

# A STATISTICAL FORMULATION OF VISCOPLASTIC BEHAVIOR IN HETEROGENEOUS POLYCRYSTALS

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A formulation for viscoplastic behavior of heterogeneous polycrystals is presented based upon the familiar constructs of statistical continuum theory. The non-local interaction law is derived which relates properties of the local velocity field to correlation functions of the local microstructure. It is demonstrated that correlation functions, based upon the two-point orientation coherence function, are required in a theory which considers first-order deviations from Taylor's 1938 uniform strain (rate) assumption. The evolution of the coherence function with deformation is also briefly considered.

**KEY WORDS** Micromechanics, crystallographic texture, viscoplasticity, correlation functions.

## 1. INTRODUCTION

During the past three decades, the modern texture theory, with its emphasis upon the crystallite orientation distribution function (o.d.f.), has been established as a cornerstone in the theory of polycrystalline plasticity. Of particular significance is the prediction of mechanical anisotropy based upon various averaging schemes incorporating the o.d.f. Models based upon Taylor's 1938 assumption of uniform strain have often demonstrated first-order agreement with the measured anisotropic response. Comparisons between simulated and measured texture evolution with these models have also exhibited first-order agreement. The predictive power of this generation of models often falls short of our expectations, however, and consequently model refinement is of considerable interest.

The viewpoint espoused in this paper is that improved models must necessarily include some information about the heterogeneity of strain (and stress) in the polycrystal. Once Taylor's uniform strain approximation is abandoned, then the traditional measures of microstructure, such as the o.d.f., are no longer adequate. Consistent with the increasing complexity required to describe non-local interactions between material particles (giving rise to the experimentally observed heterogeneities), is the requirement for microstructural measures of increasing sophistication. It will be demonstrated in this paper that these measures must describe, not only lattice orientations, but their spatial correlations.

During the past three years, we have advocated a two-point probability density function, named the orientation coherence function (o.c.f.), as a logical first step towards more sophisticated microstructural measures (Adams *et al.*, 1987; Adams, Wang and Morris, 1988; Morris, Wang and Adams, 1988). The o.c.f. describes the correlation of lattice orientations between points in the polycrystal separated by a specified vector. Whereas the o.d.f. can be conveniently defined in a three dimensional manifold parameterized by Euler angles, the o.c.f. requires nine parameters—three describing the lattice orientation at each point, and three defining their spatial relationship with respect to one-another. Obviously this represents a very substantial increase in the degree of complexity faced in describing microstructures; pictorial representations of the o.c.f. become rather burdensome, for example. However, with simultaneous advances in micro-diffraction technology and computing hardware, it has been possible to measure the o.c.f. for several materials, and it is not difficult to envision that the o.c.f. (and even higher-order density functions of the microstructure) may be measured in automated fashion in the near future.

In order to illustrate the imperative need for the o.c.f., this paper will describe a new statistical theory for viscoplastic response in polycrystals. The approach taken parallels the constructs in the statistical continuum theory for linear-elastic polycrystals (Beran, 1968; Kröner, 1972; McCoy, 1981; Kröner, 1987). The secant modulus formulation of the single-crystal constitutive law, described by Hutchinson (1976), is chosen for its simplicity. A parallel tangent-modulus approach to large-strain viscoplastic behavior is presented elsewhere (Molinari, Canova and Ahzi, 1987; Canova, Molinari, Ahzi and Adams, 1989). As shown here, the theory considers the inelastic heterogeneity in the context of perturbations from the uniform Taylor polycrystal. This approach makes a very clear connection with the previous uniform strain-rate upper-bound model. In contrast to the self-consistent theory, originating with Hill (1965) and implemented by Hutchinson (1976), the statistical theory is explicit. For example, if the o.c.f. is known, then the theory provides the complete macroscopic constitutive law, linking the applied stress and the macroscopic strain-rate tensors, in closed form. In another application of the theory, local stresses and strain-rates are estimated based upon non-local interactions with neighboring crystallites.

Although the focus here is upon steady creep of polycrystals, the form of the interaction law is observed in a variety of inelastic models. Integral equations of the form proposed by Zeller and Dederichs (1973) occur not only in viscous theories, but also in the low temperature elasto-plastic models (e.g., Berveiller *et al.*, 1987). These, however, have not yet been extended into the realm of statistical continuum theory.

The Einstein summation convention is used extensively in the following development. Summation is implied over repeated subscripts. A comma among the subscripts denotes differentiation relative to the independent variables associated with the subscripts following the comma. Cartesian tensors of arbitrary rank (but not their components) are given in bold letters for clarity.

## 2. SINGLE CRYSTAL VISCOPLASTIC BEHAVIOR AT CONSTANT TEMPERATURE

The model employed is identical to that defined by Hutchinson (1976) for power-law steady creep by slip. For a resolved shear stress,  $\tau^{(k)}$ , acting on the  $k$ th

slip system, the slip rate,  $\gamma^{(k)}$ , is connected by the equation

$$\tau^{(k)}/\tau_0^{(k)} = (\gamma^{(k)}/\gamma_0)^m \quad (2.1)$$

where  $m$  is the rate sensitivity parameter,  $\tau_0^{(k)}$  is the reference stress, and  $\gamma_0$  is an arbitrary reference slip-rate. This modellization assumes that the dependence of  $\gamma^{(k)}$  upon the slip activity on other systems can be incorporated completely in  $\tau_0^{(k)}$ . Although it is not explicitly represented in Eq. (2.1), the slip-rate must have the same sign as the resolved shear stress.

The total deviatoric strain-rate in the crystal,  $\epsilon$ , is determined by summing over the contribution from all slip systems:

$$\epsilon_{ij} = \sum_k \mu_{ij}^{(k)} \gamma^{(k)} = M_{ijkl} \sigma_{kl} \quad (2.2)$$

where

$$\mu_{ij}^{(k)} = \frac{1}{2}(b_i^{(k)} n_j^{(k)} + b_j^{(k)} n_i^{(k)}). \quad (2.3)$$

The unit vectors  $\mathbf{n}^{(k)}$  and  $\mathbf{b}^{(k)}$  signify, respectively, the slip-plane normal and slip direction for the  $k$ th slip system.  $\sigma$  is the deviatoric Cauchy stress tensor. Combining Eqs (2.1) and (2.2), and noting that

$$\tau^{(k)} = \mu_{ij}^{(k)} \sigma_{ij}, \quad (2.4)$$

the components of the fourth rank tensor of creep compliances,  $M_{ijkl}$ , can be written as

$$M_{ijkl} = \sum_k (\gamma_0/\tau_0^{(k)}) |\mu_{rs}^{(k)} \sigma_{rs}/\tau_0^{(k)}|^{n-1} \mu_{ij}^{(k)} \mu_{kl}^{(k)}. \quad (2.5)$$

The dissipation-rate is given by

$$\sigma_{ij} \epsilon_{ij} = W = \sigma_{ij} M_{ijkl} \sigma_{kl}. \quad (2.6)$$

$W$  is positive for any non-zero choice of  $\sigma$ , hence  $\mathbf{M}$  is positive definite. Furthermore, the stress potential ( $= (1/m + 1)W$ ) is convex which assures that the functional dependence between deviatoric stress and deviatoric strain-rate is one-to-one. Consequently, the inverse relationship to Eq. (2.2) exists, and is given as

$$\sigma_{ij} = N_{ijkl} \epsilon_{kl} \quad (2.7)$$

where  $\mathbf{N} = \mathbf{M}^{-1}$ .

The creep compliances are homogeneous of degree  $n - 1$  ( $n = 1/m$ ) in the stress, and therefore the creep moduli are homogeneous of degree  $(1 - n)/n$ :

$$\mathbf{M}(\lambda\sigma) = \lambda^{n-1} \mathbf{M}(\sigma), \quad \mathbf{N}(\lambda\epsilon) = \lambda^{(1-n)/n} \mathbf{N}(\epsilon). \quad (2.8)$$

The major focus in this paper will be upon Eq. (2.7). The creep moduli are obtained by inverting Eq. (2.5) for fixed stress. Equation (2.8) is then used to minimize the computational requirement. The secant modulus tensor presents the following symmetry properties.

$$N_{ijkl} = N_{jikl} = N_{ijlk} = N_{klij} \quad (2.9)$$

A fully Cauchy stress tensor,  $\mathbf{T}$ , is obtained by the addition of a hydrostatic pressure,  $p$ , which does not contribute to the dissipation-rate due to the inherent

incompressibility of the present model.

$$T_{ij} = N_{ijkl}\epsilon_{kl} - p\delta_{ij} = N_{ijkl}L_{kl} - p\delta_{ij} \quad (2.10)$$

This hydrostatic pressure can only be prescribed through the equilibrium equations and boundary conditions associated with the problem; this is addressed more completely in a subsequent section.

### 3. THE INTERACTION LAW FOR POLYCRYSTALS

Having established the local behavior through Eq. (2.10) the response of the polycrystal is sought. Define the polycrystal to be an aggregate of very many perfectly bonded space filling single crystallites. A uniform macroscopic velocity gradient,  $\bar{\mathbf{L}}$  and an arbitrary macroscopic pressure,  $\bar{p}$ , are imposed upon the aggregate at infinity. Incompressibility requires that  $\bar{\mathbf{L}}_{ii} = 0$ . Locally, equilibrium is required throughout the polycrystal, hence from Eq. (2.10)

$$T_{ij,j} = (N_{ijkl}L_{kl})_{,j} - p_{,i} = 0 \quad (3.1)$$

In the spirit of the statistical continuum theory, define a convenient “reference” or “comparison” medium, which manifests a constitutive law which, in general, differs from the macroscopic law. The secant moduli of the references medium are defined as

$$N_{ijkl}^R = \int_{h \in H} f(h) N_{ijkl}(\bar{\mathbf{L}}, h) dh \quad (3.2)$$

where  $h$  represents the relevant set of state variables defining the secant moduli. This includes the set of reference shear stresses,  $\tau_0^{(k)}$ , and the lattice orientation,  $g$ , which fixes  $\mu_{ij}^{(k)}$ . Reference to Eq. (2.5) makes this very clear. Thus  $h = \{\tau_0^{(k)}, g\}$  where  $g$  represents the usual set of three Euler angles defining the rotation of the crystal lattice from a chosen macroscopic reference frame. The domain of local state variables is  $H \subset R^k \times SO(3)$ , where  $R^k$  is the  $k$ -dimensional real domain of reference stresses for  $k$  slip systems and  $SO(3)$  is the special orthogonal group of rigid body rotations.  $f(h)$  is the probability density for the occurrence of state  $h$  in the polycrystal.

When steady creep is of primary interest, it has been common to assume that  $\tau_0^{(s)}$ , is uniform, not only in individual crystallites, but throughout the polycrystal. When this assumption is justified Eq. (3.2) reduces to

$$N_{ijkl}^R = \int_{g \in SO(3)} f(g) N_{ijkl}(\bar{\mathbf{L}}, \tau_0^*, g) dh \quad (3.3)$$

where  $\tau_0^*$  is constant. Experimental justification for this assumption is rather sparse, but observations of dislocation cell size in crept polycrystals appear to be quite uniform, which suggests that the assumption may not be in serious error. For the development given here the assumption is adopted.

Next, decompose the secant modulus tensor to define a polarized modulus,  $\tilde{N}$ , according to

$$\tilde{N}_{ijkl}(\mathbf{L}, \tau_0^*, g) = N_{ijkl}(\mathbf{L}, \tau_0^*, g) - N_{ijkl}^R \quad (3.4)$$

Also define a polarized deviatoric stress tensor,

$$\tilde{\sigma}_{ij}(\mathbf{L}, \tau_0^*, g) = \sigma_{ij}(\mathbf{L}, \tau_0^*, g) - \sigma_{ij}^R(\mathbf{L}, \tau_0^*), \quad (3.5)$$

where the reference stress is defined for the reference medium according to the relation

$$\sigma_{ij}^R(\mathbf{L}, \tau_0^*) = N_{ijkl}^R L_{kl}. \quad (3.6)$$

Further reference to  $\tau_0^*$  will hereafter be omitted since there is little possibility of confusion.

Substitution of Eq. (3.4) into (3.1) leads to the equations

$$N_{ijkl}^R L_{kl,j} - p_{,i} + f_i = 0 \quad (3.7)$$

where  $f_i$  can be considered as the components of a "fictitious" body force defined as

$$f_i = [\tilde{N}_{ijkl}(\mathbf{L}, g) L_{kl}]_{,j} \quad (3.8)$$

The incompressibility condition requires that

$$L_{ii} = 0. \quad (3.9)$$

Thus Eqs (3.7) and (3.9) define a system of four equations to be solved for the four unknowns  $v_i$  (velocity) and  $p$ .

Following the development previously given by Molinari *et al.* (1987), this set of equations is solved using the Green's function method. The Green's functions in the infinite space are  $G_{ij}(\mathbf{r} - \mathbf{r}')$  and  $H_k(\mathbf{r} - \mathbf{r}')$  where  $\mathbf{r}$  and  $\mathbf{r}'$  represent points in the space. As  $|\mathbf{r} - \mathbf{r}'|$  goes to infinity  $G$  and  $H$  are expected to equal zero. The functions are solutions to equation's which parallel 3.7 and 3.9:

$$N_{ijkl}^R G_{km,tj}(\mathbf{r} - \mathbf{r}') - H_{m,i}(\mathbf{r} - \mathbf{r}') + \delta_{im} \delta(\mathbf{r} - \mathbf{r}') = 0 \quad (3.10)$$

and

$$G_{im,i}(\mathbf{r} - \mathbf{r}') = 0 \quad (3.11)$$

The function  $\delta(\mathbf{r} - \mathbf{r}')$  is the Dirac function centered at  $\mathbf{r}'$  and the term  $\delta_{im} \delta(\mathbf{r} - \mathbf{r}')$  represents the  $i$ th component of a unit force acting at  $\mathbf{r}'$  for fixed  $m$ . Of particular importance is the fact that  $G$  and  $H$  depend only upon reference secant moduli  $N^R$  and the aforementioned boundary condition. The formal solution to the problem is well known.

$$v_i(\mathbf{r}) = \bar{v}_i + \int_{\mathbf{r}' \in V} G_{ij}(\mathbf{r} - \mathbf{r}') f_j(\mathbf{r}') dr'^3 \quad (3.12)$$

$$p(\mathbf{r}) = \bar{p} + \int_{\mathbf{r}' \in V} H_i(\mathbf{r} - \mathbf{r}') f_i(\mathbf{r}') dr'^3 \quad (3.13)$$

It is convenient to express Eq. (3.12) in terms of the local and macroscopic velocity gradient tensors. Taking the derivative with respect to the components of  $\mathbf{r}$ , and then reforming the left side of the equation, integrating by parts, the fundamental interaction law is obtained:

$$L_{ik}(\mathbf{r}) = \bar{L}_{ik} + \int_{\mathbf{r}' \in V} G_{ij,kl}(\mathbf{r} - \mathbf{r}') \tilde{N}_{jtrs}(\mathbf{L}(\mathbf{r}'), g(\mathbf{r}')) L_{rs}(\mathbf{r}') dr'^3 \quad (3.14)$$

Note the physical interpretation of the interaction law. The local velocity gradient at  $\mathbf{r}$  differs from the imposed macroscopic velocity gradient by the convolution over the infinite volume  $V$  of a polarized deviatoric stress,  $\tilde{\boldsymbol{\sigma}}$ , which depends upon the local velocity gradient and lattice orientation at  $\mathbf{r}' \in V$ . This polarized stress is defined as

$$\tilde{\sigma}_{ji}(\mathbf{r}') = \tilde{N}_{jirs}(\mathbf{L}(\mathbf{r}'), g(\mathbf{r}'))L_{rs}(\mathbf{r}'); \quad (3.15)$$

it represents the difference between the local response and the reference response to the local velocity gradient at  $\mathbf{r}'$ .

The inherent singularity of derivatives of the Green's function at  $\mathbf{r} = \mathbf{r}'$  must be handled with some care (McCoy, 1981). This is typical of many boundary value problems in physics. One way to circumvent problems with the singularity is to construct solutions for a finite volume surrounding point  $\mathbf{r}$ . Examine an arbitrarily small volume  $V_c$  surrounding point  $\mathbf{r}$ . The average velocity gradient in  $V_c$  is calculated from Eq. (3.14). Let  $\mathbf{L}^0(\mathbf{r})$  now represent this averaged value in the near neighborhood of  $\mathbf{r}$ , then for  $V_c$  sufficiently small we have

$$L_{ik}^0(\mathbf{r}) = \bar{L}_{ik} + \frac{1}{V_c} \int_{\mathbf{r} \in V_c} \int_{\mathbf{r}' \in V} G_{ij,kl}(\mathbf{r} - \mathbf{r}') \tilde{N}_{jirs}(\mathbf{L}^0(\mathbf{r}'), g(\mathbf{r}')) L_{rs}^0(\mathbf{r}') dr'^3 dr^3 \quad (3.16)$$

Hereafter, wherever possible an abbreviated notation for Eq. (3.16) will be employed:

$$\mathbf{L}^0(\mathbf{r}) = \bar{\mathbf{L}} + G(\mathbf{r} - \mathbf{r}') * \tilde{\mathbf{N}}(\mathbf{r}') \mathbf{L}^0(\mathbf{r}') \quad (3.17)$$

The symmetrical part of 3.17 defines the local strain-rate tensor

$$\boldsymbol{\varepsilon}^0(\mathbf{r}) = \bar{\boldsymbol{\varepsilon}} + \Gamma(\mathbf{r} - \mathbf{r}') * \tilde{\mathbf{N}}(\mathbf{r}') \boldsymbol{\varepsilon}^0(\mathbf{r}') \quad (3.18)$$

where

$$\Gamma_{ijkl} = \frac{1}{4}(G_{ij,kl} + G_{jk,il} + G_{il,jk} + G_{jl,ik}) \quad (3.19)$$

The antisymmetrical portion returns the total rate-of-rotation tensor

$$\boldsymbol{\omega}^0(\mathbf{r}) = \bar{\boldsymbol{\omega}} + \Lambda(\mathbf{r} - \mathbf{r}') * \tilde{\mathbf{N}}(\mathbf{r}') \mathbf{L}^0(\mathbf{r}') \quad (3.20)$$

where

$$\Lambda_{ijkl} = \frac{1}{4}(G_{ij,kl} - G_{jk,il} + G_{il,jk} - G_{jl,ik}) \quad (3.21)$$

The rate-of-lattice-rotation in  $V_c$  is  $\boldsymbol{\omega}^{0*}(\mathbf{r})$  where

$$\boldsymbol{\omega}^{0*}(\mathbf{r}) = \boldsymbol{\omega}^0(\mathbf{r}) - \boldsymbol{\omega}^{op}(\mathbf{r}) \quad (3.22)$$

and

$$\omega_{ij}^{op} = \frac{1}{2} \sum_k (b_i^{(k)} n_j^{(k)} - b_j^{(k)} n_i^{(k)}) \gamma^{(k)} \quad (3.23)$$

The slip-rates  $\gamma^{(k)}$  are calculated using Eqs (2.1), (2.4), and (2.7), and hence the rate-of-lattice rotation is readily obtained.

As a practical matter, the Green's functions required in the localization law can be obtained from the Fourier transforms of Eqs (3.10) and (3.11):

$$-N_{ijkl}^R k_j k_l \tilde{G}_{km}(\mathbf{k}) + ik_i \tilde{H}_m(\mathbf{k}) + \delta_{im} = 0 \quad (3.24)$$

and

$$k_k \tilde{G}_{km}(\mathbf{k}) = 0. \quad (3.25)$$

Thus, in  $\mathbf{k}$ -space the differential equations defining the Green's function are replaced with a system of linear equations which are solved for  $k^2 \tilde{G}_{km}(\mathbf{k})$  and  $ik \tilde{H}(\mathbf{k})$ . In direct space the required Green's functions are given by

$$G_{ij,kl}(\mathbf{r} - \mathbf{r}') = \frac{-1}{8\pi^3} \int_{\mathbf{k} \in K^3} k_k k_l \tilde{G}_{ij}(\mathbf{k}) e^{-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} d\mathbf{k}^3 \quad (3.26)$$

and

$$H_{m,i}(\mathbf{r} - \mathbf{r}') = \frac{-i}{8\pi^3} \int_{\mathbf{k} \in K^3} k_i \tilde{H}_m(\mathbf{k}) e^{-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} d\mathbf{k}^3 \quad (3.27)$$

Self-consistent iterative schemes can be pursued to solve the implicit interaction law (Eq. (3.17)) for prescribed microstructures. This approach is described by Molinari *et al.* (1987) in order to simulate texture evolution in fcc metals. Here, a statistical description of microstructures is preferred, and this is described in the subsequent section.

#### 4. A STATISTICAL FORMULATION OF THE VISCOELASTIC THEORY

Consider variations of the velocity-gradient field away from the uniform field of the Taylor polycrystal. Assume that the polarized deviatoric stress,  $\tilde{\sigma}$ , does not deviate "too far" from its value at  $\mathbf{L}$ , i.e.,

$$\left| \frac{\tilde{\sigma}_{ij}(\mathbf{L}, g) - \tilde{\sigma}_{ij}(\tilde{\mathbf{L}}, g)}{\tilde{\sigma}_{ij}(\tilde{\mathbf{L}}, g)} \right| \ll 1 \text{ for all } i, j \text{ and } g. \quad (4.1)$$

For these circumstances Eq. (3.17) can be written, omitting reference to spatial position and lattice orientation, as Taylor series expansion about  $\tilde{\mathbf{L}}$ , retaining only the first few terms:

$$\mathbf{L}^0 = \tilde{\mathbf{L}} + G * (\tilde{\sigma}(\tilde{\mathbf{L}}) + \tilde{\sigma}'(\tilde{\mathbf{L}})\tilde{\mathbf{L}}^0 + \frac{1}{2!}\tilde{\sigma}''(\tilde{\mathbf{L}})\tilde{\mathbf{L}}^{02} + \geq 0(\tilde{\mathbf{L}}^0)^3) \quad (4.2)$$

where

$$\tilde{\sigma}_{ijrs}''(\tilde{\mathbf{L}}) = \left( \frac{\partial \tilde{\sigma}_{ij}}{\partial L_{rs}}(\tilde{\mathbf{L}}) \right) \quad \text{and} \quad \tilde{\sigma}_{ijrstu}''(\tilde{\mathbf{L}}) = \left( \frac{\partial^2 \tilde{\sigma}_{ij}}{\partial L_{rs} \partial L_{tu}}(\tilde{\mathbf{L}}) \right) \quad (4.3)$$

Equation 4.2 can be explicitly iterated by reintroducing the expression for  $\tilde{\mathbf{L}}^0$  ( $= \mathbf{L}^0 - \tilde{\mathbf{L}}$ ) into itself on the right hand side as many times as necessary. This increases the required order of integration since the convolution implied by \* occurs more than one time in higher-order tensors. Note, however, that this iteration removes dependence of the equation upon  $\mathbf{L}^0$  if sufficient iterations are taken. This implicit character of the equation is replaced by an explicit one. The price which is exacted is an increasing order of complexity in the integrations required.

Taking only the zeroth-order term in Eq. (4.2) we obtain the condition  $\mathbf{L}^0 = \tilde{\mathbf{L}}$  which is recognized to be the Taylor approximation. Here the focus will be upon

the first-order correction to the homogeneous Taylor solution; hereafter  $\mathbf{L}^0$  is approximated with the equation

$$\begin{aligned}\mathbf{L}^0(\mathbf{r}) &= \bar{\mathbf{L}} + G(\mathbf{r} - \mathbf{r}') * \bar{\sigma}(\bar{\mathbf{L}}, h(\mathbf{r}')) \\ &= \bar{\mathbf{L}} + G(\mathbf{r} - \mathbf{r}') * \bar{\mathbf{N}}(\bar{\mathbf{L}}, h(\mathbf{r}'))\bar{\mathbf{L}}\end{aligned}\quad (4.4)$$

A further connection with statistical theory is obtained by considering the ensemble average of the local velocity gradient associated with very many particles of state  $h = (\tau_0^*, g)$ . Each particle will be surrounded by a structure which is, in some respects, different from all other particles having the same lattice orientation and reference shear stress. Consequently it is expected that each particle will exhibit a distinctive velocity gradient. The expectation value for the ensemble of particles of equivalent state is also expected to be different from that obtained for other ensembles of particles exhibiting different state. Of primary focus here, is this latter difference. The former variation would also be of interest in a more comprehensive theory.

Let the brackets  $\langle \rangle_h$  denote the ensemble average over particles at state  $h$ :

$$\langle ( )_i \rangle_h = \frac{1}{N} \sum_{i=1}^N ( )_i \quad (4.5)$$

Noting that ensemble averaging commutes with integration, form the ensemble average of the velocity gradient for particles at state  $h$ :

$$\begin{aligned}\langle \mathbf{L}^0(\mathbf{r}) \rangle_h &= \bar{\mathbf{L}} + G(\mathbf{r} - \mathbf{r}') * \langle \bar{\sigma}(\bar{\mathbf{L}}, h(\mathbf{r}')) \rangle_h \\ &= \bar{\mathbf{L}} + G(\mathbf{r} - \mathbf{r}') * \langle \bar{\mathbf{N}}(\bar{\mathbf{L}}, h(\mathbf{r}')) \rangle_h \bar{\mathbf{L}}\end{aligned}\quad (4.6)$$

To be consistent with our assumption of uniformity in the reference shear stress, let  $h(\mathbf{r}') = (\tau_0^*, g')$ . The ensemble average of the polarized creep modulus is conveniently expressed in terms of the conditional 2-point probability density function of lattice orientations:

$$\langle \bar{\mathbf{N}}(\bar{\mathbf{L}}, g') \rangle_h = \int_{g' \in SO(3)} f_2(g', \mathbf{r}' - \mathbf{r} | g) \bar{\mathbf{N}}(\bar{\mathbf{L}}, g') dg' \quad (4.7)$$

The function  $f_2(g', \mathbf{r}' - \mathbf{r} | g)$  represents the probability density for the occurrence of lattice orientation  $g'$  at point  $\mathbf{r}'$  given that orientation  $g$  occurs at  $\mathbf{r}$ . The point  $\mathbf{r}$  must be taken to be any arbitrary point in the microstructure where lattice orientation  $g$  occurs. Thus, the structure is assumed to exhibit spatial stationarity. The two-point function is normalized according to

$$\int_{g' \in SO(3)} f_2(g', \mathbf{r}' - \mathbf{r} | g) dg' = 1 \quad \text{for all } \mathbf{r}' - \mathbf{r} \quad (4.8)$$

Additional details about the 2-point function their determination and their representation, were previously published [Adams, Morris, Wang, Willden and Wright 1987; Adams, Wang and Morris 1988; Morris, Wang and Adams 1988]. Equation (4.6) constitutes the first-order statistical localization law. A similar first-order localization law can be derived for the local pressure in the particle,  $\langle p^0 \rangle_h$ :

$$\langle p^0 \rangle_h = \bar{p} + H(\mathbf{r} - \mathbf{r}') * \langle \bar{\mathbf{N}}(\bar{\mathbf{L}}, h(\mathbf{r}')) \rangle_h \bar{\mathbf{L}} \quad (4.9)$$

Here  $H(\mathbf{r} - \mathbf{r}')$  denotes the partial derivatives of the Green's tensor  $H$  with respect to  $x_j$ . The components are  $H_{i,j}(\mathbf{r} - \mathbf{r}')$ .

Physically,  $\langle \tilde{\mathbf{N}}(\bar{\mathbf{L}}, h(\mathbf{r}')) \rangle_h$  represents the correlation of polarized moduli at  $\mathbf{r}'$  when a particle of state  $h$  exists at  $\mathbf{r}$ . It is customary to refer to entities of this character as "correlation functions," or more precisely "microstructural correlation functions." If higher order terms were taken in theory, either by including more terms of the iteration of equation 4.2 or by incorporating higher-order terms in the Taylor expansion of  $\tilde{\sigma}(\bar{\mathbf{L}})$ , then correlation functions of higher-order would naturally occur. The explicit determination of these terms would require orientation coherence functions of more than two points.

## 5. ESTIMATES OF THE MACROSCOPIC CONSTITUTIVE LAW

Assuming that  $\langle \mathbf{L}^0 \rangle_h$  is adequate to describe the velocity gradient in particles of state  $h$  (neglecting local variations due to local microstructure), a straight forward estimate of the macroscopic constitutive law is easily constructed. Let  $\Sigma$  represent the macroscopic deviatoric Cauchy stress, which must be equated to the volume averaged local stresses:

$$\begin{aligned} \Sigma_{ij} &= \int_{h \in H} f(h) \langle \sigma_{ij} \rangle_h dh \\ &= \int_{h \in H} f(h) N_{ijkl}(\bar{\mathbf{L}}, h) \langle L_{kl}^0 \rangle_h dh \end{aligned} \quad (5.1)$$

Incorporating Eqs (3.3), (4.6) and the assumption of uniform reference stresses, this becomes

$$\Sigma_{ij} = N_{ijkl}^R(\bar{\mathbf{L}}) \bar{L}_{kl} + G_{km,ln}(\mathbf{r} - \mathbf{r}') * C_{ijklmnpq}^{N\tilde{N}} \bar{L}_{pq} \quad (5.2)$$

$C^{N\tilde{N}}$  is the microstructural correlation function defined by

$$C_{ijklmnpq}^{N\tilde{N}}(\bar{\mathbf{L}}) = \int_{h \in H} \int_{h' \in H} f_2(h', \mathbf{r}' - \mathbf{r}, h) N_{ijkl}(\bar{\mathbf{L}}, h) \tilde{N}_{mnpq}(\bar{\mathbf{L}}, h') dh' dh \quad (5.3)$$

where the  $C^{N\tilde{N}}$  is a function of  $\mathbf{r} - \mathbf{r}'$ ; its calculation requires the two-point o.c.f. which is related to the conditional form used in Eq. (4.7) by the relation

$$f_2(h', \mathbf{r}' - \mathbf{r}, h) = f_2(h', \mathbf{r}' - \mathbf{r}, |h) \cdot f(h) \quad (5.4)$$

Physically,  $C^{N\tilde{N}}$  represents the expected correlation of  $\mathbf{N}$  and  $\tilde{\mathbf{N}}$  given that they are separated by  $\mathbf{r}' - \mathbf{r}$  in the microstructure.

Equation (5.2) is the estimated macroscopic constitutive law connecting macroscopic stress  $\Sigma$  with the imposed macroscopic velocity gradient  $\bar{\mathbf{L}}$ . The symmetry of  $\Sigma$  is carried in  $N^R$  and  $C^{N\tilde{N}}$ . It is notable that the macroscopic law has the same form as the local law. If the term containing the correlation  $C^{N\tilde{N}}$  is neglected, the macroscopic constitutive law reduces to Hutchinson's (1976) uniform strain-rate upper bound for creep.

## 6. EVOLUTION OF THE ORIENTATION COHERENCE FUNCTION

The previous sections have illustrated the use of microstructural correlation functions to estimate constitutive behavior in polycrystals. Although the theory

presented retained only first-order terms in the Green's functions (resulting in analysis requiring the o.c.f. to obtain two-point correlation functions) second-order and higher-order terms are easily incorporated in the theory. These would require higher-order microstructural correlation functions. As the structure deforms with loading these correlation functions are naturally expected to evolve. Changes in lattice orientation and crystallite shape will cause this evolution in the correlation functions. A theory which is useful at finite strain must include means for describing this evolution.

In this section some preliminary analysis of this evolution is described; a more comprehensive treatment is desirable but is deferred to a subsequent paper. For the assumption of uniform reference stresses, the evolution of the local state variable,  $h$ , reduces to the evolution of the lattice orientation,  $g$ . This is completely described by Eq. (3.22) which relates lattice spin to local and macroscopic rotation rates. A description of the rate-of-change of  $\xi = r' - r$  is also required. Here it is demonstrated that a rigorous treatment of this requires a three-point probability density function; but the evolution of the three-point function is then required to complete the problem. This would require a four-point density function, and so forth. Thus a complete treatment of the problem requires probability density functions in the state variables of infinite order.

A practical question is whether approximations of this evolution based upon finite-order probability density functions is sufficient. This is the problem of closure which is central to the theory. Here, an approximation to the evolution problem requiring only the two-point o.c.f. is presented. The limitations associated with an approximation of this nature must be given further theoretical and experimental scrutiny.

Referring to Figure 1, consider the material derivative of an infinitesimal vector  $d\xi$  lying upon the vector  $\xi = r' - r$ :

$$\frac{D(d\xi)}{Dt} = L(r + \lambda\xi) \cdot d\xi \tag{6.1}$$

The parameter  $\lambda$  lies in the range  $0 \leq \lambda \leq 1$  and fixes the location of  $d\xi$  upon  $\xi$ . In

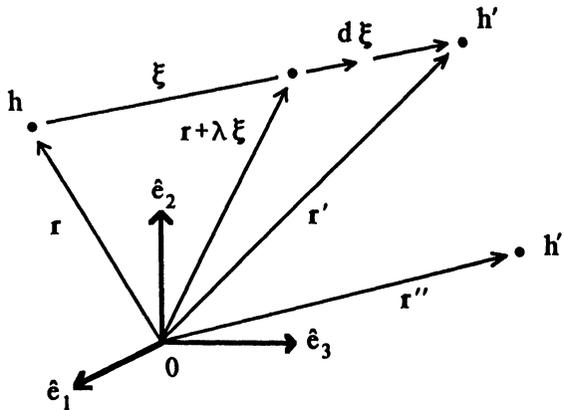


Figure 1 Definition of parameters associated with the evolution equations.

component form the overall evolution of  $\xi$  is given by

$$\dot{\xi}_i = \frac{D\xi_i}{Dt} = \int_0^1 L_{ij}(\mathbf{r} + \lambda\xi) \xi_j d\lambda \quad (6.2)$$

Define  $\langle \mathbf{L}^0(\mathbf{r} + \lambda\xi) \rangle_{h,h'}$  to be expected value of the velocity gradient in a particle located at  $\mathbf{r} + \lambda\xi$  given that state  $h$  occurs at  $\mathbf{r}$  and  $h'$  occurs at  $\mathbf{r} + \xi$ . The explicit definition of  $\langle \mathbf{L}^0(\mathbf{r} + \lambda\xi) \rangle_{h,h'}$  follows from the construction in Section 4. Analogous to Eqs (4.6) and (4.7) it follows that

$$\langle \mathbf{L}^0(\mathbf{r} + \lambda\xi) \rangle_{h,h'} = \bar{\mathbf{L}} + G(\mathbf{r} + \lambda\xi - \mathbf{r}') * \langle \tilde{\mathbf{N}}(\bar{\mathbf{L}}, h''(\mathbf{r}'')) \rangle_{h,h'} \bar{\mathbf{L}} \quad (6.3)$$

and

$$\langle \tilde{\mathbf{N}}(\bar{\mathbf{L}}, h''(\mathbf{r}'')) \rangle_{h,h'} = \int_{h'' \in H} f_3(h'', \mathbf{r}'' | h', \mathbf{r}', h, \mathbf{r}) \tilde{\mathbf{N}}(\bar{\mathbf{L}}, h'') dh''. \quad (6.4)$$

Notice that Eq. (6.4) now contains the three-point conditional probability density function which gives the probability of occurrence of  $h''$  at  $\mathbf{r}''$  given that  $h'$  and  $h$  have occurred at  $\mathbf{r}'$  and  $\mathbf{r}$  respectively.

The expectation value for  $\xi$ , given that  $h$  and  $h'$  occur at its endpoints, is estimated by introducing Eq. (6.3) into 6.2:

$$\langle \dot{\xi} \rangle_{h,h'} = \bar{\mathbf{L}} \cdot \xi + \left[ \int_0^1 G(\mathbf{r} + \lambda\xi - \mathbf{r}') * \langle \tilde{\mathbf{N}}(\bar{\mathbf{L}}, h''(\mathbf{r}'')) \rangle_{h,h'} d\lambda \right] \bar{\mathbf{L}} \cdot \xi \quad (6.5)$$

As it has been typical in the entire theory, the first term on the right hand side of Eq. (6.5) contains the uniform velocity gradient effect, and the second term addresses the difference due to local microstructures in the vicinity of a pair of material particles at states  $h$  and  $h'$  separated by  $\xi$ .

At this junction it should be clear that describing the evolution of all types of vectors  $\xi$  naturally requires three-point microstructural functions, but the evolution of these would require 4-point functions, etc. The strategy is therefore open. Intuitively, however, we must anticipate that for some order of these functions,  $O$ , it will be possible to construct (to the desired degree of accuracy) all functions of order  $> O$  with those of order  $O$ . This order of closure will depend upon the degree of accuracy required in the theory. Suppose that order two is sufficient for present purposes. Then an adequate approximation for the evolution of the two-point functions is obtained by introducing the approximation

$$f_3(h'', \mathbf{r}'' | h', \mathbf{r}', h, \mathbf{r}) \cong \frac{1}{2}(f_2(h'', \mathbf{r}'' - \mathbf{r}' | h') + f_2(h'', \mathbf{r}'' - \mathbf{r} | h)) \quad (6.6)$$

into Eq. (6.4). The extension to closures of higher order is evident.

## 7. SUMMARY AND CONCLUSIONS

The preceding development demonstrates the construction of a new theory of viscoplasticity in polycrystalline materials. Its form parallels the statistical theory for heterogeneous elastic media. For example, the interaction law (Eq. (3.14)) has algebraic form identical to the Zeller–Dederichs equation in the elastic theory (Zeller and Dederichs, 1973). The present theory emphasizes the secant-modulus

form of the single-crystal constitutive law originating with the work of Hutchinson (1976). The secant modulus formulation is best suited to the problem of creep, since the stresses typically remain a fraction of the yield stress. For large stress/large strain-rate problems a similar development, originating with the work of Molinari *et al.* (1987), and using the tangent-modulus, is more suitable. This development can also be treated in the framework of the statistical theory (Canova, Molinari, Ahzi and Adams, 1989).

The present theory focuses upon perturbations away from the uniform strain-rate approximation of the Taylor polycrystal. When these deviations are too large (according to Eq. (4.1)) then the theory breaks down. In any case, since only first-order terms correcting the uniform strain-rate solution are retained in the solution, the theory should only be viewed as a first-order correction to the Taylor-like theories.

The emergence of microstructural correlation functions is a central characteristic of the theory. The connection between these correlation functions and the ensemble averages is typified by Eq. (4.7). Notably, the passage between the ensemble average on the left hand side of this equation, to the correlation function on the right, requires use of the ergodic hypothesis. This hypothesis is central to the present theory, and to many other statistical theories. The passage from hypothesis to proof has been elusive in all but the simplest theories, but its intuitive appeal is strong. For further discussion on this issue the reader is referred to Beran (1968).

It is of particular significance that the theory includes predictions of the local velocity gradient and stress (Eq. (4.6)) and the local pressure (Eq. (4.9)) as a function of the microstructure surrounding a material particle. These localization effects are of great interest in modelling damage localization (e.g., creep cavitation damage). The non-local interaction derives from the stress-equilibrium requirement which is not imposed in the uniform strain-rate theory. From a particular vantage point the present theory constitutes a relaxation of the fully constrained uniform strain-rate theory. This relaxation is not arbitrary, however, since it must occur in a manner which drives the stress field towards equilibrium. The assumption of a universal, uniform reference shear stress in the theory is not required. If further information is available this assumption can easily be relaxed.

It is also useful to compare the present theory with the self-consistent theory (Hill, 1965; Hutchinson, 1976). The major difference is in including the explicit distribution of microstructure surrounding the particle. The self-consistent theories are based upon the solution of Eshelby for the interaction of an ellipsoidal inclusion embedded in a homogeneous medium. The properties of the medium are taken to be the average properties associated with the assemblage of inclusions. In this situation the convolution integral of Eq. (4.4) includes no contribution from particles at  $\mathbf{r}'$  lying outside of the ellipsoidal inclusion since  $\tilde{\mathbf{N}}$  is zero for these particles. This would only be valid when the microstructure outside the ellipsoid is perfectly disordered. The present theory makes no such restriction, and is therefore more general than the self-consistent theory.

The connections of the theory with macroscopic constitutive laws, shown in section 5, are not unique. The approximations represented in connecting only average or expectation values of tensors defined at a fixed state, is the simplest construction which can be considered. The primary limitation comes from the order of microstructural functions we are prepared to consider; and this is

presently limited by experimental capability. These limitations are also evident in the question of evolution of structures as treated in Section 6.

The major results of the theory, contained in Eqs (4.6, 4.9, 5.2 and 6.5), require the evaluation of the convolution integrals of the form  $\mathbf{G} * \mathbf{F}$ . A convenient method for evaluation the convolution integrals is to set  $V_c$  to be a cube of dimension  $\Delta$  with uniform state  $h$ , and then to evaluate the interaction of other individual cubes of the same dimension located in arbitrary locations upon a cubic lattice of dimension  $\Delta$  in the infinite space  $V$ . The microstructural correlation functions are assumed to be constant over these volumes relative to  $V_c$ . Summing the interactions over the lattice completes the evaluation of the convolution integral. Some details of the numerical solution for the interaction of two cubes are given in the appendix.

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### APPENDIX

Evaluate convolution integrals of the form

$$G_{ni,mj}(\mathbf{r}' - \mathbf{r}) * F_{ij}(\mathbf{r}' - \mathbf{r}) = \frac{1}{V_c} \int_{\mathbf{r} \in V_c} \int_{\mathbf{r}' \in V'_c} G_{ni,mj}(\mathbf{r}' - \mathbf{r}) * F_{ij}(\mathbf{r}' - \mathbf{r}) d\mathbf{r}'^3 d\mathbf{r}^3 \tag{A.1}$$

where  $V_c$  and  $V'_c$  are cubes of volume  $\Delta^3$  centered at  $c$  and  $c'$ , respectively, in the infinite volume  $V$  (Figure A.1). The correlation function  $F_{ij}$  is taken to be

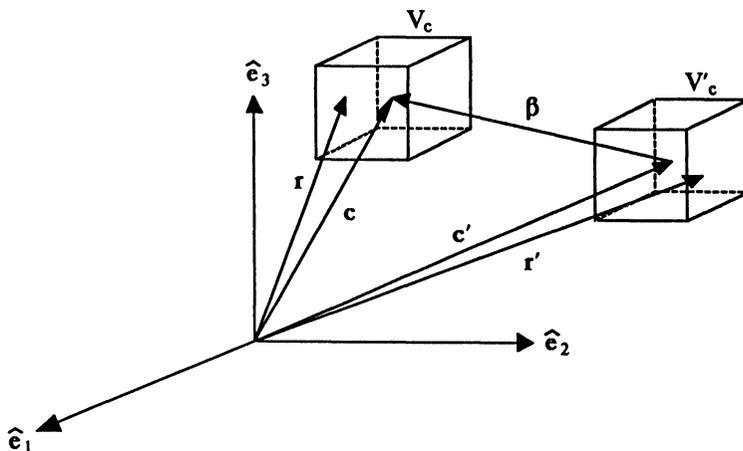


Figure A.1 Geometry of the convolution integral problem  $\mathbf{G} * \mathbf{F}$ .

constant over  $V'_c$  relative to  $V_c$ . Introducing the Fourier transform of  $G$ , Eq. (A.1) becomes

$$G_{ni,mj} * F_{ij} = \frac{-F_{ij}}{8\pi^3 \Delta^3} \int_{k \in R^3} k_m k_j \tilde{G}_{ni}(k) \int_{\mathbf{r} \in V_c} e^{-i\mathbf{k} \cdot \mathbf{r}} d\mathbf{r}^3 \int_{\mathbf{r}' \in V'_c} e^{-i\mathbf{k} \cdot \mathbf{r}'} d\mathbf{r}'^3 dk^3 \quad (\text{A.2})$$

where the integral over  $\mathbf{k}$  extends over the infinite space  $R^3$ . Next, set  $\mathbf{k} = k\hat{\alpha}$  where  $\hat{\alpha}$  is the unit vector defined in spherical angles  $\theta$  and  $\psi$  as  $[\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta]$ . Set  $\boldsymbol{\beta} = \mathbf{c} - \mathbf{c}'$  and evaluate the integrals over  $\mathbf{r}$  and  $\mathbf{r}'$ . Equation (A.2) becomes

$$G_{ni,mj} * F_{ij} = \frac{F_{ij}}{8\pi^3 \Delta^3} \int_0^{2\pi} \int_0^\pi \left[ \frac{\alpha_m \alpha_j}{\alpha_1^2 \alpha_2^2 \alpha_3^2} \right] [k^2 \tilde{G}_{ni}] \int_0^\infty \frac{1}{k^4} [e^{-ik[\alpha_1 \beta_1 + \alpha_2 \beta_2 \alpha_3 \beta_3]}] \\ \times [-8 + 4\{\text{six terms of the form } e^{\pm ik \Delta \alpha_s}\} \\ - 2\{\text{twelve terms of the form } e^{ik\Delta[\pm \alpha_s \pm \alpha_t]}_{s \neq t}\} \\ + \{\text{eight terms of the form } e^{ik\Delta[\pm \alpha_s \pm \alpha_t \pm \alpha_u]}_{s \neq t \neq u}\}] \\ \times dk \sin \theta d\theta d\psi \quad (\text{A.3})$$

The terms  $[k^2 \tilde{G}_{ni}]$  are real, and depend only upon  $\mathbf{N}^R$  and the angles  $\theta$  and  $\psi$ .

Since  $\mathbf{G} * \mathbf{F}$  is real we only need to evaluate the real part of the integral over  $k$ . This leads to integrals of the form

$$\int_0^\infty \frac{\cos k \phi}{k^4} dk \quad \text{where} \quad \phi = \phi(\hat{\alpha}, \boldsymbol{\beta}, \Delta) \quad (\text{A.4})$$

Evaluate the integral by expanding  $\cos k\phi$  about zero and then analyzing the remainder terms at a convenient order of expansion.

$$\int_0^\infty \frac{\cos k \phi}{k^4} dk = \lim_{\varepsilon \rightarrow 0} \int_\varepsilon^\infty \frac{\cos k \phi}{k^4} dk \\ = \lim_{\varepsilon \rightarrow 0} \left[ \frac{-\phi^2}{2\varepsilon} + \frac{1}{3\varepsilon^2} + O(\varepsilon) \right] + \frac{\phi^3}{6} \int_0^\infty \frac{\sin k \phi}{k} dk \quad (\text{A.5})$$

Obviously, in the limit as  $\varepsilon \rightarrow 0$  the first two terms of the right hand side of Eq. (A.5) diverge, but the fourth term becomes  $\pi \phi^3 \text{sign}(\phi)/12$ . When all sixty four terms of Eq. (A.3) are summed, however, the first three terms in the expansion sum to zero. This leads to the final result, which remains numerical in the variables  $\theta$  and  $\psi$ :

$$G_{ni,mj}(\mathbf{r}' - \mathbf{r}) * F_{ij}(\mathbf{r}' - \mathbf{r}) = \frac{F_{ij}}{96\pi^2 \Delta^3} \int_0^{2\pi} \int_0^\pi \left[ \frac{\alpha_m \alpha_j k^2 \tilde{G}_{ni}}{\alpha_1^2 \alpha_2^2 \alpha_3^2} \right] \\ [-8 |\hat{\alpha} \cdot \boldsymbol{\beta}|^3 + 4\{|\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_1|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_3|^3 \\ + |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_1|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_3|^3\} \\ - 2\{|\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_1 - \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_2 - \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} - \Delta \alpha_1 - \Delta \alpha_3|^3 \\ \times |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_1 + \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_2 + \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \boldsymbol{\beta} + \Delta \alpha_1 + \Delta \alpha_3|^3\}]$$

$$\begin{aligned}
& \times |\hat{\alpha} \cdot \beta - \Delta \alpha_1 + \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \beta - \Delta \alpha_2 + \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \beta - \Delta \alpha_1 + \Delta \alpha_3|^3 \\
& \times \{ |\hat{\alpha} \cdot \beta + \Delta \alpha_1 - \Delta \alpha_2|^3 + |\hat{\alpha} \cdot \beta + \Delta \alpha_2 - \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \beta + \Delta \alpha_1 - \Delta \alpha_3|^3 \} \\
& \quad + \{ |\hat{\alpha} \cdot \beta - \Delta \alpha_1 - \Delta \alpha_2 - \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \beta + \Delta \alpha_1 + \Delta \alpha_2 + \Delta \alpha_3|^3 \\
& \quad \quad + |\hat{\alpha} \cdot \beta - \Delta \alpha_1 + \Delta \alpha_2 - \Delta \alpha_3|^3 \\
& \quad \quad |\hat{\alpha} \cdot \beta + \Delta \alpha_1 - \Delta \alpha_2 + \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \beta + \Delta \alpha_1 - \Delta \alpha_2 - \Delta \alpha_3|^3 \\
& \quad \quad + |\hat{\alpha} \cdot \beta - \Delta \alpha_1 + \Delta \alpha_2 + \Delta \alpha_3|^3 \\
& \times |\hat{\alpha} \cdot \beta - \Delta \alpha_1 - \Delta \alpha_2 + \Delta \alpha_3|^3 + |\hat{\alpha} \cdot \beta + \Delta \alpha_1 + \Delta \alpha_2 - \Delta \alpha_3|^3 \} \sin \theta \, d\theta \, d\psi
\end{aligned} \tag{A.6}$$

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