On The Development of a Multi-Scale Continuum Model for Anisotropic Plasticity Due to Texture

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Abstract

An internal state variable constitutive theory provides a robust framework for incorporating irreversible, path dependent behavior. It contains developing a consistent kinematics based on the defined degree of freedom, chose the state variables and a function for free energy equation that shows the amount of energy inside material to do the work that is a function of defined state variables, evaluation of thermodynamics laws and drive the constraint equation and finally develop the constitutive equation.

In this report, an anisotropic ISV based material model is developed. The deformation state is decomposed into elastic and plastic part and the kinematics quantities such as deformation gradients and their time derivatives in intermediate configuration are developed using proper mapping in terms of push forward and pullback operations section.1. Then, in section 2, based on the definition of the free energy in the intermediate configuration, and the thermodynamics laws, thermodynamics restrictions are defined to develop the constitutive relations. Anisotropic texture is considered based on a series of tensorial statistical distribution function that contains the information on grain orientations in the representative volume element (section 3). The first two terms in the series of the distribution function are considered that contains a scalar and a second rank tensor known as structure tensor. The evolution equation of structure tensor is shown and a closure approximation (section 3.1) is used to prevent the appearance of higher order terms of the series in the evolution equation of structure tensor. At the end, the whole set of constitutive equation to integrate is shown in section 4

1. Multiplicative decomposition of the deformation gradient

The multiplicative decomposition of the deformation gradient into elastic and plastic parts (figure.1) is postulated as

$$F = F^e F^p \quad (1)$$

This can be described by a typical behavior in metallic materials which the material behaves elastically up to a certain point and then plastically deforms. The elastic part is defined as $F^e = \frac{dx}{d\overline{X}}$ and the plastic part is $F^p = \frac{d\overline{X}}{dX}$ then in order to reproduce F through this decomposition and based on the chain rule we have $F = \frac{dx}{dX} = \frac{dx}{d\overline{X}}\frac{d\overline{X}}{dX} = F^e F^p$ based on the this decomposition three configurations can be identified for the deformation as the reference, intermediate and current configurations. F maps the infinitesimal line segment dX from the reference configuration $\mathbf{B}_0$ to the infinitesimal line segment dx in the current configuration $\mathbf{B}_0$. The multiplicative decomposition introduces a new configuration known as the intermediate configuration and is represented as $\overline{B}_0$. Similarly F^p maps dX to $d\overline{X}$ and F^e maps $d\overline{X}$ to dx.

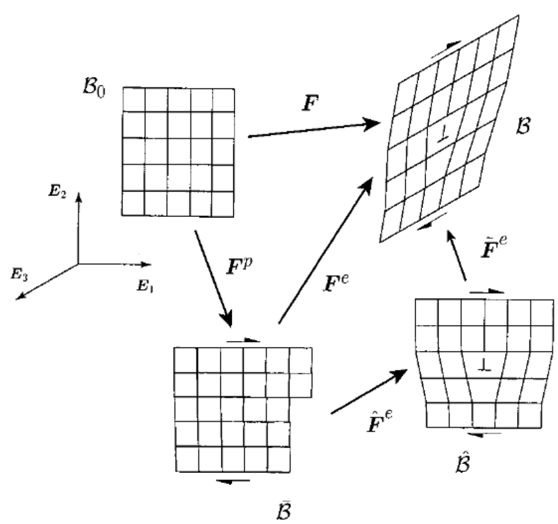

Figure 1 Multiplicative decomposition of the deformation gradient [Regueiro et al. 2001]

Velocity gradient defined in the current configuration is $l = \dot{F} F^{-1}$ which can be represented through the decomposition as

$$l = \dot{F}^e F^{e^{-1}} + F^e \dot{F}^p F^{p^{-1}} F^{e^{-1}} = l^e + l^p \quad (2)$$

Similarly the plastic velocity gradient in the intermediate configuration is

$$\overline{L}^p = \dot{F}^p F^{p^{-1}} \quad (3)$$

Pulling back the velocity gradient in the current configuration to intermediate configuration the velocity gradient can be decomposed into pure elastic and pure plastic components. In this context the pure plastic and pure elastic means that all required map is defined by plastic and elastic deformation gradient respectively.

$$\overline{L} = F^{e^{-1}} l \, F^e = F^{e^{-1}} \dot{F}^e + \dot{F}^p F^{p^{-1}} = \overline{L}^e + \overline{L}^p \quad (4)$$

Therefore, the elastic velocity gradient which can be identified as pure elastic velocity gradient is defined by

$$\overline{L}^e = F^{e^{-1}} \dot{F}^e \quad (5)$$

The velocity gradient can be decomposed into the summation of symmetric and skew-symmetric deformation. The pure plastic velocity gradient can be written as:

$$\overline{L}^p = \overline{D}^p + \overline{W}^p \quad (6)$$

The symmetric part is defined as rate of deformation tensor and the skew-symmetric part is the spin or in this case pure plastic spin. These quantities can be derived from

$$\overline{D}^p = \frac{1}{2}\left(\overline{L}^p + \overline{L}^{p^T}\right) \quad (7)$$

$$\overline{W}^p = \frac{1}{2}\left(\overline{L}^p - \overline{L}^{p^T}\right) \quad (8)$$

and $\overline{L}^p$ can be mapped to the current configuration using the relation below

$$l^p = F^e \, \overline{L}^p \, F^{e^{-1}} \quad (9)$$

The elastic strains in intermediate and current configuration are:

$$\overline{E}^{e}=\frac{1}{2}\left(F^{e^{T}}F^{e}-I\right) \qquad (10)$$

$$e^{e}=F^{e^{-T}}\overline{E}^{e}\,F^{e^{-1}}=\frac{1}{2}\left(I-F^{e^{-T}}F^{e^{-1}}\right) \qquad (11)$$

F will be determined by balance of linear momentum l is derived, having $\overline{D}^{p}$ and $\overline{W}^{p}$ from constitutive equations then elastic velocity gradient in current configuration is derived $l^{e}=l-l^{p}$

2. Thermodynamics

In this section, the thermodynamic in intermediate configuration is shown by the transformation of all the components in the thermodynamic laws from the current configuration based on the work of Regueiro et al 2001. The first law of thermodynamics for a body in current configuration states that the total energy rate is equal to the power input plus the heat input rate as

$$\frac{d}{dt}\int_{B}\left(\frac{1}{2}\rho v.v+\rho e\right)dv=\frac{d}{dt}\int_{B}\left(\frac{1}{2}\rho v.v\right)dv+\int_{B}\sigma:l\,dv-\int_{\partial B}q.n\,da+\int_{B}r\,d\,dv \qquad (12)$$

where ρ is the mass density, v is velocity, e is internal energy per unit mass, σ is Cauchy stress, l is the velocity gradient, q is the heat flux into **B**, n is unit normal to ∂B pointing out of **B**, and r is the internal heat supply per unit mass. Using the definition of material time derivative and cancelling the term of kinetic energy term in both sides, the first law can be written as

$$\int_{B}\left(\rho\frac{de}{dt}\right)dv=\int_{B}\sigma:l\,dv-\int_{\partial B}q.n\,da+\int_{B}\rho\,r\,dv \qquad (13)$$

The thermodynamics in intermediate configuration is derived using following transformations:

$$,\ dv=J^{e}\,dV,\ J^{e}(F^{e^{-1}}.q)=\overline{Q},\ \sigma=(1/J^{e})F^{e}.\overline{S}.F^{e^{T}}\ ,\ N\,dA=1/J^{p}(F^{p^{T}}.\overline{N})d\overline{A} \qquad (14)$$

$$l=F\,\overline{L}\ F^{-1},\ \overline{\rho}=\rho J^{e}$$

$$\int_{\overline{B}}\left(\overline{\rho}\frac{de}{dt}\right)d\overline{V}=\int_{\overline{B}}\overline{L}:(\overline{C}^{e}.\overline{S})\,d\overline{V}-\int_{\partial\overline{B}}\overline{Q}.\overline{N}\,d\overline{A}+\int_{B}\overline{\rho}\,r\,d\overline{V} \qquad (15)$$

where $(\overline{C}^e.\overline{S})$ is the Mandel stress and $\overline{S}$ is the second Piola-Kirchhoff stress in intermediate configuration. Applying the divergence theorem and rewriting the equations into the local form the first law of thermodynamic can be shown as

$$\overline{\rho}\,\dot{e} = \overline{L} : (\overline{C}^e.\overline{S}) - \overline{\nabla}\,\overline{Q} + \overline{\rho}\,r \qquad (16)$$

The second law states that over a body **B** in the current configuration the rate of entropy increase is greater or equal to the time rate of entropy that enters to the system

$$\frac{d}{dt}\int_B \rho\,\eta\,dv \geq \int_B \rho\frac{r}{\theta}dv - \int_{\partial B}\frac{1}{\theta}q.n\,da \qquad (17)$$

η is the entropy per unit mass, and θ is the absolute temperature. Mapping the second law of thermodynamics using the above transformations into the intermediate configuration results into the following equation

$$\int_{\overline{B}} \overline{\rho}\,\frac{\partial\eta}{\partial t}d\overline{V} \geq \int_{\overline{B}} \overline{\rho}\frac{r}{\theta}d\overline{V} - \int_{\partial\overline{B}}\frac{\overline{Q}}{\theta}.\overline{N}\,d\overline{A} \qquad (18)$$

The local form of the second law in the intermediate configuration is

$$\overline{\rho}\,\dot{\eta} \geq \overline{\rho}\frac{r}{\theta} - \overline{\nabla}.\left(\frac{\overline{Q}}{\theta}\right) \qquad (19)$$

The Helmoltz free energy per unit mass in the current configuration is ψ

$$\psi = e - \eta\theta \qquad (20)$$

Let's assume that the free energy in the intermediate configuration can be described solely by elastic strain energy and thermal internal energy. Therefore, the free energy in the intermediate configuration is a function of compatible lattice deformation due to external mechanical forces, $\overline{E}^e$, lattice deformation due to the presence of statistically stored dislocations, $\overline{\boldsymbol{\varepsilon}}_{ss}$, incompatible lattice deformation due to the presence of geometric necessary dislocation at grain boundaries and around second phase particles, $\overline{\alpha}_l^e$, and absolute temperature, θ:

$$\bar{\rho}\bar{\psi} = \bar{\rho}\bar{\psi}(\bar{E}^e, \bar{\varepsilon}_{ss}, \bar{\alpha}_l^e, \theta) \qquad (21)$$

The free energy in the current and intermediate configuration has the relation below

$$\bar{\rho}\bar{\psi}(\bar{E}^e, \bar{\varepsilon}_{ss}, \bar{\alpha}_l^e, \theta) = \bar{\rho}\psi(e^e, \varepsilon_{ss}, \alpha_l^e, \theta) \qquad (22)$$

Combining the definition of Helmholtz free energy and first law of thermodynamics in the intermediate configuration in the second law in the intermediate configuration the Clausius-Duhem inequality in the intermediate configuration is

$$-\bar{\rho}\dot{\psi} - \bar{\rho}\eta\dot{\theta} + \bar{L} : (\bar{C}^e . \bar{S}) - \frac{1}{\theta}\bar{Q}\,\bar{\nabla}\theta \geq 0 \qquad (23)$$

From the chain rule the time derivative of the free energy in intermediate configuration is

$$\dot{\bar{\psi}} = \frac{\partial\bar{\psi}}{\partial\bar{E}^e} : \dot{\bar{E}}^e + \frac{\partial\bar{\psi}}{\partial\bar{\alpha}_l^e} : \dot{\bar{\alpha}}_l^e + \frac{\partial\bar{\psi}}{\partial\bar{\varepsilon}_{ss}}\dot{\bar{\varepsilon}}_{ss} + \frac{\partial\bar{\psi}}{\partial\theta}\dot{\theta} \qquad (24)$$

By expending $\bar{L} : (\bar{C}^e . \bar{S}) = \bar{S} : \dot{\bar{E}}^e + (\bar{C}^e . \bar{S}) : \bar{L}^p$

$$\left(-\bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{E}^e} + \bar{S}\right) : \dot{\bar{E}}^e - \bar{\rho}\left(\frac{\partial\bar{\psi}}{\partial\theta} + \eta\right)\dot{\theta} - \bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{\alpha}_l^e} : \dot{\bar{\alpha}}_l^e - \bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{\varepsilon}_{ss}}\dot{\bar{\varepsilon}}_{ss} + (\bar{C}^e . \bar{S}) : \bar{L}^p - \frac{1}{\theta}\bar{Q}\,\bar{\nabla}\theta \geq 0 \qquad (25)$$

Following Coleman and Noll, Coleman and Gurtin the to have an arbitrary value for the $\bar{E}^e$ and θ the below constrain equations should be hold

$$,\ \eta = -\frac{\partial\bar{\psi}}{\partial\theta}\ \bar{S} = \bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{E}^e} \qquad (26)$$

The stress like internal state variables conjugates to $\dot{\bar{\alpha}}_l^e$ and $\dot{\bar{\varepsilon}}_{ss}$ can be introduced as

$$,\ \bar{\kappa} = \bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{\varepsilon}_{ss}}\ \bar{\zeta} = \bar{\rho}\frac{\partial\bar{\psi}}{\partial\bar{\alpha}_l^e} \qquad (27)$$

where $\bar{\kappa}$ is the scalar internal stress field in the lattice due to statistically store disolocations, and $\bar{\zeta}$ is the internal dislocation stress field due to geometrically necessary dislocations. The dissipation inequality then reduces to

$$\bar{S} : \bar{D}^p - \bar{\zeta} : \dot{\bar{\alpha}}_l^e - \bar{\kappa}\dot{\bar{\varepsilon}}_{ss} - \frac{1}{\theta}\bar{Q}\,\bar{\nabla}\theta \geq 0 \qquad (28)$$

The stored elastic energy within the crystal lattice and thermal internal energy are representing the Helmholtz free energy in the intermediate configuration assuming small elastic stretch

$$\bar{\rho}\bar{\psi} = \frac{1}{2}\bar{E}^e : \bar{\mathrm{C}}^e(\theta) : \bar{E}^e + \frac{1}{2}c_\kappa \mu(\theta)\bar{\varepsilon}_{ss}{}^2 + \frac{1}{2}c_\zeta \mu(\theta)\bar{\alpha}_l^e : \bar{\alpha}_l^e + \bar{g}(\theta) \qquad (29)$$

Where $\bar{\mathrm{C}}^e(\theta) = \lambda(\theta)\bar{1} \otimes \bar{1} + 2\mu(\theta)\bar{I}$ is the modulus tensor assuming linear isotropic elasticity, $\lambda(\theta)$ and $\mu(\theta)$ are temperature dependent Lame parameters and $\mu(\theta)$ is the shear modulus, c_κ and c_ζ are material constants and $\bar{g}(\theta)$ is the internal thermal energy.

$$\bar{S} = \bar{\mathrm{C}}^e : \bar{E}^e \qquad (30)$$

$$\bar{\eta} = -\frac{\partial \bar{\psi}}{\partial \theta} \qquad (31)$$

$$\bar{\kappa} = c_k\, \mu(\theta)\bar{\varepsilon}_{ss} \qquad (32)$$

$$\bar{\zeta} = c_\zeta\, \mu(\theta)\bar{\alpha}_l^e \qquad (33)$$

The evolution for the lattice due to the evolution of the statically-stored dislocation density for representing both thermally activated hardening and dynamic recovery (first term) along with the static recovery from thermal diffusion of dislocations (second term) as

$$\dot{\bar{\varepsilon}}_{ss} = [\hat{H} - R_d(\theta)\bar{\varepsilon}_{ss}]\,\dot{\bar{\varepsilon}}^{p,eff} - R_s(\theta)\bar{\varepsilon}_{ss}\, sinh(\hat{Q}_s(\theta)\,\bar{\varepsilon}_{ss}) \qquad (34)$$

where $\hat{H}$ is the dimensionless hardening constant, $R_d(\theta)$ and $R_s(\theta)$ are the dynamic and static recovery function.

3. Incorporating anisotropic plasticity

The goal here is to derive the incorporate the anisotropic plasticity due to texture. Two important parameters for plasticity model is derived in this section are the plastic rate of deformation $\bar{D}^p$ and plastic spin $\bar{W}^p$.

It is assumed that the orientation of grains in aggregates are represented by a continuous function representing the crystal orientation as orientation distribution function (ODF). In general the estimation of distribution is first determined by achieving a model or parametric form function that describes the orientation distribution. Assume that $\Gamma(\alpha)$ is the given distribution density, and we want to approximate the distribution density by $A(\alpha)$ which involves an indeterminate parameters. In this study, ODF represented by an infinite series in polynomial form shown below:

$$A(\alpha) = A + A_{ij}\,\alpha_i\,\alpha_j + A_{ijkl}\,\alpha_i\,\alpha_j\,\alpha_k\,\alpha_l + \ldots \qquad (35)$$

We also need a criterion to be able to estimate the ODF parameters. The typical approximation is to minimize the least square approximation as

$$\int \left[A(\alpha) - \Gamma(\alpha)\right]^2 d\alpha \to Min \qquad (36)$$

The ODF satisfies the conservative equation owing to the fact that the number of crystals in any initial interval of orientation does not change.

It is assumed that the ODF has the periodicity property which indicates that

$$A(\alpha) = A(-\alpha) \qquad (37)$$

It can be normalized by

$$\text{where } \oint dS = \int_{\phi=0}^{3\pi} \int_{\theta=0}^{\pi} \sin\theta\, d\theta\, d\phi = 4\pi \oint A(\alpha)\, dS = 1 \qquad (38)$$

Prantil et al (1993) showed that ODF satisfies the continuity equation as

$$\dot{A}(\alpha) + A(\alpha)\, div(\dot{\alpha}) = 0 \qquad (39)$$

The parameters in equation (35) known as fabric tensor of third kind proposed by Kanatani (1984) can be derived from equation below:

$$A_{i_1, i_2, \ldots, i_n} = \oint \Gamma(\alpha) \left\{\alpha_{i_1} \alpha_{i_2} \ldots \alpha_{i_n}\right\} d\alpha \qquad (40)$$

which $\left\{\alpha_{i_1} \alpha_{i_2} \ldots \alpha_{i_n}\right\}$ is the deviatoric part of $\alpha_{i_1} \alpha_{i_2} \ldots \alpha_{i_n}$ tensor

Using the first two terms and by truncating the higher order terms, the ODF becomes

$$A(\alpha) = \frac{1}{2\pi} + \frac{2}{\pi} A_{ij}\, f_{ij}(\alpha) \qquad (41)$$

where

$$f_{ij}(\alpha)=\alpha_i\alpha_j-\frac{1}{3}\delta_{ij} \qquad (42)$$

$$A_{ij}=\oint\Gamma(\alpha)\,f_{ij}(\alpha)\,d\alpha \qquad (43)$$

where A_{ij} is called the structure tensor. Therefore, the orientation of actual experimental data represented by $\Gamma(\alpha)$ helps to identify a second rank tensor. Then, the statistical distribution of the orientation can be represented by equation (41).

While the stress varies during the deformation process in material, the crystal structure may orient in different directions. The reorientation of the crystal indicates that the tonsorial constant A_{ij} in the ODF should vary in order to carry out the information of the orientation of the crystal in aggregate. For this we intend to formulate an evolution equation for the structure tensor to be able to carry the anisotropic texture information during deformation process.

The continuity equation (39) indicates that the grain orientation update $\dot{\alpha}$ should be determined. The plastic spin $\overline{W}^p$ is the main cause of the grain reorientation. Then the grain orientation update equation can be written as

$$\dot{\alpha}=\overline{W}^p\,\alpha \qquad (44)$$

The Jaummann derivative of the grain orientation can be written as

$$\breve{\alpha}=\dot{\alpha}-W\,\alpha=\lambda_g\left[\,\overline{D}^p(\alpha\otimes\alpha)-(\alpha\otimes\alpha)\,\overline{D}^p\,\right]=\lambda_g\,\overline{D}^p\alpha-\lambda_g(\alpha.\overline{D}^p\alpha)\alpha \qquad (45)$$

Substituting above equation into the continuity equation gives

$$\dot{A}(\alpha)+A(\alpha)div(\dot{\alpha})=0 \qquad (46)$$

$$\begin{aligned} div(\breve{\alpha})&=div\left(\lambda_g\,\overline{D}^p\alpha-\lambda_g(\alpha.\overline{D}^p\alpha)\alpha\right)=\lambda_g\,div(\overline{D}^p\alpha)-\lambda_g(\alpha.\overline{D}^p\alpha)div(\alpha)\\ &=\lambda_g\left(Tr(\overline{D}^p)-(\alpha.\overline{D}^p\alpha)\right)-\lambda_g(\alpha.\overline{D}^p\alpha)=-2\lambda_g(\alpha.\overline{D}^p\alpha)\end{aligned} \qquad (47)$$

$$\dot{A}(\alpha)=A(\alpha)\left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right) \qquad (48)$$

The material time derivative of the structure tensor definition is

$$\dot{A}_{ij} = \overset{\bullet}{\overline{\oint A(\alpha)\, f_{ij}(\alpha)\, d\alpha}} = \oint \dot{A}(\alpha)\, f_{ij}(\alpha)\, d\alpha + \oint A(\alpha)\, \dot{f}_{ij}(\alpha)\, d\alpha \qquad (49)$$

From the grain orientation update equation (45)

$$\begin{aligned} \dot{f}_{ij}(\alpha) &= \dot{\alpha}\otimes\alpha + \alpha\otimes\dot{\alpha} = \lambda_g\left((\alpha\otimes\alpha - I)\,\overline{D}^p\alpha\right)\otimes\alpha + \lambda_g\alpha\otimes\left((\alpha\otimes\alpha - I)\,\overline{D}^p\alpha\right) \\ &= \lambda_g\left(\overline{D}^p\alpha\otimes\alpha + \alpha\otimes\overline{D}^p\alpha - 2(\alpha.\overline{D}^p\alpha)(\alpha\otimes\alpha)\right) \end{aligned} \qquad (50)$$

$$\begin{aligned} \dot{A}_{ij} &= \overset{\bullet}{\overline{\oint A(\alpha)\, f_{ij}(\alpha)\, d\alpha}} = \oint \dot{A}(\alpha)\, f_{ij}(\alpha)\, d\alpha + \oint A(\alpha)\, \dot{f}_{ij}(\alpha)\, d\alpha \\ &= \oint A(\alpha)\left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right) f_{ij}(\alpha)\, d\alpha \\ &+ \oint A(\alpha)\,\lambda_g\left(\overline{D}^p\alpha\otimes\alpha + \alpha\otimes\overline{D}^p\alpha - 2(\alpha.\overline{D}^p\alpha)(\alpha\otimes\alpha)\right) d\alpha \\ &= \left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right)\oint A(\alpha)\, f_{ij}(\alpha)\, d\alpha \\ &+ \lambda_g\oint A(\alpha)\left(\overline{D}^p\alpha\otimes\alpha + \alpha\otimes\overline{D}^p\alpha - 2(\alpha.\overline{D}^p\alpha)(\alpha\otimes\alpha)\right) d\alpha \\ &= \left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right)A_{ij} + \lambda_g\oint A(\alpha)\left(\overline{D}^p\alpha\otimes\alpha + \alpha\otimes\overline{D}^p\alpha - 2(\alpha.\overline{D}^p\alpha)(\alpha\otimes\alpha)\right) d\alpha \\ &= \left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right)A_{ij} + \lambda_g\oint A(\alpha)\left(\overline{D}^p\alpha\otimes\alpha + \alpha\otimes\overline{D}^p\alpha\right) d\alpha \\ &- 2\lambda_g(\alpha.\overline{D}^p\alpha)\oint A(\alpha)(\alpha\otimes\alpha - \frac{1}{3}\delta_{ij} + \frac{1}{3}\delta_{ij})\, d\alpha \\ &= -\left(2\lambda_g(\alpha.\overline{D}^p\alpha)\right)A_{ij} + \lambda_g(A\overline{D}^p + \overline{D}^p A + \frac{2}{3}\overline{D}^p) + \frac{2}{3}\lambda_g(\alpha.\overline{D}^p\alpha)\oint A(\alpha)\delta_{ij}\, d\alpha \\ \overset{\bullet}{A} &= -2\lambda_g b : \overline{D}^p + \lambda_g(A\overline{D}^p + \overline{D}^p A + \frac{2}{3}\overline{D}^p) + \frac{2}{3}\lambda_g(\alpha.\overline{D}^p\alpha)\delta_{ij} \end{aligned} \qquad (51)$$

Having A in the intermediate configuration:

Based on the multiplicative decomposition of the deformation gradient into elastic and plastic parts $F = F^e F^p$ the evolution equation for the structure tensor in intermediate configuration is

$$\overset{\circ}{A} = F^p(\overset{\bullet}{\overline{F^{p^{-1}}\overline{A}\; F^p}})\, F^{p^{-1}} = \overset{\bullet}{\overline{A}} - \overline{L}^p\overline{A} + \overline{A}\,\overline{L}^p \qquad (52)$$

Considering the symmetric $\overline{A}^T = \overline{A}$ therefore the evolution equation can be represented

$$\overset{\circ}{\overline{A}} = \overset{\bullet}{\overline{A}} - \overline{W}^p\overline{A} + \overline{A}\,\overline{W}^p \qquad (53)$$

Combining equations (51) and (53) the evolution equation of the structure tensor is

$$\overset{\circ}{\overline{A}} = \dot{\overline{A}} - \overline{W}^{p}\overline{A} + \overline{A}\,\overline{W}^{p} = \overline{A}\,\overline{W}^{p} - \overline{W}^{p}\overline{A} + \lambda_g(A\overline{D}^{p} + \overline{D}^{p}A + \frac{2}{3}\overline{D}^{p}) + \frac{2}{3}\lambda_g(\alpha.\overline{D}^{p}\alpha)\delta_{ij} - 2\lambda_g b : \overline{D}^{p} \tag{54}$$

where b is a fourth rank tensor defined as

$$b_{ijkl} = \oint A(\alpha)\alpha_i\,\alpha_j\,\alpha_k\,\alpha_l\,d\theta \tag{55}$$

3.1 Closure Approximation

The structure tensor A_{ij} is the moment of the distribution function $A(\alpha)$, and the evolution equation of A presents a closure problem. The evolution equation (54) for any tensor in the set always contains the next higher even-order tensor (Advani&Tucker 1987). Therefore, the evolution equation of second order structure tensor contains a fourth order tensor b_{ijkl} . It is required to develop some approximation to obtain a close set of evolution equation. The closure approximation should contain several facts including:

1- The approximation must only be from the lower order orientation tensors and the unit tensor.

2- The approximation must satisfy normalization conditions in equations (56) and (57)

$$A_{ii} = 1 \qquad (56)$$

$$b_{ijkk} = A_{ij} \qquad (57)$$

3- The approximation should maintain the symmetry of orientation tensor (equations (58) and (59))

$$A_{ij} = A_{ij} \qquad (58)$$

$$b_{ijkl} = b_{jikl} = b_{kijl} = b_{lijk} = b_{klij} \qquad (59)$$

Hand (1962) proposed a closure approximation known as the linear closure approximation for fourth order tensor b_{ijkl} using all of the products of A_{ij} and δ_{ij}. Applying Normalization and symmetry requirements (equations 56 - 59) shows that the only linear terms may be used that is called linear closure approximation shown by $\hat{b}_{ijkl}$

For three-dimensional orientation the linear approximation of fourth order tensor becomes

$$\hat{b}_{ijkl} = -\frac{1}{35}\left(\delta_{ij}\,\delta_{kl} + \delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk}\right) + \frac{1}{7}\left(A_{ij}\delta_{kl} + A_{ik}\delta_{jl} + A_{il}\delta_{jk} + A_{kl}\delta_{ij} + A_{jl}\delta_{ik} + A_{jk}\delta_{il}\right) \qquad (60)$$

Another way to form a closure approximation is to omit the linear terms and take the product of lower order tensors. This is known as quadratic closure, $\tilde{b}_{ijkl}$, which is proposed by several authors (Doi 1981, Marrucci & Grizzuti 1984)

$$\tilde{b}_{ijkl} = A_{ij}\, A_{kl} \tag{61}$$

The quadratic closure does not have all the symmetries of b_{ijkl} (equation 59) but it has the symmetries of elasticity tensor and presents no difficulty for mechanical property predictions. It is worth mentioning that once this approximation is used in the evolution equation, it preserves the symmetry of A_{ij}.

In dilute short fiber composites, it is shown that the linear closure approximations are exact for a completely random distribution of fiber orientation while the quadratic closure approximations are exact for perfect uniaxial alignments of the fibers. Hence, the combination of the two closure approximations can offer the orientation information for the entire range of orientations. A hybrid closure approximation $\bar{b}_{ijkl}$ is constructed by combining the two presented approximation as

$$\bar{b}_{ijkl} = (1-f)\,\hat{b}_{ijkl} + f\,\tilde{b}_{ijkl} \tag{62}$$

where f is a generalization of Herman's orientation factor; it is equal to zero for randomly oriented inclusions and unity for perfectly aligned inclusions. The scalar measure f is defined as

$$f = C_1\, A_{ij}\, A_{ji} - C_2 = \frac{3}{2} A_{ij}\, A_{ji} - \frac{1}{2} \tag{63}$$

for three dimensional orientation which is an invariant of A_{ij}.

Applying the closure approximation to the last term in equation (54)

$$\bar{b} : \bar{D}^p = b_{ijkl}\, \bar{D}^p{}_{kl} = \left[(1-f)\left(-\frac{1}{35}\left(\delta_{ij}\,\delta_{kl} + \delta_{ik}\,\delta_{jl} + \delta_{il}\,\delta_{jk}\right) + \frac{1}{7}\left(A_{ij}\delta_{kl} + A_{ik}\delta_{jl} + A_{il}\delta_{jk} + A_{kl}\delta_{ij} + A_{jl}\delta_{ik} + A_{jk}\delta_{il}\right)\right) + f\, A_{ij}\, A_{kl} \right] \bar{D}^p{}_{kl}$$

$$= (1-f)\left(-\frac{1}{35}\left(\delta_{ij}\, Tr(\bar{D}^p) + \bar{D}^p + \bar{D}^p\right) + \frac{1}{7}\left(A\, Tr(\bar{D}^p) + \bar{D}^p A + A\bar{D}^p + \left(A : \bar{D}^p\right)\delta_{ij} + A\bar{D}^p + \bar{D}^p A\right)\right) + f\left(A : \bar{D}^p\right) A_{ij}$$

$$\bar{b} : \bar{D}^p = (1-f)\left(-\frac{1}{35}\left(2\bar{D}^p\right) + \frac{1}{7}\left(A\bar{D}^p + A\bar{D}^p + \left(A : \bar{D}^p\right)\delta_{ij} + \bar{D}^p A + \bar{D}^p A\right)\right) + f\left(A : \bar{D}^p\right) A_{ij}$$

$$\bar{b} : \bar{D}^p = (1-f)\left(-\frac{1}{35}\left(2\bar{D}^p\right) + \frac{1}{7}\left(2A\bar{D}^p + \left(A : \bar{D}^p\right)\delta_{ij} + 2\,\bar{D}^p A\right)\right) + f\left(A : \bar{D}^p\right) A \tag{64}$$

Hence, the final evolution equation of the structure tensor reads

$$\overset{\circ}{\overline{A}} = \dot{\overline{A}} - \overline{W}^p \overline{A} + \overline{A}\,\overline{W}^p =$$
$$-2\lambda_g \left((1-f)\left(-\frac{1}{35}\left(2\overline{D}^p\right) + \frac{1}{7}\left(2A\overline{D}^p + \left(A:\overline{D}^p\right)\delta_{ij} + 2\overline{D}^p A\right)\right) + f\left(A:\overline{D}^p\right)A \right) \tag{65}$$
$$+\lambda_g \left(A\overline{D}^p + \overline{D}^p A + \frac{2}{3}\overline{D}^p \right) + \frac{2}{3}\lambda_g \left(A:\overline{D}^p\right)\delta_{ij} - \overline{W}^p \overline{A} + \overline{A}\,\overline{W}^p$$

$$\left(A:\overline{D}^p\right) = \alpha.\overline{D}^p \alpha \tag{66}$$

λ_g is a geometry parameter dependent on slip system orientation. The plastic spin of the aggregate in the intermediate configuration is defined by averaging the plastic spin in each grain using ODF as

$$\overline{W}^p = \oint A(\alpha) W_g^p(\alpha)\, d\alpha = \lambda_g \left(\overline{A}\,\overline{D}^p - \overline{D}^p \overline{A}\right) \tag{67}$$

The asymmetric part of the velocity gradient should be added to the skew-symmetric part to obtain the velocity gradient in the deformation process.

$$\overline{l^p} = \overline{D}^p + \overline{W}^p \tag{68}$$

The symmetric part of velocity gradient $\overline{D}^p$ is defined separately by its magnitude $\left\|\overline{D}^p\right\|$ and its direction $\overline{N}^p$.

$$\overline{D}^p = \left\|\overline{D}^p\right\| \overline{N}^p \tag{69}$$

The magnitude of the symmetric part of the velocity gradient which is called the evolution of plastic flow is written in the unified creep plasticity form as

$$\left\|\overline{D}^p\right\| = \sqrt{\frac{3}{2}}\, f(\theta)\left(sinh\,\overline{\Phi}\right)^m \tag{70}$$

where the function $f(\theta)$ determines the strain rate at which the model transitions from rate-independent to rate-dependent behavior, m is the rate sensitivity parameter and, the term inside the hyperbolic sine function called the plastic potential $\overline{\Phi}$ function is defined by

$$\overline{\Phi} = \left[\frac{\Xi^{eff}}{\overline{\chi}\,\overline{\kappa}} - 1 \right] \tag{71}$$

and $\overline{\Xi}^{eff}$ the magnitude of a second rank tensor including the deviatoric part of the Piola-Kirchhoff stress and the back stress defined below

$$\overline{\Xi}^{eff} = \sqrt{\frac{3}{2}}\left\|\overline{\Xi}\right\| \qquad (72)$$

$$\overline{\Xi} = dev\,\overline{S} - dev\,\overline{\zeta} \qquad (73)$$

$$dev\,\overline{S} = \overline{S} - \frac{1}{3}tr(\overline{S}) \qquad (74)$$

$$dev\,\overline{\zeta} = \overline{\zeta} - \frac{1}{3}tr(\overline{\zeta}) \qquad (75)$$

Two terms in the denominator of equation (71) are $\overline{\kappa}$ and $\overline{\chi}$ that are for stress like parameter related to the dislocation density (equation 32) and directional distortion (eq.76).

The directional distortion is defined based on the cosine series as

$$\overline{\chi} = 1 + a_1 \cos\overline{\eta} + a_2 \cos 2\overline{\eta} + a_3 \cos 3\overline{\eta} + a_4 \cos 4\overline{\eta} \qquad (76)$$

The angles in the cosine series is calculated from the angle between the stress tensor $\overline{\Xi}$ and the structure tensor $\overline{A}$ (Regueiro et al. 2001). Similar treatment in term of the distortional yield surface is shown by Ortiz and Popov (1983)

$$\cos\overline{\eta} = \frac{\overline{\Xi} : \overline{A}}{\left\|\overline{\Xi}\right\|\left\|\overline{A}\right\|} \qquad (77)$$

Since there is no flow surface defined for this model, the plastic potential function $\overline{\Phi}$ is used to define the direction of the plastic flow. The direction of plastic flow $\overline{N}^p$ derived as

$$\overline{N}^p = sym\left(\frac{\partial\overline{\Phi}}{\partial\overline{\Xi}}\right) \Big/ \left\| sym\left(\frac{\partial\overline{\Phi}}{\partial\overline{\Xi}}\right)\right\| \qquad (78)$$

$$\frac{\partial\overline{\Phi}}{\partial\overline{\Xi}} = \partial\left[\frac{\overline{\Xi}^{eff}}{\overline{\chi}\,\overline{\kappa}} - 1\right] \Big/ \partial\overline{\Xi} = \left(\frac{\partial\overline{\Xi}^{eff}}{\partial\overline{\Xi}}\overline{\chi}\,\overline{\kappa} - \overline{\kappa}\frac{\partial\overline{\chi}}{\partial\overline{\Xi}}\overline{\Xi}^{eff}\right) \Big/ (\overline{\chi}\,\overline{\kappa})^2$$
$$= \frac{1}{\overline{\chi}\overline{\kappa}}\left(\frac{\partial\overline{\Xi}^{eff}}{\partial\overline{\Xi}} - \frac{1}{\overline{\chi}}\frac{\partial\overline{\chi}}{\partial\overline{\Xi}}\overline{\Xi}^{eff}\right) = \frac{1}{\overline{\chi}\overline{\kappa}}\left(\frac{\partial\overline{\Xi}^{eff}}{\partial\overline{\Xi}} - \frac{\overline{\Xi}^{eff}}{\overline{\chi}}\frac{\partial\overline{\chi}}{\partial\overline{\Xi}}\right) \qquad (79)$$

Where $\bar{\chi}$ and $\bar{\kappa}$ are scalars.

$$\bar{N}^{p} = sym\left(\frac{\partial\bar{\Phi}}{\partial\bar{\Xi}}\right) \Big/ \left\| sym\left(\frac{\partial\bar{\Phi}}{\partial\bar{\Xi}}\right)\right\| = \frac{1}{\bar{\chi}\bar{\kappa}}\, sym\left(\frac{\partial\bar{\Xi}^{eff}}{\partial\bar{\Xi}} - \frac{\bar{\Xi}^{eff}}{\bar{\chi}}\frac{\partial\bar{\chi}}{\partial\bar{\Xi}}\right) \Big/ \frac{1}{\bar{\chi}\bar{\kappa}}\left\| sym\left(\frac{\partial\bar{\Xi}^{eff}}{\partial\bar{\Xi}} - \frac{\bar{\Xi}^{eff}}{\bar{\chi}}\frac{\partial\bar{\chi}}{\partial\bar{\Xi}}\right)\right\| \tag{80}$$

$$\frac{\partial\bar{\Xi}^{eff}}{\partial\bar{\Xi}} = \sqrt{\frac{3}{2}}\,\frac{\bar{\Xi}}{\|\bar{\Xi}\|} \tag{81}$$

And

$$\begin{aligned}
\frac{\partial\bar{\chi}}{\partial\bar{\Xi}} &= \frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\frac{\partial\cos\bar{\eta}}{\partial\bar{\Xi}} = \frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\,\partial\left(\frac{\bar{\Xi}:\bar{A}}{\|\bar{\Xi}\|\|\bar{A}\|}\right)\Big/\partial\bar{\Xi} \\
&= \frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\left(\frac{\partial\left(\bar{\Xi}:\bar{A}\right)}{\partial\bar{\Xi}}\|\bar{\Xi}\|\|\bar{A}\| - \frac{\partial\left(\|\bar{\Xi}\|\|\bar{A}\|\right)}{\partial\bar{\Xi}}\left(\bar{\Xi}:\bar{A}\right)\right)\Big/\|\bar{\Xi}\|^{2}\|\bar{A}\|^{2} \\
&= \frac{1}{\|\bar{\Xi}\|\|\bar{A}\|}\frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\left[\frac{\partial\left(\bar{\Xi}:\bar{A}\right)}{\partial\bar{\Xi}} - \frac{\partial\left(\|\bar{\Xi}\|\|\bar{A}\|\right)}{\partial\bar{\Xi}}\frac{\left(\bar{\Xi}:\bar{A}\right)}{\|\bar{\Xi}\|\|\bar{A}\|}\right] \\
&= \frac{1}{\|\bar{\Xi}\|\|\bar{A}\|}\frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\left[\bar{A} - \frac{\partial\left(\|\bar{\Xi}\|\|\bar{A}\|\right)}{\partial\bar{\Xi}}\frac{\left(\bar{\Xi}:\bar{A}\right)}{\|\bar{\Xi}\|\|\bar{A}\|}\right] = \frac{1}{\|\bar{\Xi}\|\|\bar{A}\|}\frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\left[\bar{A} - \frac{\bar{\Xi}}{\|\bar{\Xi}\|}\frac{\left(\bar{\Xi}:\bar{A}\right)}{\|\bar{\Xi}\|}\right] \\
&= \frac{1}{\|\bar{\Xi}\|\|\bar{A}\|}\frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}}\left[\bar{A} - \left(\frac{\bar{\Xi}:\bar{A}}{\bar{\Xi}:\bar{\Xi}}\right)\bar{\Xi}\right] \\
&= \frac{a_1 + 4\,a_2\cos\bar{\eta} + 3\,a_3\left(4\cos^{2}\bar{\eta} - 1\right) + 16\,a_4\,\cos\bar{\eta}\left(4\cos^{2}\bar{\eta} - 1\right)}{\|\bar{\Xi}\|\|\bar{A}\|}\left[\bar{A} - \left(\frac{\bar{\Xi}:\bar{A}}{\bar{\Xi}:\bar{\Xi}}\right)\bar{\Xi}\right]
\end{aligned} \tag{82}$$

where these relations are hold

$$\text{and } \frac{\partial\left(\|\bar{\Xi}\|\|\bar{A}\|\right)}{\partial\bar{\Xi}} = \frac{\partial\left(\|\bar{\Xi}\|\right)}{\partial\bar{\Xi}}\|\bar{A}\| = \frac{\bar{\Xi}}{\|\bar{\Xi}\|}\|\bar{A}\| \text{ and } \|\bar{\Xi}\|\|\bar{\Xi}\| = \bar{\Xi}:\bar{\Xi} \quad \frac{\partial\left(\bar{\Xi}:\bar{A}\right)}{\partial\bar{\Xi}} = \bar{A} \tag{83}$$

$$\frac{\partial\bar{\chi}}{\partial\cos\bar{\eta}} = a_1 + 4\,a_2\cos\bar{\eta} + 3\,a_3\left(4\cos^{2}\bar{\eta} - 1\right) + 16\,a_4\,\cos\bar{\eta}\left(4\cos^{2}\bar{\eta} - 1\right) \tag{84}$$

4. **Summary**

The constitutive equation can be summarized as

Kinematics:

$$\overline{l^p} = \overline{D}^p + \overline{W}^p \text{ , } \bar{l} = \overline{l^p} + \overline{l^e} \quad (85)$$

Elastic law:

$$\overline{S} = \overline{\mathrm{C}}^e : \overline{E}^e \quad (86)$$

Flow rule:

$$\left\|\overline{D}^p\right\| = \sqrt{\frac{3}{2}} f(\theta)\left(sinh\overline{\Phi}\right)^m \text{ , } \overline{D}^p = \left\|\overline{D}^p\right\| \overline{N}^p \quad (87)$$

Plastic potential:

$$\overline{\Phi} = \left[\frac{\overline{\Xi}^{eff}}{\overline{\chi}\,\overline{\kappa}} - 1\right] \quad (88)$$

$$\Xi^{eff} = \sqrt{\frac{3}{2}}\left\|\Xi\right\| \quad (89)$$

$$\overline{\Xi} = dev\,\overline{S} - dev\,\overline{\zeta} \quad (90)$$

$$dev\,\overline{S} = \overline{S} - \frac{1}{3}tr(\overline{S}) \quad (91)$$

$$dev\,\overline{\zeta} = \overline{\zeta} - \frac{1}{3}tr(\overline{\zeta}) \quad (92)$$

Texture evolution:

$$\begin{aligned}\overset{\circ}{\overline{A}} =& -2\lambda_g\left((1-f)\left(-\frac{1}{35}\left(2\overline{D}^p\right) + \frac{1}{7}\left(2A\overline{D}^p + \left(A:\overline{D}^p\right)\delta_{ij} + 2\,\overline{D}^p A\right)\right) + f\left(A:\overline{D}^p\right)A\right) \\ &+ \lambda_g\left(A\overline{D}^p + \overline{D}^p A + \frac{2}{3}\overline{D}^p\right) + \frac{2}{3}\lambda_g\left(A:\overline{D}^p\right)\delta_{ij} - \overline{W}^p\overline{A} + \overline{A}\,\overline{W}^p\end{aligned} \quad (93)$$

$$\overline{\chi} = 1 + a_1 cos\overline{\eta} + a_2 cos 2\overline{\eta} + a_3 cos 3\overline{\eta} + a_4 cos 4\overline{\eta} \quad (94)$$

$$cos\,\overline{\eta} = \frac{\overline{\Xi} : \overline{A}}{\left\|\overline{\Xi}\right\|\left\|\overline{A}\right\|} \qquad (95)$$

$$\overline{N}^{\,p} = \frac{1}{\overline{\chi}\overline{\kappa}}\, sym\left(\frac{\partial\overline{\Xi}^{eff}}{\partial\overline{\Xi}} - \frac{\overline{\Xi}^{eff}}{\overline{\chi}}\frac{\partial\overline{\chi}}{\partial\overline{\Xi}}\right) \Big/ \frac{1}{\overline{\chi}\overline{\kappa}}\left\| sym\left(\frac{\partial\overline{\Xi}^{eff}}{\partial\overline{\Xi}} - \frac{\overline{\Xi}^{eff}}{\overline{\chi}}\frac{\partial\overline{\chi}}{\partial\overline{\Xi}}\right)\right\| \qquad (96)$$

$$\frac{\partial\overline{\chi}}{\partial\overline{\Xi}} = \frac{a_1 + 4\,a_2\,cos\,\overline{\eta} + 3\,a_3\left(4cos^2\,\overline{\eta} - 1\right) + 16\,a_4\;\;cos\,\overline{\eta}\left(4cos^2\,\overline{\eta} - 1\right)}{\left\|\overline{\Xi}\right\|\left\|\overline{A}\right\|}\left[\overline{A} - \left(\frac{\overline{\Xi} : \overline{A}}{\overline{\Xi} : \overline{\Xi}}\right)\overline{\Xi}\right] \qquad (97)$$

$$\overline{W}^{\,p} = \lambda_g\left(\overline{A}\,\overline{D}^{\,p} - \overline{D}^{\,p}\overline{A}\right) \qquad (98)$$

Hardening rule:

$$\overline{\eta} = -\frac{\partial\overline{\psi}}{\partial\theta} \qquad (99)$$

$$\overline{\kappa} = c_k\,\mu(\theta)\overline{\varepsilon}_{ss} \qquad (100)$$

$$\overline{\zeta} = c_\zeta\,\mu(\theta)\overline{\alpha}_l^e \qquad (101)$$

$$\dot{\overline{\varepsilon}}_{ss} = [\,\hat{H} - R_d\,(\theta)\overline{\varepsilon}_{ss}\,]\left\|\overline{D}^{\,p}\right\| - R_s\,(\theta)\overline{\varepsilon}_{ss}\,sinh(\hat{Q}_s(\theta)\;\overline{\varepsilon}_{ss}\,) \qquad (102)$$