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Estimation of Yield Function for Anisotropic Aggregate of FCC Crystallites

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Abstract: In this paper, we give an simple but approximate yield surface for single FCC crystals in Hill's criterion form by Schmid's law and nonlinear optimization theory. Assuming that all FCC crystallites in a polycrystal have the same (current) critical resolved shear stress τ_c for slip, we derive two closed but approximate yield functions through the orientational averaging of all FCC crystallites' yield surfaces in the polycrystal. The effect of crystallography on the two yield functions are described by the orientation distribution function.

Keywords: estimation of yield function; effective plastic anisotropy tensor; the ODF; FCC crystals

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1. Introduction

The studies of plasticity on polycrystals may be divided into two classes: the mathematical theory of plasticity and physical theory of plasticity [1–4]. The mathematical approach of plasticity is a formalization of known experimental results and does not penetrate deeply into the physical process of plastic yielding. An alternative approach to the mathematical theory of plasticity is the physical approach of plasticity. A polycrystalline material is an aggregate of tiny crystallites separated by grain boundaries. The microstructure of the polycrystal includes grain orientations and the grain boundary structure. Plastic properties of the polycrystal are related to slip mechanisms of crystallites and the microstructure of the polycrystal.

In order to study the properties of the polycrystal, we take a representative volume element (RVE) from the polycrystal. Although the volume of the RVE is small, the RVE contains information of the crystallographic texture on the polycrystal. The earlier study of polycrystalline plasticity was conducted by Sachs [5] and Taylor [6]. Sachs assumed that all crystallites in a RVE have the same stress. Taylor assumed that all crystallites in a RVE experience the same deformation. Bishop and Hill [7,8] adopted Taylor's model to calculate a yield function for an isotropic aggregate of cubic crystallites. Let τ_c denote a critical resolved shear stress. For an isotropic aggregate of FCC (face centered cubic) crystallites, assuming that all slip systems of cubic crystallites in a polycrystal have the same (current) critical resolved shear stress, the uniaxial tensile yield stresses should be $2.238\tau_c$ under Sachs' model and $3.06\tau_c$ under Taylor's model [9]. Maniatty et al. [10] employed the isotropic plasticity equivalent method, in which the actual stress tensor acting on an anisotropic material is transformed into a new stress tensor acting on an "isotropic plasticity equivalent" material, for obtaining an anisotropic yield function. Houtte [11] presented a method of obtaining the yield locus of textured polycrystals by constructing a data bank of the Taylor factors. Both Maniatty et al. and Houtte did not give closed expressions of yield functions with the effect of the texture coefficients.

The micromechanics of polycrystals is interesting only because one can measure the orientations of crystallites by orientation imaging microscopy or by X-ray diffraction. As we know, using the same manufacturing procedure, one can never make two polycrystalline samples with identical crystalline orientations. One can only make samples which seem macroscopically identical. Since the statistical information on the microstructure of a polycrystal can be described mathematically by the orientation distribution function (ODF) and since the plastic deformation of polycrystals involves slips inside crystallites, we will develop a statistical yield function with the effects of the orientation distribution function (ODF) and the the critical resolved shear stress τ_c of crystallites.

In this paper, we provide a simple method to obtain two closed but approximate yield functions with the effect of the texture coefficients for the RVE, where the volume average (i.e., orientational averaging) of all crystallites' yield surfaces is taken as a (macroscopic) yield function of the RVE. Using the physical approach to FCC crystallites, we derive a yield surface of single FCC crystals in Hill's criterion form by Schmid's law and nonlinear optimization theory, give a plastic anisotropy tensor $\mathbf{M}(\mathbf{R})$ of FCC crystallites with orientation $\mathbf{R}$, and obtain the volume average of all crystallites' yield surfaces in the RVE to obtain two closed but approximate yield functions for the RVE. The two yield functions are based on the assumption that all crystallites in the RVE have the same (current) critical resolved shear stress τ_c for slip. The effect of crystallography in the two yield functions is described by the texture coefficients. The first yield function is based on Sachs' model. The second yield function is based on the assumption that the effect of the ODF on the perturbation stress $\Delta\sigma_{ij}$ is, up to the terms, linear in the texture coefficients. Man [12–14] found that for orthorhombic aggregates of cubic crystallites, a macroscopic yield function of the RVE, up to terms, is linear in the texture coefficients.Our two yield functions are different to Man's yield function [12,13] in three aspects: (1) the two yield functions are for an anisotropic aggregate of cubic crystallites, but Man's yield function is for an orthorhombic aggregate of cubic crystallites; (2) we can determine the relations between two material parameters and the (current) critical resolved shear stress τ_c through some physical assumptions, but Man's yield function contains two unspecified parameters (Y_0 and β) and Man's yield function is independent of the physical model; (3) Man's yield function includes the effect of the ODF being, up to terms, linear in the texture coefficients,while our second yield function is quadratic texture dependence.

The critical resolved shear stress τ_c is related to the crystalline dislocation mechanism, the crystalline size, and the grain boundary structure. In this paper, however, we do not discuss the hardening process of the critical resolved shear stress τ_c during plastic deformation. Herein, we only study the constitutive form of the yield function of the FCC polycrystal for the given ODF and the given τ_c.

2. Approximate Yield Surface of FCC Crystal in Hill's Criterion form

Assume that a fixed spatial Cartesian coordinate system is chosen. To describe the orientation of a FCC crystallite in the RVE, we pick as a reference a FCC crystallite $\mathbf{I}$, whose three four-fold axes of rotational symmetry coincide with the Cartesian coordinate axes. The orientation of any crystallite in the RVE is then specified by rotation $\mathbf{R}$, which takes the reference crystallite $\mathbf{I}$ to the configuration of the crystallite.

By Schmid's law, we know that yielding for the reference crystallite $\mathbf{I}$ would begin on a slip system $\mathbf{n} \otimes \mathbf{t}$ (combination of a slip plane and a slip direction) when the resolved shear stress on this slip plane and in the slip direction reaches a critical value τ_c, where the unit normal of the slip plane is denoted by $\mathbf{n}$ and the unit vector of the slip direction is denoted by $\mathbf{t}$ with $\mathbf{t} \cdot \mathbf{n} = t_i n_i = 0$. When volume average stress components in the reference crystallite $\mathbf{I}$ are denoted by $\sigma_{ij}(\mathbf{I})$, the shear stress on the slip plane and in the slip direction should be $\tau = \sigma_{ij}(\mathbf{I}) t_i n_j$. Because the shear stress of the reference crystallite on its slip planes and in its slip direction satisfies $|\tau| \leq \tau_c$, the stress components of the reference crystallite $\mathbf{I}$ are in space $\mathcal{S}$:

$$\mathcal{S} = \left\{ (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{31}, \sigma_{12}) \in \mathbb{R}^6 : \ |\tau| = |\sigma_{ij} t_i n_j| \leq \tau_c \right\}, \tag{1}$$

where σ_{ij}=$\sigma_{ij}(\mathbf{I})$. The yield surface $\partial\mathcal{S}$ of the reference crystallite **I** should be

$$\partial\mathcal{S} = \left\{ (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{23}, \sigma_{31}, \sigma_{12}) \in \mathbb{R}^6 : \ |\tau| = |\sigma_{ij} t_i n_j| = \tau_c \right\}. \tag{2}$$

The space $\mathcal{S}$ given in (1) is surrounded by a set of yield functions ($|\sigma_{ij} t_i n_j| = \tau_c$) linear in stress components.

Assume that the space $\mathcal{S}$ in (1) can be surrounded approximately by a yield surface

$$f(\sigma_{ij}(\mathbf{I})) = M_{ijkl}(\mathbf{I})\sigma_{ij}(\mathbf{I})\sigma_{kl}(\mathbf{I}) - 1 = 0, \tag{3}$$

where **I** $\in$SO(3) is the second-order identity tensor for the reference crystallite **I**, $\mathbf{M}(\mathbf{I})$ is called the plastic anisotropy tensor[4] of the reference crystallite **I** with the minor and major symmetries, $\sigma_{ij}(\mathbf{I})$ is the volume average stress in the reference crystallite **I**. Any hydrostatic stress $p\delta_{ij}$ does not change the shear stress value of the reference crystallite **I** because $\tau = (\sigma_{ij} + p\delta_{ij})t_i n_j = \sigma_{ij} t_i n_j$ by $t_i n_i$=0 for all $p \in \mathbb{R}$. Hence, we have

$$f(\sigma_{ij}(\mathbf{I})) = f(\sigma_{ij}(\mathbf{I}) + p\delta_{ij}) \ \text{ or } 2pM_{ijkl}\delta_{ij}\sigma_{kl} + p^2 M_{ijkl}\delta_{ij}\delta_{kl} = 0, \ p \in \mathbb{R} \tag{4}$$

which leads to the traceless condition $M_{iikl}(\mathbf{I}) = 0$ for any pair of indices k and l.

When the reference crystallite **I** and the traction acting on the reference crystallite **I** have a rotation **R**, the stress tensor in the reference crystallite **I** becomes $\sigma^{\mathbf{R}}_{ij} = R_{is}R_{jt}\sigma_{st}(\mathbf{I})$, and the plastic anisotropy tensor $\mathbf{M}(\mathbf{I})$ becomes $\mathbf{M}^{\mathbf{R}}$ with constitutive restriction:

$$f(\sigma_{ij}(\mathbf{I})) = M_{pqnm}(\mathbf{I})\sigma_{pq}(\mathbf{I})\sigma_{nm}(\mathbf{I}) - 1 = M^{\mathbf{R}}_{ijkl}\sigma^{\mathbf{R}}_{ij}\sigma^{\mathbf{R}}_{kl} - 1 = 0. \tag{5}$$

where the three four-fold axes of rotational symmetry of the reference FCC crystallite **I** coincide with the Cartesian coordinate axes. Considering

$$\begin{aligned} M^{\mathbf{R}}_{ijkl}\sigma^{\mathbf{R}}_{ij}\sigma^{\mathbf{R}}_{kl} &= [R_{ip}R_{jq}R_{kn}R_{lm}M_{pqnm}(\mathbf{I})]\,[R_{is}R_{jt}\sigma_{st}(\mathbf{I})]\,[R_{ku}R_{lv}\sigma_{uv}(\mathbf{I})] \\ &= \delta_{sp}\delta_{tq}\delta_{un}\delta_{vm}M_{pqnm}(\mathbf{I})\sigma_{st}(\mathbf{I})\sigma_{uv}(\mathbf{I}) = M_{pqnm}(\mathbf{I})\sigma_{pq}(\mathbf{I})\sigma_{nm}(\mathbf{I}) \end{aligned} \tag{6}$$

and $R_{ip}R_{is} = \delta_{sp}$, we have $M^{\mathbf{R}}_{ijkl}$=$R_{ip}R_{jq}R_{kn}R_{lm}M_{pqnm}(\mathbf{I})$ in (5). Assuming that all crystallites in the RVE have the same (current) critical resolved shear stress τ_c for slip, we have the plastic anisotropy tensor $\mathbf{M}(\mathbf{R})$ of the crystallites with orientation **R**:

$$M_{ijkl}(\mathbf{R}) = M^{\mathbf{R}}_{ijkl} = R_{ip}R_{jq}R_{kn}R_{lm}M_{pqnm}(\mathbf{I}). \tag{7}$$

If we use $\sigma_{ij}(\mathbf{R})$ to denote the volume average stress of the crystallites with orientation **R**, the yield surface $f(\sigma_{ij}(\mathbf{R}))$ for the crystallites with orientation **R** can be expressed as

$$f(\sigma_{ij}(\mathbf{R})) = M_{ijkl}(\mathbf{R})\sigma_{ij}(\mathbf{R})\sigma_{kl}(\mathbf{R}) - 1 = 0 \tag{8}$$

by (5) and (7). Since the reference FCC crystallite **I** has the octahedral symmetry O, the plastic anisotropy tensor should satisfy $M^{\mathbf{R}}_{ijkl}$=$M_{ijkl}(\mathbf{I})$ for each rotation tensor **R** $\in O$, which with the minor and major symmetries of $\mathbf{M}(\mathbf{I})$ reads [15]

$$[M_{IJ}(\mathbf{I})] = \begin{pmatrix} m_{11} & m_{12} & m_{12} & 0 & 0 & 0 \\ m_{12} & m_{11} & m_{12} & 0 & 0 & 0 \\ m_{12} & m_{12} & m_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & m_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & m_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & m_{44} \end{pmatrix}, \tag{9}$$

where $[M_{IJ}(\mathbf{I})]$ is the matrix form of $\mathbf{M}(\mathbf{I})$ in Voigt's notation (i.e., indices ij and kl in M_{ijkl} are denoted by indices I and J of M_{IJ} with convention $11 \to 1,\ 22 \to 2,\ 33 \to 3,\ 23 \to 4,\ 13 \to 5,\ 12 \to 6$; for instances, $M_{1122} = M_{12}$, $M_{1123} = M_{14}$), m_{11}, m_{12}, and m_{44} are the material parameters of the reference crystallite $\mathbf{I}$. The plastic anisotropy tensor $[M_{IJ}(\mathbf{I})]$ in (9) can be decomposed into [16]

$$[M_{IJ}(\mathbf{I})] = m_{12}\left[B^{(1)}_{IJ}\right] + 2m_{44}\left[B^{(2)}_{IJ}\right] + (m_{11} - m_{12} - 2m_{44})\left[B^{(3)}_{IJ}(\mathbf{I})\right] \tag{10}$$

where $\left[B^{(1)}_{IJ}\right]$, $\left[B^{(2)}_{IJ}\right]$, and $\left[B^{(3)}_{IJ}(\mathbf{I})\right]$ are the matrix form of the following tensors in Voigt's notation, respectively

$$B^{(1)}_{ijkl} = \delta_{ij}\delta_{kl},\ B^{(2)}_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),\ B^{(3)}_{ijkl}(\mathbf{I}) = \sum_{\alpha=1}^{3} \delta_{\alpha i}\delta_{\alpha j}\delta_{\alpha k}\delta_{\alpha l}, \tag{11}$$

$\mathbf{B}^{(1)}$ and $\mathbf{B}^{(2)}$ are isotropic fourth-order tensor bases, $\mathbf{B}^{(3)}(\mathbf{I})$ is a fourth-order tensor basis for cubic crystals. The traceless condition $M_{iikl}(\mathbf{I}) = 0$ makes the plastic anisotropy tensor $\mathbf{M}(\mathbf{I})$ in (10) become

$$M_{ijkl}(\mathbf{I}) = m_{12}B^{(1)}_{ijkl} + 2m_{44}B^{(2)}_{ijkl} + (-3m_{12} - 2m_{44})B^{(3)}_{ijkl}(\mathbf{I}) \tag{12}$$

because of $m_{11} = -2m_{12}$ which makes that

$$M_{iikl}(\mathbf{I}) = m_{12}(3\delta_{kl}) + 2m_{44}\delta_{kl} + (m_{11} - m_{12} - 2m_{44})\delta_{kl} \equiv 0 \tag{13}$$

holds.

Putting (12) into (3), we find a yield surface of the reference crystallite $\mathbf{I}$ in Hill's criterion form

$$\begin{aligned} f(\sigma(\mathbf{I})) &= m_{12}\sigma_{ii}\sigma_{kk} + 2m_{44}\sigma_{ij}\sigma_{ij} + (-3m_{12} - 2m_{44})\left(\sigma_{11}^2 + \sigma_{22}^2 + \sigma_{33}^2\right) \\ &= \frac{1}{\eta^2}\left[(\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + (\sigma_{11} - \sigma_{22})^2\right] + \frac{1}{\varsigma^2}\left[\sigma_{23}^2 + \sigma_{31}^2 + \sigma_{12}^2\right] - 1 = 0 \end{aligned} \tag{14}$$

because

$$B^{(1)}_{ijkl}\sigma_{ij}\sigma_{kl} = \sigma_{ii}\sigma_{kk},\ B^{(2)}_{ijkl}\sigma_{ij}\sigma_{kl} = \sigma_{ij}\sigma_{ij},\ B^{(3)}_{ijkl}(\mathbf{I})\sigma_{ij}\sigma_{kl} = \sigma_{11}^2 + \sigma_{22}^2 + \sigma_{33}^2, \tag{15}$$

where $\sigma_{ij} = \sigma_{ij}(\mathbf{I})$ and

$$\eta^2 = -\frac{1}{m_{12}},\ \varsigma^2 = \frac{1}{4m_{44}}. \tag{16}$$

When $-3m_{12} - 2m_{44} = 0$, $\mathbf{M}(\mathbf{I})$ in (12) is an isotropic tensor whose corresponding yield surface is von Mises' yield criterion.

For the reference FCC crystallite $\mathbf{I}$, the slip occurs on {111} planes in <110> directions. The unit normal $\mathbf{n}$ of the slip planes and the unit vector $\mathbf{t}$ of the slip directions constitute the 24 slip systems $\mathbf{n} \otimes \mathbf{t}$ [9]

$$\{\mathbf{n} \otimes \mathbf{t}\} = \{\pm\frac{1}{\sqrt{3}}(111) \otimes \frac{1}{\sqrt{2}}[1\bar{1}0], \ldots, \pm\frac{1}{\sqrt{3}}(11\bar{1}) \otimes \frac{1}{\sqrt{2}}[011]\}, \tag{17}$$

in which there is $\mathbf{t} \cdot \mathbf{n} = 0$ for each slip system. Substituting (17) into $|\tau| = |\sigma_{ij}t_i n_j| \le \tau_c$ in (1), one can obtain 24 inequalities that are linear in stress components

$$
\begin{aligned}
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{22}-\sigma_{33})+\sigma_{31}\pm\sigma_{12}| \leq \ \tau_c, \\
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{22}-\sigma_{33})-\sigma_{31}\pm\sigma_{12}| \leq \ \tau_c, \\
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{33}-\sigma_{11})+\sigma_{12}\pm\sigma_{23}| \leq \ \tau_c, \\
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{33}-\sigma_{11})-\sigma_{12}\pm\sigma_{23}| \leq \ \tau_c, \\
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{11}-\sigma_{22})+\sigma_{31}\pm\sigma_{23}| \leq \tau_c, \\
|\tau| &= \frac{1}{\sqrt{6}}|(\sigma_{11}-\sigma_{22})-\sigma_{31}\pm\sigma_{23}| \leq \tau_c
\end{aligned}
\tag{18}
$$

which constitute the the stress space $\mathcal{S}$.

Now we assume that the stress space $\mathcal{S}$ in (1) can approximately be surrounded by a function in Hill's criterion form (14). In order to determine η and ς in (14), we introduce two subspaces of $\mathcal{S}$ in (1)

$$
\begin{aligned}
\mathcal{S}_1 &= \Big\{(\sigma_{11},\sigma_{22},\sigma_{33},0,0,0) \in \mathbb{R}^6 : \ |\tau| = |\,\sigma_{ij}t_i n_j| \leq \tau_c\Big\}, \\
\mathcal{S}_2 &= \Big\{(0,0,0,\sigma_{23},\sigma_{31},\sigma_{12}) \in \mathbb{R}^6 : |\tau| = |\,\sigma_{ij}t_i n_j| \leq \tau_c\Big\}
\end{aligned}
\tag{19}
$$

and two subspaces in $\mathbb{R}^6$

$$
\begin{aligned}
\mathcal{M}(\eta) &= \{(\sigma_{11},\sigma_{22},\sigma_{33},0,0,0) \in \mathbb{R}^6 : (\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2+(\sigma_{11}-\sigma_{22})^2-\eta^2 \leq 0\}, \\
\mathcal{N}(\varsigma) &= \Big\{(0,0,0,\sigma_{23},\sigma_{31},\sigma_{12}) \in \mathbb{R}^6 : \sigma_{23}^2+\sigma_{31}^2+\sigma_{12}^2-\varsigma^2 \leq 0\Big\}.
\end{aligned}
\tag{20}
$$

The maximum and minimum values of η and ς in (20) are defined by

$$
\begin{aligned}
\eta_{\max} &= \inf\{\eta : \mathcal{M}(\eta) \supset \mathcal{S}_1\}, \ \ \varsigma_{\max} = \inf\{\eta : \mathcal{N}(\varsigma) \supset \mathcal{S}_2\}, \\
\eta_{\min} &= \sup\{\eta : \mathcal{M}(\eta) \subset \mathcal{S}_1\}, \ \ \varsigma_{\min} = \sup\{\varsigma : \ \mathcal{N}(\varsigma) \subset \mathcal{S}_2\},
\end{aligned}
\tag{21}
$$

where we determine η and ς in (14) through multi-axial tensions and pure shears, respectively. The proceeding maximum and minimum problems in (21) belong to nonlinear optimization problems. The relations (19) and (20) are used to obtain the best fitting of the FCC crystal yield surface $|\,\sigma_{ij}t_i n_j| \leq \tau_c$.

We use Microsoft Excel to solve the problems (21) with (20) and (18). Then we obtain the maximum and minimum values of η and ς

$$
\eta_{\min} = 3\,\tau_c, \ \eta_{\max} = \sqrt{12}\,\tau_c, \ \varsigma_{\min} = \sqrt{3}\,\tau_c, \ \varsigma_{\max} = \sqrt{6}\tau_c. \tag{22}
$$

Putting $\eta = \eta_{\max}$ and $\varsigma = \varsigma_{\max}$ into (14), we find a yield surface of FCC crystals for the reference FCC crystallite **I**

$$
\frac{1}{12\,\tau_c^2}\Big[(\sigma_{22}-\sigma_{33})^2+(\sigma_{33}-\sigma_{11})^2+(\sigma_{11}-\sigma_{22})^2\Big]+\frac{1}{6\,\tau_c^2}\Big[\sigma_{23}^2+\sigma_{31}^2+\sigma_{12}^2\Big]-1=0 \tag{23}
$$

which is just the same as that of Maniatty et al. [10].

Since the goal of the paper is to estimate a macroscopic yield function of the RVE, let us choose η and ς in (14) as follows:

$$
\eta = \frac{1}{2}(\eta_{\min}+\eta_{\max}) = 3.232\tau_c, \ \varsigma = \frac{1}{2}(\varsigma_{\min}+\varsigma_{\max}) = 2.091\tau_c. \tag{24}
$$

If all crystallites in the RVE have the same (current) critical resolved shear stress τ_c for slip, we combine (7) with (12), (16) and (24) to obtain the plastic anisotropy tensor

$$M_{ijkl}(\mathbf{R}) = -\frac{1}{\eta^2}B^{(1)}_{ijkl} + \frac{1}{2\varsigma^2}B^{(2)}_{ijkl} + \omega B^{(3)}_{ijkl}(\mathbf{R}) \tag{25}$$

and the yield surface $f(\sigma_{ij}(\mathbf{R}))$ for FCC crystallites with orientation $\mathbf{R}$

$$f(\sigma_{ij}(\mathbf{R})) = -\frac{1}{\eta^2}(\sigma_{ii}(\mathbf{R}))^2 + \frac{1}{2\varsigma^2}\sigma_{ij}(\mathbf{R})\sigma_{ij}(\mathbf{R}) + \omega B^{(3)}_{ijkl}(\mathbf{R})\sigma_{ij}(\mathbf{R})\sigma_{kl}(\mathbf{R}) - 1 = 0 \tag{26}$$

where $\omega = \frac{3}{\eta^2} - \frac{1}{2\varsigma^2}$ and

$$\begin{aligned} B^{(\alpha)}_{ijkl}(\mathbf{R}) &= R_{ip}R_{jq}R_{kn}R_{lm}B^{(\alpha)}_{pqnm} = B^{(\alpha)}_{ijkl}, \ \alpha = 1, 2, \\ B^{(3)}_{ijkl}(\mathbf{R}) &= R_{ip}R_{jq}R_{kn}R_{lm}B^{(3)}_{pqnm}(\mathbf{I}) = \sum_{\alpha=1}^{3} R_{i\alpha}R_{j\alpha}R_{k\alpha}R_{l\alpha}. \end{aligned} \tag{27}$$

3. Yield Function and Effective Plastic Anisotropy Tensor of RVE

The crystallographic texture of a polycrystal is described by the orientation distribution function (ODF). The ODF is used to describe the probability density of finding a crystallite with orientation $\mathbf{R}$ in the RVE. The mechanical anisotropy of the RVE is caused mainly by its crystallographic texture and plastic anisotropy of crystallites. Let $w(\mathbf{R})$ be the orientation distribution function. If $L^2(\mathrm{SO}(3))$ is the space of the square-integrable complex-valued functions, $w \in L^2(\mathrm{SO}(3))$ can be expanded as an infinite series in terms of the Wigner $D-$functions [17,18]

$$w(\mathbf{R}) = w_{\text{iso}} + \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\sum_{n=-l}^{l} c^l_{mn}D^l_{mn}(\mathbf{R}), \ c^l_{mn} = (-1)^{m-n}(c^l_{\bar{m}\bar{n}})^*, \tag{28}$$

where $w_{\text{iso}} = \frac{1}{8\pi^2}$, c^l_{mn} $(l \geq 1)$ are the texture coefficients, $(c^l_{\bar{m}\bar{n}})^*$ denote the complex conjugate of the complex number $c^l_{\bar{m}\bar{n}}$, $\bar{n} = -n$. The Wigner D-functions D^l_{mn} constitute an orthogonal basis in $L^2(\mathrm{SO}(3))$. The texture coefficients that we shall need can easily be measured by $X-$ray diffraction. The texture coefficients c^l_{mn} are related to Roe's W_{lmn} coefficients by formula [19]

$$W_{lmn} = (-1)^{n-m}\sqrt{\frac{2}{2l+1}}\,c^l_{mn}. \tag{29}$$

The micromechanics of polycrystals becomes interesting only because one can obtain statistical information of the orientations by X-ray diffraction or measure the orientations of pcrystallites, pointwise, by orientation imaging microscopy. For the measurement of X-ray diffraction, one measures the specimen surface's, $\frac{1}{4}$ depth's, and $\frac{1}{2}$ depth's texture coefficients, respectively, by sanding the specimen of sheets. The mean values of the texture coefficients on the surface, $\frac{1}{4}$ depth, and $\frac{1}{2}$ depth of the specimen are taken as the texture coefficients of the specimen. For the measurement of the orientation imaging microscopy, one obtains the orientation (Euler angles ψ_p, θ_p, ϕ_p) of each crystallite Ω_p in the specimen. Since the FCC polycrystal can be taken as an aggregate of cubic crystallites (i.e., $\Omega = \cup_{p=1}^{N}\Omega_p$), the texture coefficients of the specimen are given by [20]

$$c^l_{mn} = \frac{1}{|\Omega|}\sum_{p=1}^{N}|\Omega_p|c^4_{mn}(\mathbf{R}_p) \tag{30}$$

with

$$c^l_{mn}(\mathbf{R}_p) = \frac{2l+1}{8\pi^2} \cdot \frac{1}{24} \sum_{i=1}^{24} \left(D^l_{mn}(\mathbf{R}_p \mathbf{Q}^{(i)}_{\text{cr}}) \right)^*, \ \forall \mathbf{Q}^{(i)}_{\text{cr}} \in O, \tag{31}$$

where $\mathbf{R}_p = \mathbf{R}(\psi_p, \theta_p, \phi_p)$ and O is the group of cubic crystal symmetry.

Let $\overline{\sigma}_{ij}$ be the volume average stress components of the RVE. By definition of the ODF, the orientational (volume) average stress can be obtained by

$$\overline{\sigma}_{ij} = \int_{\text{SO}(3)} \sigma_{ij}(\mathbf{R}) w(\mathbf{R}) dg, \tag{32}$$

where $g = 8\pi^2 g_H$, g_H is the Haar measure on SO(3) with $g_H(\text{SO}(3)) = 1$, $\sigma_{ij}(\mathbf{R})$ is the volume average stress tensor of crystallites with orientation $\mathbf{R}$ in the RVE. When $\mathbf{R}$ is defined by Roe's notation [18], there is $dg = \sin\theta d\psi d\theta d\phi$.

When all crystallites in the RVE have the same (current) critical resolved shear stress τ_c for slip, the yield surface $f(\sigma_{ij}(\mathbf{R}))$ of crystallites with orientation $\mathbf{R}$ is determined by (26). By the ODF definition, the volume average $\overline{f(\sigma_{ij}(\mathbf{R}))}$ of all crystallites in the RVE can be expressed as

$$\overline{f(\sigma_{ij}(\mathbf{R}))} = \int_{\text{SO}(3)} f(\sigma_{ij}(\mathbf{R})) w(\mathbf{R}) dg = \int_0^{2\pi} \int_0^{\pi} \int_0^{2\pi} f(\sigma_{ij}(\mathbf{R})) w(\mathbf{R}) \sin\theta d\psi d\theta d\phi = 0 \tag{33}$$

which can be taken as the macroscopic yield function of the RVE.

If the macroscopic yield function $\overline{f(\sigma_{ij}(\mathbf{R}))}$ can be expressed as

$$\overline{f(\sigma_{ij}(\mathbf{R}))} = \overline{\sigma}_{ij} M^{\text{eff}}_{ijkl} \overline{\sigma}_{kl} - 1 = 0 \tag{34}$$

in Hill's criterion form, then we call $\mathbf{M}^{\text{eff}}$ in (34) the effective plastic anisotropy tensor of the RVE. The effective plastic anisotropy tensor $\mathbf{M}^{\text{eff}}$ gives the relationship between the macroscopic yield function and the volume average stress of the RVE. One recipe to compute the effective plastic anisotropy tensor $\mathbf{M}^{\text{eff}}$ in (34) is by way of putting (8) into (33)

$$\overline{\sigma}_{ij} M^{\text{eff}}_{ijkl} \overline{\sigma}_{kl} = \int_{\text{SO}(3)} \sigma_{ij}(\mathbf{R}) M_{ijkl}(\mathbf{R}) \sigma_{kl}(\mathbf{R}) w(\mathbf{R}) dg. \tag{35}$$

4. Volume Average of Plastic Anisotropy Tensor

The basic assumption for Sachs' model [5] is that all crystallites in the RVE experience the same state of stress (i.e., $\sigma_{ij}(\mathbf{R}) = \overline{\sigma}_{ij}$, $\forall \mathbf{R} \in \text{SO}(3)$). Substituting $\sigma_{ij}(\mathbf{R}) = \overline{\sigma}_{ij}$ into (35) reads $\overline{\sigma}_{ij} M^{\text{eff}}_{ijkl} \overline{\sigma}_{kl} = \int_{\text{SO}(3)} \overline{\sigma}_{ij} M_{ijkl}(\mathbf{R}) \overline{\sigma}_{kl} w(\mathbf{R}) dg$. Since the equation holds for each $\overline{\sigma}_{ij}$, the effective plastic anisotropy tensor has to be the volume average plastic anisotropy tensor $\overline{\mathbf{M}}$ of the RVE

$$\begin{aligned} \overline{M}_{ijkl} &= \int_{\text{SO}(3)} M_{ijkl}(\mathbf{R}) w(\mathbf{R}) dg \\ &= \int_{\text{SO}(3)} \left(-\frac{1}{\eta^2} B^{(1)}_{ijkl} + \frac{1}{2\varsigma^2} B^{(2)}_{ijkl} + \omega B^{(3)}_{ijkl}(\mathbf{R}) \right) w(\mathbf{R}) dg \end{aligned} \tag{36}$$

by (25).

From the results given by Huang and Man [21] and Huang [16,22], we know

$$\int_{\text{SO}(3)} B^{(1)}_{ijkl} w(\mathbf{R}) dg = B^{(1)}_{ijkl}, \ \int_{\text{SO}(3)} B^{(2)}_{ijkl} w(\mathbf{R}) dg = B^{(2)}_{ijkl} \tag{37}$$

because of $B^{(1)}_{ijkl}$ and $B^{(2)}_{ijkl}$ being isotropic fourth order tensors and

$$\begin{aligned}\int_{\mathrm{SO}(3)} B^{(3)}_{ijkl}(\mathbf{R})w(\mathbf{R})dg &= \left(\sum_{\alpha=1}^{3}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} R_{i\alpha}R_{j\alpha}R_{k\alpha}R_{l\alpha}\frac{1}{8\pi^2}\sin\theta d\psi d\theta d\phi\right) \\ &+ \sum_{s=1}^{\infty}\sum_{m=-s}^{s}\sum_{n=-s}^{s} c^s_{mn}\sum_{\alpha=1}^{3}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} R_{i\alpha}R_{j\alpha}R_{k\alpha}R_{l\alpha}D^s_{mn}(\mathbf{R})\sin\theta d\psi d\theta d\phi \\ &= \left(\frac{1}{5}B^{(1)}_{ijkl} + \frac{2}{5}B^{(2)}_{ijkl}\right) + \Phi_{ijkl},\end{aligned} \tag{38}$$

because of the relation [19]

$$\int_{\mathrm{SO}(3)} B^{(3)}_{ijkl}(\mathbf{R})D^s_{mn}(\mathbf{R})dg = 0, \text{ when } s > 4 \tag{39}$$

where $B^{(3)}_{ijkl}(\mathbf{R})$ is a fourth-order tensor. For an anisotropic aggregate of cubic crystallites, $\mathbf{\Phi}$ in (38) is totally symmetric (i.e., $\Phi_{i_1i_2i_3i_4} = \Phi_{i_{\tau(1)}i_{\tau(2)}i_{\tau(3)}i_{\tau(4)}}$ for any permutation τ of $\{1, 2, 3, 4\}$) and traceless with non-trivial components [21]:

$$\begin{aligned}&\Phi_{2233} = a_1,\ \Phi_{1133} = a_2,\ \Phi_{1122} = a_3, \\ &\Phi_{1123} = a_5 - a_8,\ \Phi_{1113} = -a_7 + 3a_4,\ \Phi_{1112} = -a_6 + a_9, \\ &\Phi_{3323} = -4a_5,\ \Phi_{3313} = -4a_4,\ \Phi_{3312} = 2a_6\end{aligned} \tag{40}$$

and

$$\begin{aligned}&a_1 = -\frac{32\pi^2}{105}(c^4_{00} + \sqrt{\frac{5}{2}}\,\mathrm{Re}\,c^4_{20}),\ a_2 = -\frac{32\pi^2}{105}(c^4_{00} - \sqrt{\frac{5}{2}}\,\mathrm{Re}\,c^4_{20}), \\ &a_3 = \frac{8\pi^2}{105}(c^4_{00} - \sqrt{70}\,\mathrm{Re}\,c^4_{40}),\ a_4 = \frac{8\sqrt{5}\pi^2}{105}\mathrm{Re}\,c^4_{10},\ a_5 = \frac{8\sqrt{5}\pi^2}{105}\mathrm{Im}\,c^4_{10}, \\ &a_6 = \frac{8\sqrt{10}\pi^2}{105}\mathrm{Im}\,c^4_{20},\ a_7 = \frac{8\sqrt{35}\pi^2}{105}\mathrm{Re}\,c^4_{30},\ a_8 = \frac{8\sqrt{35}\pi^2}{105}\mathrm{Im}\,c^4_{30},\ a_9 = \frac{8\sqrt{70}\pi^2}{105}\mathrm{Im}\,c^4_{40}.\end{aligned} \tag{41}$$

Here $\mathrm{Re}\,c^4_{m0}$ and $\mathrm{Im}\,c^4_{m0}$ denote the real and imaginary parts of the complex number c^4_{m0}, respectively. c^4_{00} is a real number because of $(28)_2$.

Putting (37) and (38) into (36), we obtain an effective plastic anisotropy tensor $\mathbf{M}^{\mathrm{eff}}$ of the RVE under the Sachs' model

$$M^{\mathrm{eff}}_{ijkl} = \overline{M}_{ijkl} = -\rho B^{(1)}_{ijkl} + 3\rho B^{(2)}_{ijkl} + \omega\Phi_{ijkl} \tag{42}$$

with

$$\begin{aligned}\rho &= \frac{1}{5}(\frac{2}{\eta^2} + \frac{1}{2\varsigma^2}) = \frac{1}{16.348\tau_c^2}, \\ \omega &= \frac{3}{\eta^2} - \frac{1}{2\varsigma^2} = \frac{1}{5.786\tau_c^2}.\end{aligned} \tag{43}$$

The texture coefficients c^4_{m0} above can be measured by the $X-$ray diffraction and inversion of pole figures (Roe, 1965 [18]). Obviously, the effective plastic anisotropy tensor satisfies the traceless condition $M^{\mathrm{eff}}_{iikl} = 0$ because of $\Phi_{iikl} = 0$. Substituting (42) and $(15)_{1,2}$ into (34), we obtain a macroscopic yield function of the RVE

$$\begin{aligned}\overline{f(\sigma_{ij}(\mathbf{R}))} &= -\rho\overline{\sigma}_{ii}\overline{\sigma}_{jj} + 3\rho\overline{\sigma}_{ij}\overline{\sigma}_{ij} + \omega\Phi_{ijkl}\overline{\sigma}_{ij}\overline{\sigma}_{kl} \\ &= \frac{1}{Y_0^2}\left(\frac{3}{2}\overline{\sigma}_{ij}\overline{\sigma}_{ij} - \frac{1}{2}\overline{\sigma}_{ii}\overline{\sigma}_{jj} + \beta\Phi_{ijkl}\overline{\sigma}_{ij}\overline{\sigma}_{kl}\right) - 1 = 0\end{aligned} \tag{44}$$

where

$$Y_0 = \frac{1}{\sqrt{2\rho}} = 2.859\tau_c\,,\ \beta = \frac{\omega}{2\rho} = 1.413. \tag{45}$$

The macroscopic yield function $\overline{f(\sigma_{ij}(\mathbf{R}))}$ of the RVE with a group of texture symmetry $\mathcal{G}_{\text{tex}}$ can be obtained from the constraints imposed by $\mathcal{G}_{\text{tex}}$ on the texture coefficients. For instance, if the coordinate axes are the two-fold axes of orthorhombic symmetry of the texture, then $c^4_{m0} = 0$ for odd m and $\operatorname{Im} c^4_{m0} = 0$ for all m. Substituting these restriction into (44) and (41), we obtain the macroscopic yield function of the RVE in the Hill's criterion form

$$\overline{f(\sigma_{ij}(\mathbf{R}))} = F(\overline{\sigma}_{22} - \overline{\sigma}_{33})^2 + G(\overline{\sigma}_{33} - \overline{\sigma}_{11})^2 + H(\overline{\sigma}_{11} - \overline{\sigma}_{22})^2 + 2L\overline{\sigma}^2_{23} + 2M\,\overline{\sigma}^2_{31} + 2N\,\overline{\sigma}^2_{12} - 1 = 0 \tag{46}$$

for an orthorhombic aggregate of FCC crystallites, where

$$\begin{aligned}(F, G, H) &= \frac{1}{Y_0^2}\left(\frac{1}{2}(1,1,1) - \beta(a_1, a_2, a_3)\right),\\ (L, M, N) &= \frac{1}{Y_0^2}\left(\frac{3}{2}(1,1,1) + 2\beta(a_1, a_2, a_3)\right).\end{aligned} \tag{47}$$

a_1, a_2, and a_3 in (41) are determined by the texture coefficients. Y_0 and β in (45) are dependent on the (current) critical resolved shear stress τ_c. The formula (46) is the same as that of Man [12,13] in form. However, Man's yield function is independent of the physical model; hence Y_0 and β for Man's yield function are two unspecified material parameters.

5. Yield Function with Quadratic Texture Dependence

Under Sachs' model, the effective plastic anisotropy tensor $\mathbf{M}^{\text{eff}}$ is the volume average plastic anisotropy tensor of the RVE. Man's yield function [12,13] and the yield function (46) contain the effect of the ODF only being, up to terms, linear in the texture coefficients, which may not suffice for strongly textured polycrystals [20]. In this section, we will establish a new physical model for deriving a macroscopic yield function of the RVE. The macroscopic yield function delineates the effect of the crystallographic texture on the plastic anisotropy up to terms quadratic in the texture coefficients.

Considering the collection of crystallites with orientation $\mathbf{R}$ in the RVE and using $\sigma_{ij}(\mathbf{R})$ to denote the volume average stress in these crystallites, we have the average perturbation stress of these crystallites

$$\Delta\sigma_{ij} = \sigma_{ij}(\mathbf{R}) - \overline{\sigma}_{ij}, \tag{48}$$

where $\overline{\sigma}_{ij}$ is given in (32). We assume that the average perturbation stress $\Delta\sigma_{ij}$ of crystallites with orientation $\mathbf{R}$ are governed by a constitutive relation of the form

$$\Delta\sigma_{ij} = \Delta\sigma_{ij}(\mathbf{R}, w, \overline{\sigma}_{kl}) \tag{49}$$

with constraint

$$\Delta\sigma_{ij}(\mathbf{R}, w, 0) = 0. \tag{50}$$

From (32) and (48), we have

$$\int_{\text{SO}(3)} \Delta\sigma_{ij}(\mathbf{R}, w, \overline{\sigma}_{kl}) w(\mathbf{R}) dg = 0. \tag{51}$$

Similar to the process of deriving the HV-V model given by Huang and Man [21], the average perturbation stress $\Delta\sigma_{ij}$ of the crystallites with orientation $\mathbf{R}$ can approximately be expressed as

$$\Delta\sigma_{ij} = \kappa\Big(\Psi_{ijkl}(\mathbf{R}) - \Phi_{ijkl}\Big)\overline{\sigma}_{kl}, \tag{52}$$

where we consider the effect of the ODF to $\Delta\sigma_{ij}$ being, up to terms, linear in the texture coefficients,

$$\Psi_{ijkl}(\mathbf{R}) = -\frac{1}{5}B^{(1)}_{ijkl} - \frac{2}{5}B^{(2)}_{ijkl} + B^{(3)}_{ijkl}(\mathbf{R}), \tag{53}$$

and κ is an unspecified material parameter. From (37) and (38), we know that $\Delta\sigma_{ij}$ in (52) satisfy the relation (51).

Through (35) and (48), we obtain an effective plastic anisotropy tensor by relation

$$\begin{aligned}\overline{\sigma}_{ij}M^{\text{eff}}_{ijkl}\overline{\sigma}_{kl} &= \int_{\text{SO(3)}} \sigma_{ij}(\mathbf{R})M_{ijkl}(\mathbf{R})\sigma_{kl}(\mathbf{R})w(\mathbf{R})dg = \int_{\text{SO(3)}} \overline{\sigma}_{ij}M_{ijkl}(\mathbf{R})\overline{\sigma}_{kl}w(\mathbf{R})dg \\ &+ \int_{\text{SO(3)}}\Big(\Delta\sigma_{ij}M_{ijkl}(\mathbf{R})\Delta\sigma_{kl} + \Delta\sigma_{ij}M_{ijkl}(\mathbf{R})\overline{\sigma}_{kl} + \overline{\sigma}_{ij}M_{ijkl}(\mathbf{R})\Delta\sigma_{kl}\Big)w(\mathbf{R})dg.\end{aligned} \tag{54}$$

From (52) and (25), we have

$$\begin{aligned}\overline{\sigma}_{ij}M_{ijkl}(\mathbf{R})\Delta\sigma_{kl} &= \frac{\kappa}{2\varsigma^2}\overline{\sigma}_{ij}\Big(\Psi_{ijkl}(\mathbf{R}) - \Phi_{ijkl}\Big)\overline{\sigma}_{kl} \\ &+\kappa\omega\overline{\sigma}_{ij}\left(-\frac{1}{5}B^{(1)}_{ijkl} + \frac{3}{5}B^{(3)}_{ijkl}(\mathbf{R}) - B^{(3)}_{ijmn}(\mathbf{R})\Phi_{mnkl}\right)\overline{\sigma}_{kl}.\end{aligned} \tag{55}$$

by relations $B^{(1)}_{ijmn}\Psi_{mnkl}(\mathbf{R}) = B^{(1)}_{ijmn}\Phi_{mnkl} = 0$ and

$$\begin{aligned}B^{(1)}_{ijmn}B^{(1)}_{mnkl} &= 3B^{(1)}_{ijkl},\ B^{(1)}_{ijmn}B^{(3)}_{mnkl}(\mathbf{R}) = B^{(1)}_{ijkl}, \\ B^{(3)}_{ijmn}(\mathbf{R})B^{(3)}_{mnkl}(\mathbf{R}) &= B^{(3)}_{ijkl}(\mathbf{R}),\ B^{(2)}_{ijmn}B^{(\alpha)}_{mnkl}(\mathbf{R}) = B^{(\alpha)}_{ijkl}(\mathbf{R}),\ \alpha = 1,2,3.\end{aligned} \tag{56}$$

By means of the relations (37) and (38), we can complete the following integrations and obtain the volume average value on (55)

$$\begin{aligned}\int_{\text{SO(3)}} \Delta\sigma_{ij}M_{ijkl}(\mathbf{R})\overline{\sigma}_{kl}w(\mathbf{R})dg &= \int_{\text{SO(3)}} \overline{\sigma}_{ij}M_{ijkl}(\boldsymbol{R})\boldsymbol{\Delta}\sigma_{kl}w(\mathbf{R})dg \\ &= \kappa\omega\overline{\sigma}_{ij}\left(-\frac{2}{25}B^{(1)}_{ijkl} + \frac{6}{25}B^{(2)}_{ijkl} + \frac{1}{5}\Phi_{ijkl} - \Phi_{ijmn}\Phi_{mnkl}\right)\overline{\sigma}_{kl}.\end{aligned} \tag{57}$$

Similarly, from (52) and (25) we have

$$\begin{aligned}\Delta\sigma_{ij}M_{ijkl}(\boldsymbol{R})\boldsymbol{\Delta}\sigma_{kl} &= \check{}^{2}\overline{\sigma}_{ij}(\Psi_{ijpq}(\mathbf{R}) - \Phi_{ijpq})[-\frac{1}{\eta^2}B^{(1)}_{pqmn} \\ &+\frac{1}{2\varsigma^2}B^{(2)}_{pqmn} + \omega B^{(3)}_{pqmn}(\mathbf{R})](\Psi_{mnkl}(\mathbf{R}) - \Phi_{mnkl})\overline{\sigma}_{kl}\end{aligned}$$

whose volume average value is

$$\begin{aligned}&\int_{\text{SO(3)}} \Delta\sigma_{ij}M_{ijkl}(\boldsymbol{R})\boldsymbol{\Delta}\sigma_{kl}w(\mathbf{R})dg \\ &= \frac{\kappa^2}{2\varsigma^2}\overline{\sigma}_{ij}\left(-\frac{2}{25}B^{(1)}_{ijkl} + \frac{6}{25}B^{(2)}_{ijkl} + \frac{1}{5}\Phi_{ijkl} - \Phi_{ijmn}\Phi_{mnkl}\right)\overline{\sigma}_{kl} \\ &+ \kappa^2\omega\overline{\sigma}_{ij}\left(-\frac{6}{125}B^{(1)}_{ijkl} + \frac{18}{125}B^{(2)}_{ijkl} - \frac{3}{25}\Phi_{ijkl} - \frac{4}{5}\Phi_{ijmn}\Phi_{mnkl} + o(|\boldsymbol{\Phi}^2|\right)\overline{\sigma}_{kl}.\end{aligned} \tag{58}$$

Substituting (36), (42), (57), and (58) into (54), we obtain the effective plastic anisotropy tensor for anisotropic aggregates of FCC crystallites with quadratic texture dependence

$$M^{\text{eff}}_{ijkl} = -\rho^{\text{eff}}B^{(1)}_{ijkl} + 3\rho^{\text{eff}}B^{(2)}_{ijkl} + \omega^{\text{eff}}\Phi_{ijkl} + \vartheta^{\text{eff}}\Phi_{ijmn}\Phi_{mnkl} \tag{59}$$

with

$$\begin{aligned}
\rho^{\text{eff}} &= \rho + \frac{4}{25}\kappa\omega + \frac{6}{25}\kappa^2\rho + \frac{2}{125}\kappa^2\omega \\
&= (0.0612 + 0.0277\kappa + 0.0175\kappa^2)/\tau_c^2\,, \\
\omega^{\text{eff}} &= \omega + \frac{2}{5}\kappa\omega + \frac{3}{5}\kappa^2\rho - \frac{1}{5}\kappa^2\omega \\
&= 0.00213(\kappa + 29.573)(\kappa + 2.731)/\tau_c^2\,, \\
\vartheta^{\text{eff}} &= -2\kappa\omega - 3\kappa^2\rho - \frac{2}{5}\kappa^2\omega \\
&= -0.253(\kappa + 1.368)\kappa/\tau_c^2
\end{aligned} \tag{60}$$

where $\frac{1}{\varsigma^2} = \frac{2}{5}(15\rho - 2\omega)$ because of (43). Substituting (59) into (34), we obtain a macroscopic yield function of the RVE

$$\overline{f(\sigma_{ij}(\mathbf{R}))} = \frac{1}{\left(Y_0^{\text{eff}}\right)^2}\left(\frac{3}{2}\overline{\sigma}_{ij}\overline{\sigma}_{ij} - \frac{1}{2}\overline{\sigma}_{ii}\overline{\sigma}_{jj} + \beta^{\text{eff}}\Theta_{ijkl}\overline{\sigma}_{ij}\overline{\sigma}_{kl} + \gamma^{\text{eff}}\Theta_{ijmn}\Theta_{mnkl}\overline{\sigma}_{ij}\overline{\sigma}_{kl}\right) - 1 = 0 \tag{61}$$

where we discard terms $o(|\mathbf{\Phi}^2|)$ in (59) and

$$\begin{aligned}
Y_0^{\text{eff}} &= \left(2\rho^{\text{eff}}\right)^{-1/2} = 0.707\tau_c(0.0612 + 0.0277\kappa + 0.0175\kappa^2)^{-1/2}, \\
\beta^{\text{eff}} &= \frac{\omega^{\text{eff}}}{2\rho^{\text{eff}}} = \frac{0.00107(\kappa + 29.573)(\kappa + 2.731)}{0.0612 + 0.0277\kappa + 0.0175\kappa^2}, \\
\gamma^{\text{eff}} &= \frac{\vartheta^{\text{eff}}}{2\rho^{\text{eff}}} = -\frac{0.126(\kappa + 1.368)\kappa}{0.0612 + 0.0276\kappa + 0.0174\kappa^2}.
\end{aligned} \tag{62}$$

The effective plastic anisotropy tensor in (59) satisfies the traceless condition $M_{iikl}^{\text{eff}} = 0$.

In metallurgical practice, because of the effects of alloying elements, it is difficult to obtain accurate estimates of the material parameters τ_c and κ in (61). The macroscopic yield function (61) is then more properly looked upon as a representation formula with three undetermined parameters Y_0^{eff}, β^{eff} and γ^{eff}.

6. Discussion and Example

When the yield function is in Hill's criterion form, the Taylor factor $\mathcal{M}(0.5, 0)$ for an orthorhombic weakly textured aggregate of FCC crystallites can be expressed as [14]

$$\mathcal{M}(0.5, 0) = \frac{\overline{\sigma}_{11}}{\tau_c} = 3.067 - 10.095\left(W_{400} - \frac{2\sqrt{10}}{3}W_{420} + \frac{\sqrt{70}}{3}W_{440}\right), \tag{63}$$

where $\overline{\sigma}_{11}$ is a uniaxial tensile yield stress.

Under Sachs' model, we obtained the macroscopic yield function (46) for an aggregate of FCC crystallites. For uniaxial tensile problems, the yield function in (46) becomes $(G + H)(\overline{\sigma}_{11})^2 - 1 = 0$ or

$$\overline{\sigma}_{11} = (G + H)^{-1/2} = Y_0(1 - \beta(a_2 + a_3))^{-1/2} \approx Y_0\left(1 + \frac{\beta}{2}(a_2 + a_3)\right) \tag{64}$$

from (47). When the RVE is an orthorhombic aggregate of FCC crystallites, there are $\operatorname{Re} c_{20}^4 = c_{20}^4$ and $\operatorname{Re} c_{40}^4 = c_{40}^4$ (Roe, 1965 [18]) in (41). From (41), (45) and (29), we rewrite (64) into

$$\overline{\sigma}_{11} = 2.859\tau_c - 9.666\tau_c\left(W_{400} - \frac{2\sqrt{10}}{3}W_{420} + \frac{\sqrt{70}}{3}W_{440}\right) \tag{65}$$

which is close to the result (63). However, the derivation of (65) is much simpler than that of (63) because the computation of the Taylor factor for a textured polycrystal is very complicated and time consuming.

The parameter κ in (62) can be determined by an experiment. For instance, from the relation of an isotropic polycrystal (aluminum) stress–strain curve and a single crystal stress–strain curve, Taylor [6] found that $Y_0^{\text{eff}} = 3.06\tau_c$ agrees with the experimental data very well. Taking $Y_0^{\text{eff}} = 3.06\tau_c$, we obtain $\kappa = -0.365$ by solving $(62)_1$ and then get $\beta^{\text{eff}} = 1.384$ and $\gamma^{\text{eff}} = 0.866$ from $(62)_{2,3}$. For an orthorhombic weakly textured aggregate of FCC crystallites, if we discard the $o(c_{m0}^4)$ terms of the texture coefficients in (61), similar to the procedure of deriving (46) and (64) from (44), we obtain the yield stress of uniaxial tension

$$\overline{\sigma}_{11} = Y_0^{\text{eff}}\left(1 + \frac{\beta^{\text{eff}}}{2}(a_2 + a_3)\right) = 3.06\tau_c - 10.133\tau_c\left(W_{400} - \frac{2\sqrt{10}}{3}W_{420} + \frac{\sqrt{70}}{3}W_{440}\right). \tag{66}$$

The formula above is almost the same as (63). To check the form of the expression (66), we give one example as follows.

Example of yield stress under uniaxial tension of sample $\boldsymbol{\mathcal{S}_\theta}$:

Take an example $\boldsymbol{\mathcal{S}_\theta}$ from a metal sheet with the rolling direction $\boldsymbol{\theta}$ as shown in Figure 1. To obtain the expression of the uniaxial yield stress $\boldsymbol{\sigma_\theta}$ and the rolling direction $\boldsymbol{\theta}$, we give the stress tensor of a uniaxial stress $\boldsymbol{\sigma_\theta}$ on as follows

$$\boldsymbol{\sigma(\theta) = \sigma_\theta \mathbf{n} \otimes \mathbf{n} = \sigma_\theta \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta & 0 \\ \cos\theta\sin\theta & \sin^2\theta & 0 \\ 0 & 0 & 0 \end{bmatrix}} \tag{67}$$

where $\mathbf{n} = [\boldsymbol{\cos\theta, \sin\theta, 0}]^{\boldsymbol{T}}$. Similar to the derivation of (66), for an orthorhombic weakly textured aggregate of FCC crystallites, putting $\boldsymbol{\sigma_{ij}(\theta)}$ in (67) and $\boldsymbol{W_{4m0} = \sqrt{\frac{2}{9}}\, c_{m0}^4}$ in (29) into (61) and after discarding the $\boldsymbol{o(W_{m0}^4)}$ terms of the texture coefficients, we obtain the yield stress $\boldsymbol{\sigma_\theta}$ of the uniaxial tension sample $\boldsymbol{\mathcal{S}_\theta}$ as follows:

$$\boldsymbol{\sigma_\theta = 3.06\tau_c - 10.133\tau_c\left(W_{400} - \frac{2\sqrt{10}}{3}W_{420}\cos 2\theta + \frac{\sqrt{70}}{3}W_{440}\cos 4\theta\right).} \tag{68}$$

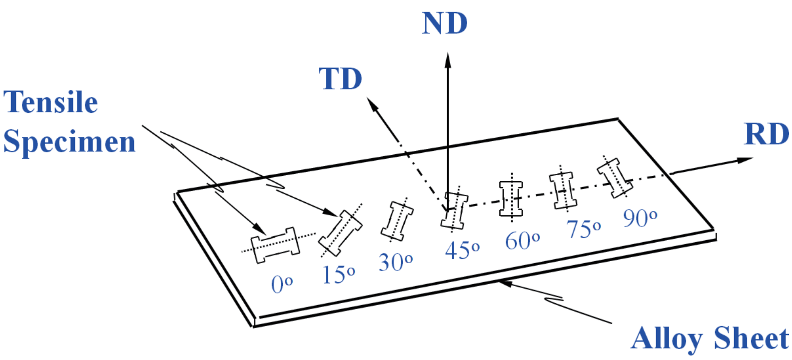

Figure 1. Samples $\boldsymbol{\mathcal{S}_\theta}$ of metal sheet.

Yu Xiang [23] in the doctoral dissertation gave the experimental data on two aluminum alloys (AA5754 hot band, AA3105 O-temper). As shown in Figure 1, uniaxial test samples were cut with tensile axis with the rolling direction (RD) $\boldsymbol{\theta = 0°, 15°, 30°, \cdots, 90°}$. For each tensile direction, measurements were made on two samples to obtain the flow stress at 4% longitudinal plastic strain. The experimental results are listed in Table 1, where the data $\boldsymbol{Y_i^{(1)}}$ and $\boldsymbol{Y_i^{(2)}}$ of Xiang's Experiment 1 and Experiment 2 are labeled with superscripts (1) and (2), respectively, and the subscript $\boldsymbol{1 \leq i \leq 7}$ indicates a sample with tensile axis making an angle $\phi_i = (i-1) \times 15°$ with the rolling direction (RD) shown in Figure 1. The texture coefficients of the two alloys were measured by X-ray diffraction as shown in Table 2.

Table 1. Flow stresses $Y_i^{(j)}$ (MPa) of two aluminum alloys.

Aluminum Alloy		0°	15°	30°	45°	60°	75°	90°
Hot Band	$Y_i^{(1)}$	282.31	279.14	274.78	258.58	259.41	270.97	279.58
AA5754	$Y_i^{(2)}$	282.00	278.82	270.15	257.99	257.53	271.77	280.87
O-temper	$Y_i^{(1)}$	126.72	125.13	124.11	122.15	124.19	124.72	126.10
AA3105	$Y_i^{(2)}$	125.19	125.43	124.82	124.50	123.91	124.65	126.04

Table 2. Texture coefficients W_{lmn} of two aluminum alloys.

AA5754 (Hot band)	$W_{400} = -0.0033$	$W_{420} = -0.0025$	$W_{440} = -0.0071$
AA3105 (O-temper)	$W_{400} = 0.0072$	$W_{420} = -0.0019$	$W_{440} = -0.0022$

To determine τ_c in (68) for the aluminum alloys from Xiang's experimental data, we introduce an objective function as follows:

$$\Pi(\tau_c) = \sum_{i=1}^{7} [\frac{1}{2}(Y_i^{(1)} + Y_i^{(2)}) - \sigma_\theta|_{\theta=\theta_i}]^2, \ \theta_i = (i-1) \times 15°. \tag{69}$$

By the method of least squares, we solve the equation $\frac{\partial \Pi(\tau_c)}{\partial \tau_c} = 0$ and obtain the critical resolved shear stress τ_c of the FCC crystals for the two aluminum alloys

$$\begin{aligned} \tau_c &= 86.93 \, \text{MPa} \quad \text{for AA5754 hot band;} \\ \tau_c &= 41.66 \, \text{MPa} \quad \text{for AA3105 O-temper.} \end{aligned} \tag{70}$$

Putting the fitted values τ_c in (70) and the texture coefficients W_{lmn} in Table 2 for the two alloys into (68), we plot the fitting results of the yield stress σ_θ on the uniaxial tension sample $\mathcal{S}_\theta$ as shown in Figure 2. The expression (68) of the yield stress σ_θ on the uniaxial tension sample $\mathcal{S}_\theta$ can fit Xiang's experimental data on two aluminum alloys (AA5754 and AA3105) very well.

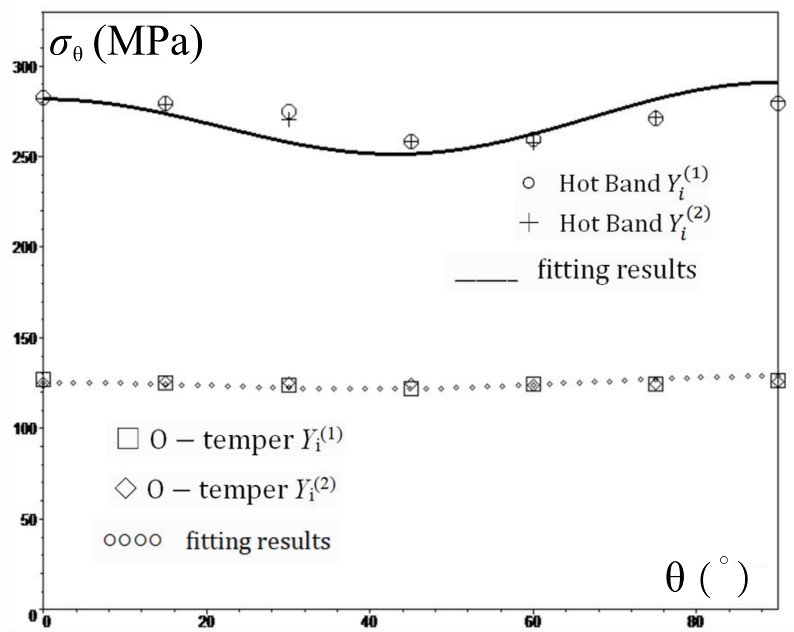

Figure 2. Experimental data of Xiang and fitting results of (68).

7. Conclusions

In this paper, we provide a simple method to obtain two closed but approximate yield functions with the effect of the texture coefficients for the RVE, where the volume average (i.e., orientational averaging) of all crystallites' yield surfaces is taken as a (macroscopic) yield function of the RVE. Through theoretical analysis, we draw the following important conclusions:

1. Assuming that all crystallites in the RVE have the same (current) critical resolved shear stress $\boldsymbol{\tau_c}$ for slip and employing Schmid's law and the nonlinear optimization theory, we give a plastic anisotropy tensor $\mathbf{M}(\mathbf{R})$ of the FCC crystals with orientation $\mathbf{R}$ and obtain the volume average of all crystallites' yield surfaces in the RVE.
2. By the Microsoft Excel, we solve nonlinear optimization problems and obtain an approximate plastic anisotropy tensor and a yield surface of FCC crystallites with orientation.
3. For an orthorhombic weakly textured aggregates of FCC crystallites, we obtain two yield stresses of uniaxial tension, respectively.
4. Through an example, we obtain the yield stress under the uniaxial tension on sample $\boldsymbol{\mathcal{S}_\theta}$. We find that the expression of the yield stress can fit Xiang's experimental data very well.

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