Research Paper

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0.1 Introduction

introduction

0.2 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

$$\boldsymbol{x} = \boldsymbol{x}(\boldsymbol{X}, t) \tag{1}$$

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

$$\boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X} = [u(\boldsymbol{X}, t), v(\boldsymbol{X}, t), w(\boldsymbol{X}, t)]^{\mathsf{T}} \tag{2}$$

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

$$\mathbf{F} = \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}} = \boldsymbol{\nabla}_{\boldsymbol{X}} \boldsymbol{u} + \mathbf{I} \tag{3}$$

$$\mathbf{E} = \frac{1}{2}(\mathbf{F}^{\mathsf{T}}\mathbf{F} - \mathbf{I}) \tag{4}$$

Assuming plane strain deformation,

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

Decomposition of deformation gradient gives,

$$\mathbf{F} = \mathbf{F}^{\mathrm{el}}\mathbf{F}^{\mathrm{inel}} \tag{6}$$

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

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

$$\mathbf{F}^{\mathrm{inel}} = \mathbf{F}^{\mathrm{c}}\mathbf{F}^{\mathrm{p}} \tag{7}$$

0.2.1 Viscoplastic Deformation

$$\dot{\mathbf{F}}^{\mathrm{p}} = (J)^{-1}\frac{3}{2}\frac{\mathbf{M}_{\mathbf{0}}^{\mathrm{el}}\mathbf{F}^{\mathrm{p}}}{\sigma_{\mathrm{eff}}}\dot{d}_0\langle\frac{\sigma_{\mathrm{eff}}}{\sigma_{\mathrm{f}}} - 1\rangle^{\mathrm{m}} \tag{8}$$

$$\text{where, } \mathbf{M}_{\mathbf{0}}^{\mathrm{el}} = J(\mathbf{F}^{\mathrm{el}})^{\mathsf{T}}\boldsymbol{\tau}(\mathbf{F}^{\mathrm{el}})^{-\mathsf{T}} \tag{9}$$

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

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

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

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

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

0.2.2 Deformation due to concentration gradient

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

$$\text{where } J^c = 1 + 3\eta\chi_{\mathrm{max}}\tilde{c} \tag{14}$$

0.2.3 Momentum Conservation

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

$$\mathbf{E}^{\mathrm{el}} = \frac{1}{2}\left[(\mathbf{F}^{\mathrm{el}})^{\mathsf{T}}\mathbf{F}^{\mathrm{el}} - \mathbf{I}\right] \tag{16}$$

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

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

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

$$\mathbf{S} = (\mathbf{F}^{\mathrm{c}})^{-1}(\mathbf{F}^{\mathrm{p}})^{-1}\mathbf{S}^{\mathrm{el}}(\mathbf{F}^{\mathrm{p}})^{-\mathsf{T}}(\mathbf{F}^{\mathrm{c}})^{-\mathsf{T}} \tag{19}$$

$$\mathbf{P} = \mathbf{F}\mathbf{S} \tag{20}$$

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

$$\boldsymbol{\sigma} = (J)^{-1}\mathbf{P}\mathbf{F}^{\mathsf{T}} \tag{21}$$

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

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

$$\tag{23}$$

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

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

$$\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \mathbf{P} = 0. \tag{25}$$

0.2.4 Mass Convservation

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \boldsymbol{j} \tag{26}$$

0.2.5 Non-Dimensionalization

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

0.2.6 Definition of the state of charge

$$\text{soc} = \frac{\int_{-L/2}^{L/2}\int_0^H \tilde{c}\,\mathrm{dydx}}{LH} \tag{27}$$

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

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

0.2.7 Equations in component form

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

$$F^{\mathrm{el}}_{11} = \frac{F_{11}\,\lambda_{22} - F_{12}\,\lambda_{21}}{{J^c}^{1/3}\,\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)} \tag{31}$$

$$F^{\mathrm{el}}_{21} = \frac{F_{21}\,\lambda_{22} - F_{22}\,\lambda_{21}}{{J^c}^{1/3}\,\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)} \tag{32}$$

$$F^{\mathrm{el}}_{12} = -\frac{F_{11}\,\lambda_{12} - F_{12}\,\lambda_{11}}{{J^c}^{1/3}\,\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)} \tag{33}$$

$$F^{\mathrm{el}}_{22} = -\frac{F_{21}\,\lambda_{12} - F_{22}\,\lambda_{11}}{{J^c}^{1/3}\,\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)} \tag{34}$$

$$F^{\mathrm{el}}_{33} = \frac{1}{{J^c}^{1/3}\,\lambda_{33}} \tag{35}$$

$$E^{\mathrm{el}}_{11} = \frac{{F^{\mathrm{el}}_{11}}^2}{2} + \frac{{F^{\mathrm{el}}_{21}}^2}{2} - \frac{1}{2} \tag{36}$$

$$E^{\mathrm{el}}_{21} = \frac{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{12}}{2} + \frac{F^{\mathrm{el}}_{21}\,F^{\mathrm{el}}_{22}}{2} \tag{37}$$

$$E^{\mathrm{el}}_{12} = \frac{F^{\mathrm{el}}_{11}\,F^{\mathrm{el}}_{12}}{2} + \frac{F^{\mathrm{el}}_{21}\,F^{\mathrm{el}}_{22}}{2} \tag{38}$$

$$E^{\mathrm{el}}_{22} = \frac{{F^{\mathrm{el}}_{12}}^2}{2} + \frac{{F^{\mathrm{el}}_{22}}^2}{2} - \frac{1}{2} \tag{39}$$

$$E^{\mathrm{el}}_{33} = \frac{{F^{\mathrm{el}}_{33}}^2}{2} - \frac{1}{2} \tag{40}$$

$$\tilde{S}^{\mathrm{el}}_{11} = J^c\,\left(2\,E^{\mathrm{el}}_{11}\,\tilde{\mu}_{\mathrm{si}} + \tilde{\lambda}_{\mathrm{si}}\,\left(E^{\mathrm{el}}_{11} + E^{\mathrm{el}}_{22} + E^{\mathrm{el}}_{33}\right)\right) \tag{41}$$

$$\tilde{S}^{\mathrm{el}}_{21} = 2\,E^{\mathrm{el}}_{21}\,J^c\,\tilde{\mu}_{\mathrm{si}} \tag{42}$$

$$\tilde{S}^{\mathrm{el}}_{12} = 2\,E^{\mathrm{el}}_{12}\,J^c\,\tilde{\mu}_{\mathrm{si}} \tag{43}$$

$$\tilde{S}^{\mathrm{el}}_{22} = J^c\,\left(2\,E^{\mathrm{el}}_{22}\,\tilde{\mu}_{\mathrm{si}} + \tilde{\lambda}_{\mathrm{si}}\,\left(E^{\mathrm{el}}_{11} + E^{\mathrm{el}}_{22} + E^{\mathrm{el}}_{33}\right)\right) \tag{44}$$

$$\tilde{S}^{\mathrm{el}}_{33} = J^c\,\left(2\,E^{\mathrm{el}}_{33}\,\tilde{\mu}_{\mathrm{si}} + \tilde{\lambda}_{\mathrm{si}}\,\left(E^{\mathrm{el}}_{11} + E^{\mathrm{el}}_{22} + E^{\mathrm{el}}_{33}\right)\right) \tag{45}$$

$$\tilde{S}_{11} = \frac{\tilde{S}^{\mathrm{el}}_{11}\,{\lambda_{22}}^2 + \tilde{S}^{\mathrm{el}}_{22}\,{\lambda_{12}}^2 - \tilde{S}^{\mathrm{el}}_{12}\,\lambda_{12}\,\lambda_{22} - \tilde{S}^{\mathrm{el}}_{21}\,\lambda_{12}\,\lambda_{22}}{J^{c\,2/3}\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)^2} \tag{46}$$

$$\tilde{S}_{21} = \frac{\tilde{S}^{\mathrm{el}}_{12}\,\lambda_{12}\,\lambda_{21} - \tilde{S}^{\mathrm{el}}_{22}\,\lambda_{11}\,\lambda_{12} - \tilde{S}^{\mathrm{el}}_{11}\,\lambda_{21}\,\lambda_{22} + \tilde{S}^{\mathrm{el}}_{21}\,\lambda_{11}\,\lambda_{22}}{J^{c\,2/3}\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)^2} \tag{47}$$

$$\tilde{S}_{12} = \frac{\tilde{S}^{\mathrm{el}}_{12}\,\lambda_{11}\,\lambda_{22} - \tilde{S}^{\mathrm{el}}_{22}\,\lambda_{11}\,\lambda_{12} - \tilde{S}^{\mathrm{el}}_{11}\,\lambda_{21}\,\lambda_{22} + \tilde{S}^{\mathrm{el}}_{21}\,\lambda_{12}\,\lambda_{21}}{J^{c\,2/3}\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)^2} \tag{48}$$

$$\tilde{S}_{22} = \frac{\tilde{S}^{\mathrm{el}}_{11}\,{\lambda_{21}}^2 + \tilde{S}^{\mathrm{el}}_{22}\,{\lambda_{11}}^2 - \tilde{S}^{\mathrm{el}}_{12}\,\lambda_{11}\,\lambda_{21} - \tilde{S}^{\mathrm{el}}_{21}\,\lambda_{11}\,\lambda_{21}}{J^{c\,2/3}\left(\lambda_{11}\,\lambda_{22} - \lambda_{12}\,\lambda_{21}\right)^2} \tag{49}$$

$$\tilde{S}_{33} = \frac{\tilde{S}^{\mathrm{el}}_{33}}{J^{c\,2/3}\,{\lambda_{33}}^2} \tag{50}$$

$$\tilde{P}_{11} = F_{11}\,\tilde{S}_{11} + F_{12}\,\tilde{S}_{21} \tag{51}$$

$$\tilde{P}_{21} = F_{21}\,\tilde{S}_{11} + F_{22}\,\tilde{S}_{21} \tag{52}$$

$$\tilde{P}_{12} = F_{11}\,\tilde{S}_{12} + F_{12}\,\tilde{S}_{22} \tag{53}$$

$$\tilde{P}_{22} = F_{21}\,\tilde{S}_{12} + F_{22}\,\tilde{S}_{22} \tag{54}$$

$$\tilde{P}_{33} = \tilde{S}_{33} \tag{55}$$

$$\tilde{\sigma}_{11} = \frac{F_{11}\,\tilde{P}_{11} + F_{12}\,\tilde{P}_{12}}{J} \tag{56}$$

$$\tilde{\sigma}_{21} = \frac{F_{11}\,\tilde{P}_{21} + F_{12}\,\tilde{P}_{22}}{J} \tag{57}$$

$$\tilde{\sigma}_{12} = \frac{F_{21}\,\tilde{P}_{11} + F_{22}\,\tilde{P}_{12}}{J} \tag{58}$$

$$\tilde{\sigma}_{22} = \frac{F_{21}\,\tilde{P}_{21} + F_{22}\,\tilde{P}_{22}}{J} \tag{59}$$

$$\tilde{\sigma}_{33} = \frac{\tilde{P}_{33}}{J} \tag{60}$$

$$\tilde{\tau}_{11} = \frac{2\,\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{33}}{3} \tag{61}$$

$$\tilde{\tau}_{21} = \tilde{\sigma}_{21} \tag{62}$$

$$\tilde{\tau}_{12} = \tilde{\sigma}_{12} \tag{63}$$

$$\tilde{\tau}_{22} = \frac{2\,\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} - \frac{\tilde{\sigma}_{33}}{3} \tag{64}$$

$$\tilde{\tau}_{33} = \frac{2\,\tilde{\sigma}_{33}}{3} - \frac{\tilde{\sigma}_{22}}{3} - \frac{\tilde{\sigma}_{11}}{3} \tag{65}$$

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

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

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

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

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

$$\tilde{M}_{33}^{el} = J\,\tilde{\tau}_{33} \tag{71}$$

Viscoplastic rates:

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

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

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

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

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

Viscoplastic rate equations in non-dimensional form:

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

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

$$\text{where, } \dot{\tilde{d}}_0 = \dot{d}_0 t_{\text{ref}} \tag{79}$$

Stress equilibrium Equation:

$$\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \mathbf{P} = \mathbf{0}. \tag{80}$$

$$\frac{\partial P_{11}}{\partial X} + \frac{\partial P_{12}}{\partial Y} = 0 \tag{81}$$

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

In non-dimensional form:

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

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

So,

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

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

Mass conservation Equation:

$$\frac{\partial c}{\partial t} = -\boldsymbol{\nabla}_{\boldsymbol{X}} \cdot \boldsymbol{j} = -(\frac{\partial j_x}{\partial X} + \frac{\partial j_y}{\partial Y}) \tag{87}$$

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

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

For one way coupling:

$$\boldsymbol{j} = -D_0 \boldsymbol{\nabla}_{\boldsymbol{X}} c \tag{90}$$

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

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

$$= -\frac{\partial \tilde{c}}{\partial \tilde{X}} \tag{93}$$

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

$$= -\frac{\partial \tilde{c}}{\partial \tilde{Y}} \tag{95}$$

For two way coupling:

$$\boldsymbol{j} = -\frac{1}{R_g T}\frac{D\chi_{\max}\tilde{c}}{V_m^b}(\mathbf{F})^{-1}(\mathbf{F})^{-\mathsf{T}}\boldsymbol{\nabla}_{\boldsymbol{X}}\mu \tag{96}$$

$$\tilde{\boldsymbol{j}} = \frac{\boldsymbol{j}H}{c_{\max}D_0} = -\frac{1}{R_g T}\tilde{D}\tilde{c}(\mathbf{F})^{-1}(\mathbf{F})^{-\mathsf{T}}\boldsymbol{\nabla}_{\boldsymbol{X}}\mu \tag{97}$$

$$D = D_0\exp(\frac{\alpha \mathrm{S_h}}{\mathrm{E_0}}) = \mathrm{D_0}\exp(\alpha\tilde{\mathrm{S}}_\mathrm{h}) \tag{98}$$

$$\mu = \mu_0 + \mu_s; \tilde{\mu} = \frac{\mu}{R_g T} \tag{99}$$

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

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

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

$$\tilde{\mu}_s = \frac{1}{R_g T}\mu_s \tag{103}$$

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

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

$$\tilde{C}_{ijkl} = \tilde{\lambda}_{si}(\tilde{c})\delta_{ij}\delta_{kl} + \tilde{\mu}_{si}(\tilde{c})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{106}$$

$$\tilde{S}_{ij}^{\mathrm{el}} = J^c\tilde{C}_{ijkl}\tilde{E}_{kl}^{\mathrm{el}} \tag{107}$$

$$\tilde{\mu}_s = \frac{1}{\chi_{\max}}\left[-\frac{1}{3J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{F}_{im}^{\mathrm{el}}\tilde{F}_{in}^{\mathrm{el}}\tilde{S}_{mn}^{\mathrm{el}} + \frac{1}{2}J^c\frac{\partial\tilde{C}_{ijkl}}{\partial\tilde{c}}\tilde{E}_{ij}^{\mathrm{el}}\tilde{E}_{kl}^{\mathrm{el}} + \frac{1}{2}\frac{\partial J^c}{\partial\tilde{c}}\tilde{C}_{ijkl}\tilde{E}_{ij}^{\mathrm{el}}\tilde{E}_{kl}^{\mathrm{el}}\right] \tag{108}$$

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

$$= \frac{1}{\chi_{\max}}\left[\frac{1}{J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{S}_{mn}^{\mathrm{el}}\left(-\frac{1}{3}\tilde{F}_{im}^{\mathrm{el}}\tilde{F}_{in}^{\mathrm{el}} + \frac{1}{2}\tilde{E}_{mn}^{\mathrm{el}}\right) + \frac{1}{2}J^c\frac{\partial\tilde{C}_{ijkl}}{\partial\tilde{c}}\tilde{E}_{ij}^{\mathrm{el}}\tilde{E}_{kl}^{\mathrm{el}}\right] \tag{110}$$

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

$$= \frac{1}{\chi_{\max}}\left[-\frac{1}{6J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{S}_{mn}^{\mathrm{el}}\tilde{E}_{mn}^{\mathrm{el}} - \frac{1}{3J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{S}_{mn}^{\mathrm{el}}\delta_{mn} + \frac{1}{2}J^c\frac{\partial\tilde{C}_{ijkl}}{\partial\tilde{c}}\tilde{E}_{ij}^{\mathrm{el}}\tilde{E}_{kl}^{\mathrm{el}}\right] \tag{112}$$

$$= \frac{1}{\chi_{\max}}\left[-\frac{1}{6J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{S}_{mn}^{\mathrm{el}}\tilde{E}_{mn}^{\mathrm{el}} - \frac{1}{3J^c}\frac{\partial J^c}{\partial\tilde{c}}\tilde{S}_{mm}^{\mathrm{el}} + \frac{1}{2}J^c\frac{\partial\tilde{C}_{ijkl}}{\partial\tilde{c}}\tilde{E}_{ij}^{\mathrm{el}}\tilde{E}_{kl}^{\mathrm{el}}\right] \tag{113}$$

$$= \frac{1}{\chi_{\max}}(\tilde{\mu}_1 + \tilde{\mu}_2 + \tilde{\mu}_3) \tag{114}$$

$$\tilde{\mu}_0 = \log(\gamma\tilde{c}) \tag{115}$$

$$\tilde{\mu}_1 = -\frac{1}{6(J^c)}\frac{\partial J^c}{\partial \tilde{c}}[\tilde{S}^{\text{el}}_{11}\tilde{E}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22}\tilde{E}^{\text{el}}_{22} + 2\tilde{S}^{\text{el}}_{12}\tilde{E}^{\text{el}}_{12} + \tilde{S}^{\text{el}}_{33}\tilde{E}^{\text{el}}_{33}] \tag{116}$$

$$\tilde{\mu}_2 = -\frac{1}{3(J^c)}\frac{\partial J^c}{\partial \tilde{c}}[\tilde{S}^{\text{el}}_{11} + \tilde{S}^{\text{el}}_{22} + \tilde{S}^{\text{el}}_{33}] \tag{117}$$

$$\tilde{\mu}_3 = \frac{1}{2}J^c\frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}}\tilde{E}^{\text{el}}_{kl}\tilde{E}^{\text{el}}_{ij} \tag{118}$$

$$\frac{\partial \tilde{C}_{ijkl}}{\partial \tilde{c}} = \frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}}\delta_{ij}\delta_{kl} + \frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{119}$$

$$\tilde{\mu}_3 = \frac{1}{2}J^c\frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}}\delta_{ij}\delta_{kl}\tilde{E}^{\text{el}}_{kl}\tilde{E}^{\text{el}}_{ij} + \frac{1}{2}J^c\frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}}(\delta_{ik}\delta_{jl}\tilde{E}^{\text{el}}_{kl}\tilde{E}^{\text{el}}_{ij} + \delta_{il}\delta_{jk}\tilde{E}^{\text{el}}_{kl}\tilde{E}^{\text{el}}_{ij}) \tag{120}$$

$$= \frac{1}{2}J^c\frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}}\tilde{E}^{\text{el}}_{kk}\tilde{E}^{\text{el}}_{ii} + \frac{1}{2}J^c\frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}}(\tilde{E}^{\text{el}}_{ij}\tilde{E}^{\text{el}}_{ij} + \tilde{E}^{\text{el}}_{ji}\tilde{E}^{\text{el}}_{ij}) \tag{121}$$

$$= \frac{1}{2}J^c\frac{\partial \tilde{\lambda}_{si}(\tilde{c})}{\partial \tilde{c}}(\text{tr}(\mathbf{E}^{\text{el}}))^2 + J^c\frac{\partial \tilde{\mu}_{si}(\tilde{c})}{\partial \tilde{c}}\tilde{E}^{\text{el}}_{ij}\tilde{E}^{\text{el}}_{ij} \tag{122}$$

$$= \frac{1}{2}J^c[\tilde{\lambda}'_{\text{si}}(c)(\tilde{E}^{\text{el}}_{11} + \tilde{E}^{\text{el}}_{22} + \tilde{E}^{\text{el}}_{33})^2 + 2\tilde{\mu}'_{\text{si}}(\tilde{c})((\tilde{E}^{\text{el}}_{11})^2 + (\tilde{E}^{\text{el}}_{22})^2 + (\tilde{E}^{\text{el}}_{33})^2 + 2(\tilde{E}^{\text{el}}_{12})^2)] \tag{123}$$

$$\boldsymbol{j} = -\frac{D\chi_{\max}\tilde{c}}{V^b_m}\tilde{\mathbf{F}}^{-1}(\tilde{\mathbf{F}}^{-1})^{\mathsf{T}}\nabla_{\boldsymbol{X}}\tilde{\mu} \tag{124}$$

$$\tilde{\boldsymbol{j}} = \boldsymbol{j}HV^b_m/(\chi_{\max}D_0) \tag{125}$$

$$= -\frac{D}{D_0}H\tilde{c}\tilde{\mathbf{F}}^{-1}(\tilde{\mathbf{F}}^{-1})^{\mathsf{T}}\nabla_{\boldsymbol{X}}\tilde{\mu} \tag{126}$$

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

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

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

$$= \frac{-\bar{D}\tilde{c}}{J^2}\left(\frac{\partial\tilde{\mu}}{\partial \tilde{Y}}(\tilde{F}^2_{11} + \tilde{F}^2_{21}) - \frac{\partial\tilde{\mu}}{\partial \tilde{X}}(\tilde{F}_{11}\tilde{F}_{12} + \tilde{F}_{21}\tilde{F}_{22})\right) \tag{130}$$

$$\tag{131}$$

0.2.8 Boundary and Initial Conditions

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

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

$$\tilde{v}(\tilde{X}, \tilde{Y}, 0) = 0 \tag{134}$$

$$\tilde{u}(\tilde{X}, 0, \tilde{t}) = \tilde{v}(\tilde{X}, 0, \tilde{t}) = 0 \tag{135}$$

$$\tilde{u}(-1/2, \tilde{Y}, \tilde{t}) = \tilde{u}(1/2, \tilde{Y}, \tilde{t}) = 0 \tag{136}$$

$$\tilde{j}_x(\tilde{X}, 1, \tilde{t}) = \tilde{j}_0(1 - \tilde{c}(\tilde{X}, 1, \tilde{t})) \tag{137}$$