

0.1 Mathematical Formulation

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

$$\mathbf{x} = \mathbf{x}(\mathbf{X}, t) \quad (1)$$

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

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X} = [u(\mathbf{X}, t), v(\mathbf{X}, t), w(\mathbf{X}, t)]^\top \quad (2)$$

Let the total deformation gradient be denoted by \mathbf{F} .

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \nabla_{\mathbf{X}} \mathbf{u} + \mathbf{I} \quad (3)$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^\top \mathbf{F} - \mathbf{I}) \quad (4)$$

Assuming plane strain deformation,

$$\mathbf{F} = \begin{bmatrix} 1 + \frac{\partial u}{\partial X} & \frac{\partial u}{\partial Y} & 0 \\ \frac{\partial v}{\partial X} & 1 + \frac{\partial v}{\partial Y} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} F_{11} & F_{12} & 0 \\ F_{21} & F_{22} & 0 \\ 0 & 0 & F_{33} \end{bmatrix} \quad (5)$$

Decomposition of deformation gradient gives,

$$\mathbf{F} = \mathbf{F}^{\text{el}} \mathbf{F}^{\text{inel}} \quad (6)$$

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} .

$$\mathbf{F}^{\text{inel}} = \mathbf{F}^{\text{c}} \mathbf{F}^{\text{p}} \quad (7)$$

0.1.1 Viscoplastic Deformation

$$\dot{\mathbf{F}}^{\text{p}} = (J)^{-1} \frac{3}{2} \frac{\mathbf{M}_0^{\text{el}} \mathbf{F}^{\text{p}}}{\sigma_{\text{eff}}} \dot{d}_0 \left\langle \frac{\sigma_{\text{eff}}}{\sigma_f} - 1 \right\rangle^m \quad (8)$$

$$\text{where, } \mathbf{M}_0^{\text{el}} = J(\mathbf{F}^{\text{el}})^\top \boldsymbol{\tau}(\mathbf{F}^{\text{el}})^{-\top} \quad (9)$$

$$J = \det(\mathbf{F}) \quad (10)$$

\mathbf{F}^p is assumed to be of the following form:

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

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

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

0.1.2 Deformation due to concentration gradient

$$\mathbf{F}^c = (J^c)^{1/3} \mathbf{I} \quad (13)$$

$$\text{where } J^c = 1 + 3\eta\chi_{\max}\tilde{c} \quad (14)$$

0.1.3 Momentum Conservation

$$\mathbf{F}^{\text{el}} = \mathbf{F}(\mathbf{F}^p \mathbf{F}^c)^{-1} \quad (15)$$

$$\mathbf{E}^{\text{el}} = \frac{1}{2} [(\mathbf{F}^{\text{el}})^\top \mathbf{F}^{\text{el}} - \mathbf{I}] \quad (16)$$

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

$$W(\mathbf{F}, c) = \frac{J^c}{2} \frac{E(c)}{1 + \nu} \left(\frac{\nu}{1 - 2\nu} (\text{tr} \mathbf{E}^{\text{el}})^2 + \text{tr}(\mathbf{E}^{\text{el}} \mathbf{E}^{\text{el}}) \right) \quad (17)$$

$$\mathbf{S}^{\text{el}} = J^c [2\mu_{\text{si}}(c) \mathbf{E}^{\text{el}} + \lambda_{\text{si}}(c) \text{tr}(\mathbf{E}^{\text{el}}) \mathbf{I}] \quad (18)$$

$$\mathbf{S} = (\mathbf{F}^c)^{-1} (\mathbf{F}^p)^{-1} \mathbf{S}^{\text{el}} (\mathbf{F}^p)^{-\top} (\mathbf{F}^c)^{-\top} \quad (19)$$

$$\mathbf{P} = \mathbf{F} \mathbf{S} \quad (20)$$

Let $\boldsymbol{\sigma}$ denote the Cauchy stress tensor. Then

$$\boldsymbol{\sigma} = (J)^{-1} \mathbf{P} \mathbf{F}^\top \quad (21)$$

Let $\boldsymbol{\tau}$ denote the deviatoric part of the Cauchy stress, $\boldsymbol{\sigma}$; then

$$\boldsymbol{\tau} = \boldsymbol{\sigma} - (1/3) \text{tr}(\boldsymbol{\sigma}) \mathbf{I} \quad (22)$$

$$(23)$$

Let σ_{eff} denote the von Mises stress. Then:

$$\sigma_{\text{eff}} = \sqrt{\frac{3}{2}(\tau_{11}^2 + \tau_{22}^2 + \tau_{33}^2 + 2\tau_{12}^2)} \quad (24)$$

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = 0. \quad (25)$$

0.1.4 Mass Convservation

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} \quad (26)$$

0.1.5 Non-Dimensionalization

$$\begin{aligned} \tilde{c} &= c/c_{\text{max}} & \tilde{\mathbf{j}} &= \mathbf{j}H/(c_{\text{max}}D_0) \\ \text{where, } c_{\text{max}} &= \chi_{\text{max}}/V_m^B \\ \tilde{u} &= u/H & \tilde{v} &= v/H \\ \tilde{X} &= X/H & \tilde{Y} &= Y/H \\ \tilde{t} &= D_0 t/H^2 & \tilde{\mu}_{\text{si}}, \tilde{\lambda}_{\text{si}} &= \mu_{\text{si}}/E_0, \lambda_{\text{si}}/E_0 \\ \tilde{E}(c) &= E_{\text{si}}(1 + \eta_E \chi_{\text{max}} \tilde{c})/E_0, \text{ where } E_0 = \frac{R_g T}{V_m^b} \end{aligned}$$

0.1.6 Definition of the state of charge

$$\text{soc} = \frac{\int_{-L/2}^{L/2} \int_0^H \tilde{c} d\tilde{y} d\tilde{x}}{LH} \quad (27)$$

$$= H^2 \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{LH} \quad (28)$$

$$= H \frac{\int_{-L/2H}^{L/2H} \int_0^1 \tilde{c}(\tilde{x}, \tilde{y}) d\tilde{y} d\tilde{x}}{L} \quad (29)$$

0.1.7 Equations in component form

$$\mathbf{F} = \begin{bmatrix} 1 + \frac{\partial \tilde{u}}{\partial \tilde{X}} & \frac{\partial \tilde{u}}{\partial \tilde{Y}} & 0 \\ \frac{\partial \tilde{v}}{\partial \tilde{X}} & 1 + \frac{\partial \tilde{v}}{\partial \tilde{Y}} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} \tilde{F}_{11} & \tilde{F}_{12} & 0 \\ \tilde{F}_{21} & \tilde{F}_{22} & 0 \\ 0 & 0 & \tilde{F}_{33} \end{bmatrix} \quad (30)$$

$$F_{11}^{\text{el}} = \frac{F_{11} \lambda_{22} - F_{12} \lambda_{21}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (31)$$

$$F_{21}^{\text{el}} = \frac{F_{21} \lambda_{22} - F_{22} \lambda_{21}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (32)$$

$$F_{12}^{\text{el}} = -\frac{F_{11} \lambda_{12} - F_{12} \lambda_{11}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (33)$$

$$F_{22}^{\text{el}} = -\frac{F_{21} \lambda_{12} - F_{22} \lambda_{11}}{J^{c^{1/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})} \quad (34)$$

$$F_{33}^{\text{el}} = \frac{1}{J^{c^{1/3}} \lambda_{33}} \quad (35)$$

$$E_{11}^{\text{el}} = \frac{F_{11}^{\text{el}^2}}{2} + \frac{F_{21}^{\text{el}^2}}{2} - \frac{1}{2} \quad (36)$$

$$E_{21}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (37)$$

$$E_{12}^{\text{el}} = \frac{F_{11}^{\text{el}} F_{12}^{\text{el}}}{2} + \frac{F_{21}^{\text{el}} F_{22}^{\text{el}}}{2} \quad (38)$$

$$E_{22}^{\text{el}} = \frac{F_{12}^{\text{el}^2}}{2} + \frac{F_{22}^{\text{el}^2}}{2} - \frac{1}{2} \quad (39)$$

$$E_{33}^{\text{el}} = \frac{F_{33}^{\text{el}^2}}{2} - \frac{1}{2} \quad (40)$$

$$\tilde{S}_{11}^{\text{el}} = J^c \left(2 E_{11}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (41)$$

$$\tilde{S}_{21}^{\text{el}} = 2 E_{21}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (42)$$

$$\tilde{S}_{12}^{\text{el}} = 2 E_{12}^{\text{el}} J^c \tilde{\mu}_{\text{si}} \quad (43)$$

$$\tilde{S}_{22}^{\text{el}} = J^c \left(2 E_{22}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (44)$$

$$\tilde{S}_{33}^{\text{el}} = J^c \left(2 E_{33}^{\text{el}} \tilde{\mu}_{\text{si}} + \tilde{\lambda}_{\text{si}} (E_{11}^{\text{el}} + E_{22}^{\text{el}} + E_{33}^{\text{el}}) \right) \quad (45)$$

$$\tilde{S}_{11} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{22}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{12}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{22} - \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (46)$$

$$\tilde{S}_{21} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{12} \lambda_{21} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{22}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (47)$$

$$\tilde{S}_{12} = \frac{\tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{22} - \tilde{S}_{22}^{\text{el}} \lambda_{11} \lambda_{12} - \tilde{S}_{11}^{\text{el}} \lambda_{21} \lambda_{22} + \tilde{S}_{21}^{\text{el}} \lambda_{12} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (48)$$

$$\tilde{S}_{22} = \frac{\tilde{S}_{11}^{\text{el}} \lambda_{21}^2 + \tilde{S}_{22}^{\text{el}} \lambda_{11}^2 - \tilde{S}_{12}^{\text{el}} \lambda_{11} \lambda_{21} - \tilde{S}_{21}^{\text{el}} \lambda_{11} \lambda_{21}}{J^{c^{2/3}} (\lambda_{11} \lambda_{22} - \lambda_{12} \lambda_{21})^2} \quad (49)$$

$$\tilde{S}_{33} = \frac{\tilde{S}_{33}^{\text{el}}}{J^{c^{2/3}} \lambda_{33}^2} \quad (50)$$

$$\tilde{P}_{11} = F_{11} \tilde{S}_{11} + F_{12} \tilde{S}_{21} \quad (51)$$

$$\tilde{P}_{21} = F_{21} \tilde{S}_{11} + F_{22} \tilde{S}_{21} \quad (52)$$

$$\tilde{P}_{12} = F_{11} \tilde{S}_{12} + F_{12} \tilde{S}_{22} \quad (53)$$

$$\tilde{P}_{22} = F_{21} \tilde{S}_{12} + F_{22} \tilde{S}_{22} \quad (54)$$

$$\tilde{P}_{33} = \tilde{S}_{33} \quad (55)$$

$$\tilde{\sigma}_{11} = \frac{F_{11} \tilde{P}_{11} + F_{12} \tilde{P}_{12}}{J} \quad (56)$$

$$\tilde{\sigma}_{21} = \frac{F_{11} \tilde{P}_{21} + F_{12} \tilde{P}_{22}}{J} \quad (57)$$

$$\tilde{\sigma}_{12} = \frac{F_{21} \tilde{P}_{11} + F_{22} \tilde{P}_{12}}{J} \quad (58)$$

$$\tilde{\sigma}_{22} = \frac{F_{21} \tilde{P}_{21} + F_{22} \tilde{P}_{22}}{J} \quad (59)$$

$$\tilde{\sigma}_{33} = \frac{\tilde{P}_{33}}{J} \quad (60)$$

$$\tilde{\tau}_{11} = \frac{2 \tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (61)$$

$$\tilde{\tau}_{21} = \tilde{\sigma}_{21} \quad (62)$$

$$\tilde{\tau}_{12} = \tilde{\sigma}_{12} \quad (63)$$

$$\tilde{\tau}_{22} = \frac{2 \tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{33}}{3} \quad (64)$$

$$\tilde{\tau}_{33} = \frac{2 \tilde{\sigma}_{33}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} \quad (65)$$

$$\tilde{\sigma}_{\text{eff}} = \sqrt{\frac{3}{2}(\tilde{\tau}_{11}^2 + \tilde{\tau}_{22}^2 + \tilde{\tau}_{33}^2 + 2\tilde{\tau}_{12}^2)} \quad (66)$$

$$\tilde{M}_{11}^{\text{el}} = -\frac{J \left(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (67)$$

$$\tilde{M}_{21}^{\text{el}} = -\frac{J \left(F_{12}^{\text{el}^2} \tilde{\tau}_{12} - F_{22}^{\text{el}^2} \tilde{\tau}_{21} - F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{11} + F_{12}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (68)$$

$$\tilde{M}_{12}^{\text{el}} = \frac{J \left(F_{11}^{\text{el}^2} \tilde{\tau}_{12} - F_{21}^{\text{el}^2} \tilde{\tau}_{21} - F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{22} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (69)$$

$$\tilde{M}_{22}^{\text{el}} = \frac{J \left(F_{11}^{\text{el}} F_{12}^{\text{el}} \tilde{\tau}_{12} - F_{12}^{\text{el}} F_{21}^{\text{el}} \tilde{\tau}_{11} + F_{11}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{22} - F_{21}^{\text{el}} F_{22}^{\text{el}} \tilde{\tau}_{21} \right)}{F_{11}^{\text{el}} F_{22}^{\text{el}} - F_{12}^{\text{el}} F_{21}^{\text{el}}} \quad (70)$$

$$\tilde{M}_{33}^{\text{el}} = J \tilde{\tau}_{33} \quad (71)$$

Viscoplastic rates:

$$\dot{F}_{11}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (72)$$

$$\dot{F}_{21}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{11}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{21}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (73)$$

$$\dot{F}_{12}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{11}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{12}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (74)$$

$$\dot{F}_{22}^{\text{p}} = \dot{d}_0 \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \left(\frac{3 \tilde{M}_{21}^{\text{el}} \lambda_{12}}{2 J \tilde{\sigma}_{\text{eff}}} + \frac{3 \tilde{M}_{22}^{\text{el}} \lambda_{22}}{2 J \tilde{\sigma}_{\text{eff}}} \right) \quad (75)$$

$$\dot{F}_{33}^{\text{p}} = \frac{3 \tilde{M}_{33}^{\text{el}} \dot{d}_0 \lambda_{33} \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m}{2 J \tilde{\sigma}_{\text{eff}}} \quad (76)$$

Viscoplastic rate equations in non-dimensional form:

$$\frac{d\lambda_{11}}{dt} = \frac{1}{t_{\text{ref}}} \frac{d\lambda_{11}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}} \lambda_{11} + \tilde{M}_{12}^{\text{el}} \lambda_{21}) \text{H} \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \quad (77)$$

$$\frac{d\lambda_{11}}{d\tilde{t}} = \frac{3\dot{d}_0}{2J\tilde{\sigma}_{\text{eff}}} (\tilde{M}_{11}^{\text{el}} \lambda_{11} + \tilde{M}_{12}^{\text{el}} \lambda_{21}) \text{H} \left(\frac{\tilde{\sigma}_{\text{eff}}}{\tilde{\sigma}_f} - 1 \right)^m \quad (78)$$

$$\text{where, } \dot{d}_0 = \dot{d}_0 t_{\text{ref}} \quad (79)$$

Stress equilibrium Equation:

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = \mathbf{0}. \quad (80)$$

$$\frac{\partial P_{11}}{\partial X} + \frac{\partial P_{12}}{\partial Y} = 0 \quad (81)$$

$$\text{and, } \frac{\partial P_{21}}{\partial X} + \frac{\partial P_{22}}{\partial Y} = 0 \quad (82)$$

In non-dimensional form:

$$\frac{E_0}{H} \frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{E_0}{H} \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (83)$$

$$\text{and, } \frac{E_0}{H} \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{E_0}{H} \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \quad (84)$$

So,

$$\frac{\partial \tilde{P}_{11}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{12}}{\partial \tilde{Y}} = 0 \quad (85)$$

$$\text{and, } \frac{\partial \tilde{P}_{21}}{\partial \tilde{X}} + \frac{\partial \tilde{P}_{22}}{\partial \tilde{Y}} = 0 \quad (86)$$

Mass conservation Equation:

$$\frac{\partial c}{\partial t} = -\nabla_{\mathbf{X}} \cdot \mathbf{j} = -\left(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y}\right) \quad (87)$$

$$c_{\max} \frac{D_0}{H^2} \frac{\partial \tilde{c}}{\partial \tilde{t}} = -\left(\frac{1}{H} \frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{1}{H} \frac{\partial \tilde{j}_y}{\partial \tilde{Y}}\right) c_{\max} \frac{D_0}{H} \quad (88)$$

$$\text{so, } \frac{\partial \tilde{c}}{\partial \tilde{t}} = -\left(\frac{\partial \tilde{j}_x}{\partial \tilde{X}} + \frac{\partial \tilde{j}_y}{\partial \tilde{Y}}\right) \quad (89)$$

For one way coupling:

$$\mathbf{j} = -D_0 \nabla_{\mathbf{X}} c \quad (90)$$

$$\tilde{j}_x = j_x H / (c_{\max} D_0) \quad (91)$$

$$= -D_0 \frac{\partial c}{\partial X} H / (c_{\max} D_0) \quad (92)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{X}} \quad (93)$$

$$\tilde{j}_y = j_y H / (c_{\max} D_0) \quad (94)$$

$$= -\frac{\partial \tilde{c}}{\partial \tilde{Y}} \quad (95)$$

For two way coupling:

$$\mathbf{j} = -\frac{1}{R_g T} \frac{D \chi_{\max} \tilde{c}}{V_m^b} (\mathbf{F})^{-1} (\mathbf{F})^{-\top} \nabla_{\mathbf{x}} \mu \quad (96)$$

$$\tilde{\mathbf{j}} = \frac{\mathbf{j}^H}{c_{\max} D_0} = -\frac{1}{R_g T} \tilde{D} \tilde{c} (\mathbf{F})^{-1} (\mathbf{F})^{-\top} \nabla_{\mathbf{x}} \mu \quad (97)$$

$$D = D_0 \exp\left(\frac{\alpha S_h}{E_0}\right) = D_0 \exp(\alpha \tilde{S}_h) = D_0 \exp\left(\alpha \frac{\tilde{S}_{11} + \tilde{S}_{33}}{2}\right) \quad (98)$$

$$\mu = \mu_0 + \mu_s; \tilde{\mu} = \frac{\mu}{R_g T} \quad (99)$$

$$\mu_0 = R_g T \log(\gamma \tilde{c}); \tilde{\mu}_0 = \log(\gamma \tilde{c}) \quad (100)$$

$$\gamma = \frac{1}{1 - \tilde{c}} \exp\left(\frac{1}{R_g T} [2(A_0 - 2B_0)\tilde{c} - 3(A_0 - B_0)(\tilde{c}^2)]\right) \quad (101)$$

$$\mu_s = \frac{V_m^b}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (102)$$

$$\tilde{\mu}_s = \frac{1}{R_g T} \mu_s \quad (103)$$

$$= \frac{V_m^b}{R_g T \chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} C_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial C_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} C_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (104)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{C}_{mnkl} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \left(J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} + \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \right) \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (105)$$

$$\tilde{C}_{ijkl} \tilde{E}_{kl}^{\text{el}} = \tilde{P}_{ij}^{\text{el}} = \tilde{S}_{ij}^{\text{el}} / J^c \implies \tilde{C}_{ijkl} = \tilde{\lambda}_{si}(\tilde{c}) \delta_{ij} \delta_{kl} + \tilde{\mu}_{si}(\tilde{c}) (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (106)$$

$$\tilde{\mu}_s = \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{C}_{ijkl} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (107)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} \tilde{P}_{mn}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} + \frac{1}{2} \frac{\partial J^c}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{P}_{kl}^{\text{el}} \right] \quad (108)$$

$$= \frac{1}{\chi_{\max}} \left[\frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left(-\frac{1}{3} \tilde{F}_{im}^{\text{el}} \tilde{F}_{in}^{\text{el}} + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (109)$$

$$= \frac{1}{\chi_{\max}} \left[\frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \left(-\frac{1}{3} (2\tilde{E}_{mn}^{\text{el}} + \delta_{mn}) + \frac{1}{2} \tilde{E}_{mn}^{\text{el}} \right) + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (110)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \delta_{mn} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (111)$$

$$= \frac{1}{\chi_{\max}} \left[-\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mn}^{\text{el}} \tilde{E}_{mn}^{\text{el}} - \frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} \tilde{P}_{mm}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{kl}^{\text{el}} \right] \quad (112)$$

$$= \frac{1}{\chi_{\max}} (\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3) \quad 8 \quad (113)$$

$$\tilde{\mu}_0 = \log(\gamma\tilde{c}) \quad (114)$$

$$\tilde{\mu}_1 = -\frac{1}{6} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} \tilde{E}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} \tilde{E}_{22}^{\text{el}} + 2\tilde{P}_{12}^{\text{el}} \tilde{E}_{12}^{\text{el}} + \tilde{P}_{33}^{\text{el}} \tilde{E}_{33}^{\text{el}}] \quad (115)$$

$$\tilde{\mu}_2 = -\frac{1}{3} \frac{\partial J^c}{\partial \tilde{c}} [\tilde{P}_{11}^{\text{el}} + \tilde{P}_{22}^{\text{el}} + \tilde{P}_{33}^{\text{el}}] \quad (116)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (117)$$

$$\frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} = \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} + \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (118)$$

$$\tilde{\mu}_3 = \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \delta_{ij} \delta_{kl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\delta_{ik} \delta_{jl} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \delta_{il} \delta_{jk} \tilde{E}_{kl}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \quad (119)$$

$$= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{kk}^{\text{el}} \tilde{E}_{ii}^{\text{el}} + \frac{1}{2} J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} (\tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} + \tilde{E}_{ji}^{\text{el}} \tilde{E}_{ij}^{\text{el}}) \quad (120)$$

$$= \frac{1}{2} J^c \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}} (\text{tr}(\mathbf{E}^{\text{el}}))^2 + J^c \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}} \tilde{E}_{ij}^{\text{el}} \tilde{E}_{ij}^{\text{el}} \quad (121)$$

$$= \frac{1}{2} J^c [\tilde{\lambda}'_{si}(\tilde{c}) (\tilde{E}_{11}^{\text{el}} + \tilde{E}_{22}^{\text{el}} + \tilde{E}_{33}^{\text{el}})^2 + 2\tilde{\mu}'_{si}(\tilde{c}) ((\tilde{E}_{11}^{\text{el}})^2 + (\tilde{E}_{22}^{\text{el}})^2 + (\tilde{E}_{33}^{\text{el}})^2 + 2(\tilde{E}_{12}^{\text{el}})^2)] \quad (122)$$

$$\mathbf{j} = -\frac{D\chi_{\max}\tilde{c}}{V_m^b} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{x}} \tilde{\mu} \quad (123)$$

$$\tilde{\mathbf{j}} = \mathbf{j} H V_m^b / (\chi_{\max} D_0) \quad (124)$$

$$= -\frac{D}{D_0} H \tilde{c} \tilde{\mathbf{F}}^{-1} (\tilde{\mathbf{F}}^{-1})^\top \nabla_{\mathbf{x}} \tilde{\mu} \quad (125)$$

$$\tilde{j}_x = \frac{-\bar{D}H\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (126)$$

$$= \frac{-\bar{D}\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{12}^2 + \tilde{F}_{22}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (127)$$

$$\tilde{j}_y = \frac{-\bar{D}H\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial Y} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial X} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (128)$$

$$= \frac{-\bar{D}\tilde{c}}{J^2} \left(\frac{\partial \tilde{\mu}}{\partial \tilde{Y}} (\tilde{F}_{11}^2 + \tilde{F}_{21}^2) - \frac{\partial \tilde{\mu}}{\partial \tilde{X}} (\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22}) \right) \quad (129)$$

0.1.8 Boundary and Initial Conditions

$$\tilde{c}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{130}$$

$$\tilde{u}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{131}$$

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{132}$$

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0 \tag{133}$$

$$\tilde{u}(-1/2, \tilde{Y}, \tilde{t}) = \tilde{u}(1/2, \tilde{Y}, \tilde{t}) = 0 \tag{134}$$

$$\tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})) \tag{135}$$