_{11}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}}\lambda_{11} + \tilde{M}_{12}^{\text{el}}\lambda_{21}) \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \text{H} \left(\frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right) \quad (1.86)$$

$$\text{where, } \dot{d}_0 = \dot{d}_0 t_{\text{ref}} \quad (1.87)$$

Momentum Conservation equations in non-dimensional form:

$$\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (1.88)$$

$$\text{and, } \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0. \quad (1.89)$$

Mass conservation Equation in non-dimensional form:

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y} \right) \quad (1.90)$$

$$\frac{\chi_{\text{max}}}{V_{\text{m}}^{\text{B}}} \frac{D_0}{H^2} \frac{\partial \tilde{c}}{\partial \tilde{t}} = -\left(\frac{1}{H} \frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{1}{H} \frac{\partial \tilde{j}_y}{\partial \tilde{Y}} \right) \frac{\chi_{\text{max}}}{V_{\text{m}}^{\text{B}}} \frac{D_0}{H} \quad (1.91)$$

$$\implies \frac{\partial \tilde{c}}{\partial \tilde{t}} = -\left(\frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{\partial \tilde{j}_y}{\partial \tilde{Y}} \right) \quad (1.92)$$

For one way coupling:

$$\mathbf{j} = -D_0 \nabla_{\mathbf{X}} c \quad (1.93)$$

$$\tilde{j}_x = j_x H / \left(\frac{\chi_{\text{max}}}{V_{\text{m}}^{\text{B}}} D_0 \right) \quad (1.94)$$

$$= -D_0 \frac{\partial c}{\partial X} H / \left(\frac{\chi_{\text{max}}}{V_{\text{m}}^{\text{B}}} D_0 \right) \quad (1.95)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{X}} \quad (1.96)$$

$$\tilde{j}_y = j_y H / \left(\frac{\chi_{\text{max}}}{V_{\text{m}}^{\text{B}}} D_0 \right) \quad (1.97)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{Y}} \quad (1.98)$$

For two way coupling:

$$\mathbf{j} = -\frac{1}{R_g T} \frac{D\chi_{\max}\tilde{c}}{V_m^b} (\mathbf{F})^{-1} (\mathbf{F})^{-\top} \nabla_{\mathbf{X}} \mu \quad (1.99)$$

$$\tilde{\mathbf{j}} = \frac{\mathbf{j}H}{\frac{\chi_{\max}}{V_m^B} D_0} = -\frac{1}{R_g T} \tilde{D}\tilde{c}(\mathbf{F})^{-1} (\mathbf{F})^{-\top} \nabla_{\mathbf{X}} \mu \quad (1.100)$$

$$D = D_0 \exp\left(\frac{\alpha \tilde{S}_h}{E_0}\right) = D_0 \exp(\alpha \tilde{S}_h) = D_0 \exp\left(\alpha \frac{\tilde{S}_{11} + \tilde{S}_{33}}{2}\right) \quad (1.101)$$

$$\mu = \mu_0 + \mu_s; \tilde{\mu} = \frac{\mu}{R_g T} \quad (1.102)$$

$$\mu_0 = R_g T \log(\gamma \tilde{c}); \tilde{\mu}_0 = \log(\gamma \tilde{c}) \quad (1.103)$$

$$\gamma = \frac{1}{1 - \tilde{c}} \exp\left(\frac{1}{R_g T} [2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]\right) \quad (1.104)$$

$$\mu_s = \frac{V_m^b}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.105)$$

$$\tilde{\mu}_s = \frac{1}{R_g T} \mu_s \quad (1.106)$$

$$= \frac{V_m^b}{R_g T \chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.107)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{C}_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.108)$$

$$\tilde{C}_{ijkl} \tilde{E}_{kl}^{\text{el}} = \tilde{P}_{ij}^{\text{el}} = \tilde{S}_{ij}^{\text{el}} / J^c \implies \tilde{C}_{ijkl} = \tilde{\lambda}_{si}(\tilde{c}) \delta_{ij} \delta_{kl} + \tilde{\mu}_{si}(\tilde{c}) (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (1.109)$$

$$\tilde{\mu}_s = \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.110)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{P}_{kl}^{\text{el}} \right] \quad (1.111)$$

$$= \frac{1}{\chi_{\max}} \left[\frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left(-\frac{1}{3} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.112)$$

$$= \frac{1}{\chi_{\max}} \left[\frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left(-\frac{1}{3} (2\tilde{E}_{mn}^{\text{el}} + \delta_{mn}) + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.113)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \delta_{mn} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.114)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mm}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (1.115)$$

$$= \frac{1}{\chi_{\max}} (\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3) \quad (1.116)$$

$$\tilde{\mu}_0 = \log(\gamma\tilde{c}) \quad (1.117)$$

$$\tilde{\mu}_1 = -\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{P}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{P}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (1.118)$$

$$\tilde{\mu}_2 = -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} + \tilde{P}_{33}^{\text{el}}] \quad (1.119)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (1.120)$$

$$\frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} = \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} + \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (1.121)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \delta_{il} \delta_{jk} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \quad (1.122)$$

$$= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{kk}^{\text{el}} \tilde{E}_{ii}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \tilde{E}_{ji}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \quad (1.123)$$

$$= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} (\text{tr}(\mathbf{E}^{\text{el}}))^2 + J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (1.124)$$

$$= \frac{1}{2} J^c [\tilde{\lambda}'_{si}(\tilde{c}) (\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}})^2 + 2\tilde{\mu}'_{si}(\tilde{c}) ((\tilde{E}_{11}^{\text{el}})^2 + (\tilde{E}_{22}^{\text{el}})^2 + (\tilde{E}_{33}^{\text{el}})^2 + 2(\tilde{E}_{12}^{\text{el}})^2)] \quad (1.125)$$

$$\mathbf{j} = -\frac{D\chi_{\max}\tilde{c}}{V_m^b} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{X}} \tilde{\mu} \quad (1.126)$$

$$\tilde{\mathbf{j}} = \mathbf{j} H V_m^b / (\chi_{\max} D_0) \quad (1.127)$$

$$= -\frac{D}{D_0} H \tilde{c} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{X}} \tilde{\mu} \quad (1.128)$$

$$\tilde{j}_x = \frac{-\bar{D}H\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (1.129)$$

$$= \frac{-\bar{D}\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (1.130)$$

$$\tilde{j}_y = \frac{-\bar{D}H\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (1.131)$$

$$= \frac{-\bar{D}\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (1.132)$$

1.8 Boundary and Initial Conditions

$$\tilde{c}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (1.133)$$

$$\tilde{u}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (1.134)$$

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0 \quad (1.135)$$

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0 \quad (1.136)$$

$$\tilde{u}(-1/2, \tilde{Y}, \tilde{t}) = \tilde{u}(1/2, \tilde{Y}, \tilde{t}) = 0 \quad (1.137)$$

$$\tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})) \quad (1.138)$$

Bibliography

Lee, E. H. (1969), 'Elastic-plastic deformation at finite strains'.