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# A micro-mechanically motivated phenomenological yield function for cubic crystal aggregates

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A micro-mechanically motivated phenomenological yield function, for polycrystalline cubic metals is presented. In the suggested yield function microstructure is taken into account by the crystallographic orientation distribution function in terms of tensorial Fourier coefficients. The yield function is presented in a polynomial form in powers of the stress state. Known group-theoretic results are used to identify isotropic and anisotropic parts in the yield function, whereby anisotropic parts are characterized by tensorial Fourier coefficients. The form of the presented yield function is inspired by the classic, phenomenological von Mises - Hill yield function first published in 1913. For a specific choice of material parameters, both functions coincide, thus a micro-mechanically motivated generalization of the von Mises - Hill yield function is presented. For the given yield function, two dimensional experimental results are sufficient, to identify a three dimensional anisotropic yield behavior. The work concludes with a treatment of the isotropic special case, i.e. a tension-compression split in yield behavior as well as parameter ranges for convexity and shapes of the yield surface.

**KEYWORDS**
anisotropic yield function, crystallographic texture, orientation distribution function, plastic anisotropy, tensorial texture coefficients

## 1 | INTRODUCTION

Generally a yield criterion is a function used to distinguish, whether the response of a material to a given stress state is reversible (elastic) or irreversible (e.g. plastic or viscoplastic) and can also be viewed as equivalent stress hypotheses [1]. Yield functions thus serve as a limit to the elastic range of the underlying material and define five dimensional hyper-surfaces in stress space [2]. In an associated plastic flow theory [3] the yield function serves as a potential for irreversible deformation. Plastic flow is thereby governed by the normal-derivative of the yield function to the current stress state. Convexity of the yield surface and normality of plastic flow to the yield surface both follow from a postulate for stable inelastic material [4].

Historically significant efforts were made to describe plastically isotropic and anisotropic material behavior via various kinds of yield functions. Publications by von Mises [5, 6] established a quadratic form of the yield function, which is still widely used today. Hill is generally viewed as having introduced the first fully anisotropic quadratic yield criterion for orthotropic materials [7], but his function can also be viewed as a special case of the quadratic von Mises yield function specified for

plastically anisotropic behavior [6]. Thus from now on we will refer to the quadratic von Mises - Hill yield function. This function can be used to describe plastically anisotropic material with an orthotropic symmetry by using six parameters for plastically incompressible behavior. Later publications aimed at generalizing the yield criterion of von Mises - Hill by using arbitrary powers of stress states instead of being purely quadratic. Examples are criteria of the Barlat class, e.g., the Barlat-05-p18 yield criterion [8], which uses 18 parameters to describe anisotropic yield. Further discussion of anisotropic yield criteria is, e.g. summarized in the work of Altenbach et al. [9].

All the mentioned criteria have in common, that they are phenomenological in nature. Thus they follow from empirical evidence and do not incorporate microstructural information into yield behavior. In addition the identification of anisotropy parameters requires a large range of experiments and these parameters often lack a clear physical interpretation [3].

In continuum mechanics $n$-point probability functions are often used to homogenize the effective properties of polycrystal materials [10]. In this work we consider the relationship between microstructure, in the form of a one-point probability distribution of crystal orientations, and macroscopic plastic yield. We present a quasi-phenomenological yield function to describe plastically anisotropic and the special case of plastically isotropic behavior. Quasi-phenomenological means, that the material model is formulated on the macroscopic scale, but the coefficients used are determined in terms of the microstructure and are therefore observable. Microstructure is accounted for by making use of the crystallite orientation distribution function and its representation by tensorial Fourier coefficients. The yield function is presented in powers of the stress direction and can be viewed as a generalization of the quadratic von Mises - Hill form. Previously published group-theoretic results allow a split into isotropic and anisotropic parts of the yield function, where texture accounts for anisotropic behavior. Main assumptions that lead to the suggested new yield function are

i) a correlation between crystallographic texture and plastic yielding,
ii) plastic incompressibility,
iii) a polynomial form in powers of stress direction,
iv) the yield condition is positively homogeneous of degree one in the absolute value of stress and
v) a weakly pronounced crystallographic texture.

**Notation.** Throughout this work a direct tensor notation is preferred. If tensor components are used, then the Einstein summation convention is applied. Scalars are denoted as small Latin or Greek letters, e.g., $c$ and $\eta$. First-order tensors are denoted by bold lower case Latin letters, e.g. $\mathbf{a}$, second-order tensors by upper case bold Latin or bold Greek letters, e.g. $\boldsymbol{\sigma}$. Arbitrary $n$th-order tensors are marked via a subscript, e.g., $\mathbb{J}_4$ for a fourth-order tensor. The Kronecker symbol is denoted by $\delta_{ij}$. The scalar and dyadic produssct are denoted by $\mathbf{a}\cdot\mathbf{b}$ and $\mathbf{a}\otimes\mathbf{b}$. The symbol $\star$ denotes the Rayleigh product, which for tensors $\mathbb{T}_n$ of arbitrary rank $n$ is defined by $\mathbf{Q}\star\mathbb{T}=T_{ij..n}(\mathbf{Q}\mathbf{e}_i)\otimes(\mathbf{Q}\mathbf{e}_j)\otimes\ldots(\mathbf{Q}\mathbf{e}_n)$. A map $\mathbf{Q}\to\mathbf{Q}^{\otimes r}$ defines a $r$ times dyadic product of the tensor $\mathbf{Q}$ with itself.

## 2 | PRELIMINARIES

### 2.1 | Crystallite orientation distribution function and its tensorial representation

A polycrystalline structure can be described by $n$-point probability functions [11]. A one-point probability function describes the volume fraction of lattice orientation and is, in engineering sciences, called crystallite orientation distribution function (CODF). For a non-uniform CODF the material is said to posses a crystallographic texture. Higher order $n$-point probability functions, ($n\geq 2$) are used to described additional aspects of grain structure, like shape and size of crystal grains (morphological texture). As morphological texture has a less pronounced influence on plastically anisotropic behavior [12] it will not be considered here.

The orientation of a single crystal can be described by a proper orthogonal tensor $\mathbf{Q}\in\mathrm{SO}(3)$ with $\mathbf{Q}=\mathbf{g}_i\otimes\mathbf{e}_i$, where the vectors $\mathbf{g}_i$ and $\mathbf{e}_i$ denote orthonormal lattice vectors and a fixed orthonormal reference basis respectively. The CODF $f(\mathbf{Q})$ specifies the volume fraction $\mathrm{d}v/v$ of all crystals with the orientation $\mathbf{Q}$ [13]. Thus $\mathrm{d}v/v(\mathbf{Q})=f(\mathbf{Q})\mathrm{d}Q$, where $\mathrm{d}Q$ is the volume element in SO(3) which ensures invariant integration over SO(3). The CODF is normalized, non-negative and reflects the symmetry of the constituting crystals $\mathbf{H}^{\mathrm{C}}$ and the sample symmetry $\mathbf{H}^{\mathrm{S}}$ resulting from processing [13]. For a uniform orientation the CODF is constant $f(\mathbf{Q})=1$.

Tensorial representations of the CODF have been established [14, 15, 38]. A Fourier series expansion of a cubic CODF is proposed as

$$\begin{aligned} f(\mathbf{Q}) &= 1 + \sum_{i=1}^{\infty} f_{\alpha_i}(\mathbf{Q}), \quad f_{\alpha_i} = \mathbb{V}'_{\alpha_i} \cdot \mathbb{F}'_{\alpha_i}(\mathbf{Q}), \\ \mathbb{F}'_{\alpha_i}(\mathbf{Q}) &= \mathbf{Q} \star \mathbb{T}'_{\alpha_i}, \end{aligned} \tag{1}$$

where $\{\alpha_i\} = \{4, 6, 8, 9, 10 \ldots\}$. For a Fourier series expansion the square integrability of $f(\mathbf{Q})$ is a necessity, which is assumed here. The $\mathbb{T}'_{\alpha_i}$ are called cubic reference tensors, are normalized to $\|\mathbb{T}'_{\alpha_i}\| = 2\alpha_i + 1$ and reflect the crystal symmetry $\mathbf{H}^{\mathrm{C}}$. The $\mathbb{V}'_{\alpha_i}$ are called tensorial Fourier or texture coefficients and reflect the sample symmetry $\mathbf{H}^{\mathrm{S}}$. For a number $N$ of discrete single crystal orientations $\mathbf{Q}_\gamma$ with volume fraction $c_\gamma$ they can be computed via [16]

$$\mathbb{V}'_{\alpha_i} = \frac{1}{2\alpha_i + 1} \sum_{\gamma=1}^{N} c_\gamma \mathbf{Q}_\gamma \star \mathbb{T}'_{\alpha_i}. \tag{2}$$

We assume the texture coefficients $\mathbb{V}'_{\alpha_i}$ to be a representation of the crystallographic texture, defined at every material point in the regarded sample. For determination of these texture coefficients pole figure data are necessary. These can be obtained, e.g., by diffraction measurements. For details regarding diffraction techniques see Kocks et al. [10] and the literature mentioned therein.

Tensors with a prime are harmonic (completely symmetric and traceless [17]), thus e.g.

$$V'_{ijkl} = V'_{jikl} = V'_{jilk} = V'_{kjil} = \cdots, \quad V'_{iikl} = 0. \tag{3}$$

The number of independent components in a harmonic tensor is

$$\dim(\mathbb{V}'_{\alpha_i}) = 2\alpha_i + 1. \tag{4}$$

Cubic base tensors of unequal rank are mutually orthogonal in the following sense [18]

$$\int_{\mathrm{SO(3)}} \frac{\mathbb{F}'_{\alpha_i}(\mathbf{Q})}{2\alpha_i + 1} \otimes \frac{\mathbb{F}'_{\beta_i}(\mathbf{Q})}{2\beta_i + 1} \mathrm{d}\mathbf{Q} = \mathbb{O}, \forall \alpha_i \neq \beta_i. \tag{5}$$

Note that the $\{\alpha_i\}$ start with index 4, which is due to the fact that a cubic reference tensor of rank 2 is zero. Also cubic texture coefficients with uneven tensor rank vanish up to rank eight [13]. The Frobenius norm of all texture coefficients is in this work (see Eq. 2) bounded by one, thus $\|\mathbb{V}'_{\alpha_i}\| \in [0, 1]$. The Frobenius norm is a measure for the anisotropy of texture [19]. As has been stated isotropic materials have an CODF equal to one, so that all texture coefficients vanish for completely random orientation distribution. For single crystals the norm of all texture coefficients is equal to one and corresponds to maximum anisotropy.

A generalization of Fourier series expansion for arbitrary crystal symmetries has been published [17, 20]. Further details concerning the CODF and its tensorial representation can be found in the works of Bunge and Zheng et al. [13, 21, 22]. An evolving texture will not be considered in this work. We restrict our derivations to the special case of a texture constant in time. However, in a tensorial setting, it is possible to derive evolution equations for texture coefficients [23]. Further work has been focused on the estimation of a CODF based on leading texture coefficients [24].

## 2.2 | Decomposition of tensors into irreducible parts

From the theory of group representations it is well known, that any finite order tensor can be decomposed into a sum of harmonic tensors. Irreducible states, that for a considered representation no proper sub representation exists [25]. The procedure of decomposing tensors into irreducible parts (where these parts are harmonic tensors) allows a separation into isotropic and anisotropic components of a given tensor and enables a more intuitive physical understanding of the decomposed tensor [17]. For the decomposition the detailed number of independent tensors and their construction is of interest. In this subsection we will use known group theoretic results, to investigate the number of independent components in a specific

**TABLE 1** Number of fundamental (N), linear independent fundamental (M) and symmetric isotropic tensors (O)

| Rank | 2 | 4 | 6 | 8 |
|---|---|---|---|---|
| $N$ | 1 | 3 | 15 | 105 |
| $M$ | 1 | 3 | 15 | 91 |
| $O$ | 1 | 2 | 3 | 5 |

representation which is of interest in the derivation of our yield function. The construction of independent tensors will be dealt with in Sec. 3.

In this work we let $T^{(r)}V$ be the space of $r$-th order tensors of a three-dimensional Euclidean space $V$. The map $\mathbf{Q} \to \mathbf{Q}^{\otimes r}$ of a rotation $\mathbf{Q}$ on $V$ defines a linear representation of the rotation group SO3 on $T^{(r)}V$. For a subspace $Z \in T^{(r)}V$ invariant under $\mathbf{Q}^{\otimes r}$ the restriction $\mathbf{Q}^{\otimes r}|_Z$ is a linear representation of the rotation group on $Z$. The decomposition of these representations, so a decomposition of tensors invariant under arbitrary rotations, will be of concern in this section.

For a given representation $\mathbf{Q}^{\otimes r}|_Z$ there exists a complete set of irreducible unitary representations $\mathcal{D}_l$ of dimension $2l+1$ which can be expressed as a sum

$$\mathbf{Q}^{\otimes r}\big|_Z = n_0\mathcal{D}_0 + n_1\mathcal{D}_1 + \cdots + n_r\mathcal{D}_r. \tag{6}$$

The $n_l$ are multiplicities of each sub representation $\mathcal{D}_l$. In this work we will be concerned with representations of harmonic tensors of ranks $4, 6$ and $8$, which are subspaces of $T^{(4)}V, T^{(6)}V$ and $T^{(8)}V$ respectively. We will denote the subspaces of harmonic tensors by $\mathcal{J}_m$ for harmonic tensors of rank $m$, which is used [17, 26, 27].

The decomposition of the rotation group restricted to harmonic tensors has been previously published [26] and [28]. The result is

$$\begin{aligned}
\mathbf{Q}^{\otimes 4}\Big|_{\mathcal{J}_4} &= \mathcal{D}_0 + \mathcal{D}_2 + \mathcal{D}_4,\\
\mathbf{Q}^{\otimes 6}\Big|_{\mathcal{J}_6} &= \mathcal{D}_0 + \mathcal{D}_2 + \mathcal{D}_4 + \mathcal{D}_6,\\
\mathbf{Q}^{\otimes 8}\Big|_{\mathcal{J}_8} &= \mathcal{D}_0 + 2\mathcal{D}_2 + 2\mathcal{D}_4 + \mathcal{D}_5 + \mathcal{D}_6 + \mathcal{D}_8.
\end{aligned} \tag{7}$$

For interpretation we examine a fourth-order tensor $\mathbb{C}_4 \in \mathcal{J}_4$. Thus $\mathbb{C}_4$ maps $\mathcal{J}_2 \to \mathcal{J}_2$. The decomposition implies, that $\mathbb{C}_4$ can be written as a sum of three harmonic fourth-order tensors in a one-, five- and nine-dimensional subspace of $\mathcal{J}_4$ respectively. Thereby parts corresponding to the irreducible representation $\mathcal{D}_0$ are isotropic tensors, whereas the remaining parts $\mathcal{D}_k, k > 0$ are anisotropic tensors.

## 2.3 | Isotropic tensors

Fundamentally isotropic tensors $\mathbb{I}_{2r}$ of rank $2r$ are linear combinations of Kronecker-deltas $\delta_{ij}^{\otimes \mathrm{r}}$ and permutations thereof [29]. So one fourth order isotropic tensor $\mathbb{I}_4$ is $I_{ijkl} = \delta_{ij}\delta_{kl}$. From this combination there exist two further permutations, so that the maximum number $N$ of fundamentally isotropic tensors of rank 4 is 3. For higher tensor ranks there exist linear dependencies between the fundamentally isotropic tensors, such that the number of linear independent fundamentally isotropic tensors $M$ is lower than $N$. In this work we will restrict ourselves to isotropic tensors with certain symmetries. These are a permutation of indices in the Kronecker-deltas and a permutation of the Kronecker-deltas themselves. The notation used will be $\mathbb{I}_\alpha^{\mathrm{S},i}$, where $\alpha$ is the tensor rank, $i$ the number of the isotropic tensor and $S$ indicates symmetries in the stated sense. If one imposes this symmetry restriction, the resulting symmetric tensors are linear combinations of the fundamentally isotropic tensors, which can be shown by a quick calculation. Thus, e.g. the second symmetric fourth order isotropic tensor is $I_{ijkl}^{\mathrm{S},2} = 1/2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. The number of symmetric isotropic tensors for a given rank is $O$ in this work. In Tab. 1 the numbers $N$, $M$ and $O$ for even isotropic tensors up to rank eight are summarized.

For later use we include the results of scalar products between the symmetric isotropic tensors $\mathbb{I}_\alpha^{\mathrm{S},i}$ and maps of symmetric second order tensors $\mathbf{A} \to \mathbf{A}^{\otimes \mathrm{r}}$, which can be easily obtained via a quick calculation. These results are summarized in Tab. 2. The main invariants of a symmetric second order tensor are denoted by $I_1, I_2$ and $I_3$. With usage of the Cayley-Hamilton theorem $\mathrm{tr}(\mathbf{A}^4)$ can be expressed via $I_1, I_2$ and $I_3$.

**TABLE 2** Results of scalar products between symmetric isotropic tensors and a symmetric second order tensor

| $\mathbb{I}_2^{S,1} \cdot \mathbf{A}$ | $= \mathrm{tr}(\mathbf{A})$ | $= I_1$ |
|---|---|---|
| $\mathbb{I}_4^{S,1} \cdot (\mathbf{A}^{\otimes 2})$ | $= \mathrm{tr}^2(\mathbf{A})$ | $= I_1^2$ |
| $\mathbb{I}_4^{S,2} \cdot (\mathbf{A}^{\otimes 2})$ | $= \mathrm{tr}(\mathbf{A}^2)$ | $= I_2$ |
| $\mathbb{I}_6^{S,1} \cdot (\mathbf{A}^{\otimes 3})$ | $= \mathrm{tr}^3(\mathbf{A})$ | $= I_1^3$ |
| $\mathbb{I}_6^{S,2} \cdot (\mathbf{A}^{\otimes 3})$ | $= \mathrm{tr}(\mathbf{A})\mathrm{tr}(\mathbf{A}^2)$ | $= I_1 I_2$ |
| $\mathbb{I}_6^{S,3} \cdot (\mathbf{A}^{\otimes 3})$ | $= \mathrm{tr}(\mathbf{A}^3)$ | $= I_3$ |
| $\mathbb{I}_8^{S,1} \cdot (\mathbf{A}^{\otimes 4})$ | $= \mathrm{tr}^4(\mathbf{A})$ | $= I_1^4$ |
| $\mathbb{I}_8^{S,2} \cdot (\mathbf{A}^{\otimes 4})$ | $= \mathrm{tr}^2(\mathbf{A})\mathrm{tr}(\mathbf{A}^2)$ | $= I_1^2 I_2$ |
| $\mathbb{I}_8^{S,3} \cdot (\mathbf{A}^{\otimes 4})$ | $= \mathrm{tr}^2(\mathbf{A}^2)$ | $= I_2^2$ |
| $\mathbb{I}_8^{S,4} \cdot (\mathbf{A}^{\otimes 4})$ | $= \mathrm{tr}(\mathbf{A})\mathrm{tr}(\mathbf{A}^3)$ | $= I_1 I_3$ |
| $\mathbb{I}_8^{S,5} \cdot (\mathbf{A}^{\otimes 4})$ | $= \mathrm{tr}(\mathbf{A}^4)$ | $= -\frac{1}{6} I_1^4 + \frac{1}{2} I_2^2 + \frac{2}{3} I_1 I_3$ |

## 3 | ANISOTROPIC YIELD FUNCTION FOR POLYCRYSTALLINE MATERIALS

In this section a micro-mechanically motivated anisotropic yield function for polycrystalline cubic metals is presented. We start by considering a yield function $\varphi$, being a function of the deviatoric stress state $\sigma'$ and CODF $f$

$$\varphi\left(\sigma', f\right). \tag{8}$$

We assume the yield function to be a smooth function $\varphi : \mathcal{I}_2 \times \mathcal{N} \to \mathbb{R}$, where $\mathcal{N}$ is a rotationally invariant neighborhood of an isotropic orientation distribution $f_{\mathrm{Iso}}$ [30]. By using assumption i) we have introduced texture by means of the CODF to macroscopic yield behavior. This assumption is frequently used in continuum mechanics [31, 32]. The usage of deviatoric stresses leads to a plastically incompressible theory (assumption ii)), where plastic deformation is purely deviatoric. This assumption is usually made for metallic materials, due to the fact that plastic deformation is governed by dislocation glide and thus volume preserving [3]. Pressure-sensitive plasticity [33] will not be considered here.

Combining assumptions i) and ii), a polynomial form in powers of stress direction (assumption iii) and a positively homogeneous function of degree one in the absolute value of $\sigma'$ (assumption iv) we conclude, that a general form of an anisotropic yield function is

$$\varphi\left(\sigma', f\right) = \frac{\|\sigma'\|}{\sigma_{\mathrm{f}}}\left(\mathbb{H}_4 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 2}\right) + \mathbb{H}_6 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 3}\right) + \mathbb{H}_8 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 4}\right)\right) \leq 1, \tag{9}$$

where $\mathbf{N}_{\sigma'} = \|\sigma'\|^{-1}\sigma'$ is the stress direction and $\sigma_{\mathrm{f}}$ is the yield stress which results from an uniaxial tensile test. Assumption iii) is motivated by the usual polynomial form of most existing phenomenological yield functions in powers of stress. Assumption iv) is similar to other existing yield functions, e.g. the von Mises - Hill criterion, which is positively homogeneous of degree one in $\|\sigma'\|$. The so far unspecified tensors $\mathbb{H}_m$ depend on the CODF and thus on the given microstructure. Their specific form will be derived in the following for aggregates of cubic crystallites. Such a restriction is in general not necessary, the tensors $\mathbb{H}_m$ can be derived explicitly for arbitrary crystal symmetries.

For analyzing the tensors $\mathbb{H}_m$ we assume the sample to be an aggregate of cubic crystals with a weakly pronounced texture (assumption v)). The implication of a weakly pronounced texture follows [31] after a Taylor series expansion in the CODF

$$\varphi\left(\sigma', f\right) = \varphi\left(\sigma', f_{\mathrm{iso}}\right) + \left.\frac{\partial \varphi}{\partial f}\right|_{f=f_{\mathrm{iso}}} \left(f - f_{\mathrm{iso}}\right) + o\left(\|f - f_{\mathrm{iso}}\|^2\right), \tag{10}$$

with the deviation $f - f_{\mathrm{iso}}$ of a CODF $f$ from an isotropic CODF $f_{\mathrm{iso}}$. For small deviations of an isotropic CODF, thus for weakly pronounced texture, dropping all terms $o(\|f - f_{\mathrm{iso}}\|^2)$ is a good approximation. Thus weak texture implies a decomposition of each $\mathbb{H}_m$ into an isotropic and an anisotropic part, which is linear in the CODF. The isotropic parts of each decomposition are isotropic tensors of rank $m$. As can be seen in Tab. 2 these tensors are $\mathbb{I}_4^{S,2}$, $\mathbb{I}_6^{S,3}$ and $\mathbb{I}_8^{S,3}$.

We now proceed to determine the anisotropic parts of each $\mathbb{H}_m$, which are linear in the CODF. Therefore we make use of the the principle of material frame indifference [34], which has to be fulfilled by any function in continuum mechanics, and the irreducible decomposition in Eq. (7). The principle of material frame indifference implies

$$\varphi\big(\mathbf{R} \star \sigma', \mathcal{T}_{\mathbf{R}}(f)\big) = \varphi\big(\sigma', f\big), \forall\, \mathbf{R} \in \mathrm{SO}(3). \tag{11}$$

Here $\mathcal{T}_{\mathbf{R}}(f)$ is the rotated CODF, defined by $\mathcal{T}_{\mathbf{R}}(f)(\mathbf{Q}) = f(\mathbf{R}^{\mathrm{T}}\mathbf{Q})$. We note, that $\mathbb{H}_m \in \mathcal{I}_m$ for $m = 4, 6$ and 8. This is due to the symmetry and tracelessness of $\mathbf{N}_{\sigma'}$. Thus the principle of material frame indifference is equivalent to the mathematical restriction of the rotation group to $\mathcal{I}_m$. This allows us to use the irreducible decomposition introduced in Eq. (7), to additively decompose each tensor $\mathbb{H}_m$. Resulting tensors in the sub representation $\mathcal{D}_0$ are the isotropic tensors already introduced. In addition, due to the assumption of a weakly pronounced texture, all sub representations $\mathcal{D}_k, k > 0$ are linear in the CODF.

For deriving the specific form of each sub representation we make use of a previously published proof [26]. The author shows, that each harmonic tensor in $\mathcal{D}_k$ depends only on certain texture coefficients. This dependency is unique up to a multiplicative constant [1]. Thus, in our framework, each harmonic tensor in $\mathcal{D}_k$ is (up to an arbitrary multiplicative constant) identical to a projection of the texture coefficient $\mathbb{V}'_k$ to the corresponding subspace $\mathcal{D}_k$.

After these considerations we conclude the following for an aggregate of cubic crystals:

- All terms corresponding to the subspace $\mathcal{D}_2$ vanish, as there is no cubic texture coefficient of rank two.
- All terms corresponding to the subspace $\mathcal{D}_l$ with $l$ uneven vanish, as there is no cubic texture coefficient of uneven rank (for ranks smaller eight).
- $\mathbb{H}_4$ can be additively decomposed into two terms, the first being isotropic and the second being equal to $\mathbb{V}'_4$.
- $\mathbb{H}_6$ can be additively decomposed into three terms, the first being isotropic, the second a sixth order anisotropic tensor depending solely on the cubic texture coefficient of rank four, which we define as $\mathbb{V}'_{6,4}(\mathbb{V}'_4)$, and $\mathbb{V}'_6$.
- $\mathbb{H}_8$ can be additively decomposed into four terms, the first being isotropic, the second an eighth order anisotropic tensor depending solely on the cubic texture coefficient of rank four $\mathbb{V}'_{8,4}(\mathbb{V}'_4)$, the third term being an eighth order anisotropic tensor depending solely on $\mathbb{V}'_6$ as in $\mathbb{V}'_{8,6}(\mathbb{V}'_6)$ and the last term being $\mathbb{V}'_8$.

Each tensor in the decomposition is explicitly determined up to a scalar constant. These constants are material parameters in the resulting yield function. Summarized, the tensors $\mathbb{H}_m$ can be decomposed as

$$\begin{aligned}
\mathbb{H}_4 &= c_1 \mathbb{I}_4^{\mathrm{S},2} + \eta_1 \mathbb{V}'_4\,, \\
\mathbb{H}_6 &= c_2 \mathbb{I}_6^{\mathrm{S},3} + \eta_2 \mathbb{V}'_{6,4} + \eta_3 \mathbb{V}'_6\,, \\
\mathbb{H}_8 &= c_3 \mathbb{I}_8^{\mathrm{S},3} + \eta_4 \mathbb{V}'_{8,4} + \eta_5 \mathbb{V}'_{8,6} + \eta_6 \mathbb{V}'_8.
\end{aligned} \tag{12}$$

For clarification the material parameters have been partitioned into isotropy ($c_i$) and anisotropy ($\eta_i$) coefficients. Thus the yield function is calibrated via three isotropy and six anisotropy coefficients.

The harmonic tensors $\mathbb{V}'_{6,4}(\mathbb{V}'_4)$, $\mathbb{V}'_{8,4}(\mathbb{V}'_4)$ and $\mathbb{V}'_{8,6}(\mathbb{V}'_6)$ are isotropic projections of the corresponding texture coefficients [26]

$$\begin{aligned}
\mathbb{V}'_{6,4}\big(\mathbb{V}'_4\big) &= \mathbb{M}_{6,4}\big[\mathbb{V}'_4\big]\,, \\
\mathbb{V}'_{8,4}\big(\mathbb{V}'_4\big) &= \mathbb{M}_{8,4}\big[\mathbb{V}'_4\big]\,, \\
\mathbb{V}'_{8,6}\big(\mathbb{V}'_6\big) &= \mathbb{M}_{8,6}\big[\mathbb{V}'_6\big]\,,
\end{aligned} \tag{13}$$

such that the resulting tensors are harmonic. With this restriction in mind, the isotropic tensors $\mathbb{M}_{6,4}, \mathbb{M}_{8,4}$ and $\mathbb{M}_{8,6}$ can be constructed as linear combinations of Kronecker-deltas. Thus all anisotropic parts of the yield function are explicitly determined through the CODF and its tensorial Fourier series representation.

After these considerations an anisotropic yield function which shows explicitly the influence of crystallographic texture on plastic behavior has been derived. It can be calibrated with three isotropy ($c_i$) and six anisotropy ($\eta_i$) material param-

[1] The author uses Wigner D-functions and spherical harmonics $W_{lmn}$ to represent CODFs. The author shows, that the irreducible representation $\mathcal{D}_k$ can depend only on those $W_{lmn}$ with $l = k$. In addition it is proven, that the relationship between $W_{lmn}$ and an anisotropic irreducible representation $\mathcal{D}_k$ is determined up to an arbitrary multiplicative constant.

eters. For using this function texture data, e.g. obtained through EBSD measurement or X-Ray diffraction, are necessary. With the texture coefficients microstructure data is inherently included in macroscopic yield behavior in a phenomenological sense.

# 4 | APPLICATIONS

## 4.1 | Comparison to existing yield functions

The derived yield function can be considered as a generalization of the quadratic yield function by von Mises - Hill. This follows after considering, that for a quadratic yield function all material parameters in Eq. (9) except $c_1$ and $\eta_1$ are set to zero. Focusing on plastically isotropic behavior first, we recognize, that for $c_1 = \sqrt{3/2}$ the proposed yield function coincides with the isotropic formulation of the well known von Mises - Hill yield function.

When $\eta_1$ differs from zero the yield function is quadratic and anisotropic. This form, where the plastic anisotropy is taken into account by the texture coefficient, has been previously used [35]. This followed as an ansatz to incorporate micro-structure to phenomenological plastically anisotropic behavior. In comparison, in this work the formulation followed after considering group-theory and the principle of material frame-indifference. It has been shown [36], that the quadratic yield function coincides with the orthotropic quadratic form by Hill and that the constants appearing in Hill's yield function can be identified with the entries of the texture coefficient $\mathbb{V}_4'$.

## 4.2 | Identification of material parameters in the yield function for sheet metals

With the presented yield function a three dimensional plastic material behavior can be modeled. The parameter identification for sheet metals is possible by comparing standard tensile tests in the sheet plane, thus two dimensional data, with simulated results. A possible procedure for a parameter identification is shown in the following.

For sheet metals it is common to experimentally determine $R$-values (also called Lankford coefficients) and yield strength values in uniaxial tensile tests, where samples with different angles to the rolling direction are used. $R$-values are often determined as ratio of plastic strain in width direction to plastic strain in thickness direction after 20% elongation. However it is advantageous to use plastic strain rates instead of plastic strain [3]. Then $R$-values follow as

$$R = \frac{\dot{\varepsilon}_\mathrm{p} \cdot \mathbf{n}_\mathrm{w} \otimes \mathbf{n}_\mathrm{w}}{\dot{\varepsilon}_\mathrm{p} \cdot \mathbf{n}_\mathrm{t} \otimes \mathbf{n}_\mathrm{t}}, \tag{14}$$

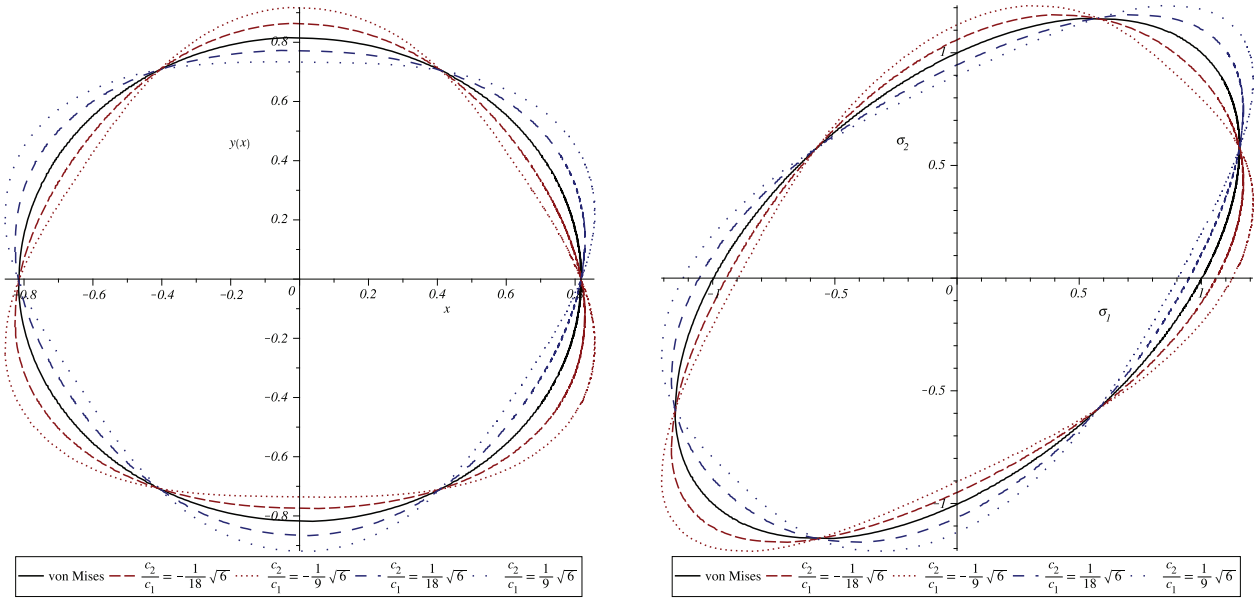
with plastic strain rate $\dot{\varepsilon}_\mathrm{p}$, width direction $\mathbf{n}_\mathrm{w}$ and thickness direction $\mathbf{n}_\mathrm{t}$. In associated flow plasticity $\dot{\varepsilon}$ follows as the derivative of the yield function to the current stress state as

$$\dot{\varepsilon}_\mathrm{p} = \lambda \frac{\partial \varphi\left(\sigma', f\right)}{\sigma'}. \tag{15}$$

These relations, combined with the stress state $\sigma = \sigma \mathbf{n}_\phi \otimes \mathbf{n}_\phi$ can be used to calculate $R$-values predicted by the yield function and compare them to experimentally determined ones. $\mathbf{n}_\phi$ is thereby the tensile direction with angle $\phi$ to rolling direction of the sheet. Due to the homogeneity of the yield function in $\|\sigma'\|$ we can use Eq. (14) without knowing the absolute value of stress state. Only the direction $\mathbf{n}_\phi \otimes \mathbf{n}_\phi$ is relevant. In addition, yield strength can be simulated with the proposed yield function via

$$\frac{\sigma\left(\mathbf{n}_\phi\right)}{\sigma_\mathrm{f}} = \sqrt{3/2}\left(\mathbb{H}_4 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 2}\right) + \mathbb{H}_6 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 3}\right) + \mathbb{H}_8 \cdot \left(\mathbf{N}_{\sigma'}^{\otimes 4}\right)\right)^{-1}. \tag{16}$$

Thus, once the texture of a material is known (e.g. through X-Ray measurement [10]) and texture coefficients are calculated according to Eq. (2) Eqs (14) and (16) can be used to simulate the in plane variation of yield stress an $R$-values for various angles to rolling direction. These results can be compared to experimental data and material parameters can be identified by minimizing the error between experimental and simulated results. This means, that it is possible to identify a three dimensional anisotropic yield behavior by simple uniaxial experiments in sheet plane.




Three dimensional stress state. Plane stress setting.

**FIGURE 1** Isotropic cubic yield function for different parameter combinations, $c_1 = \sqrt{3/2}$

## 4.3 | Discussion of the special case of an isotropic yield function

By setting all anisotropy coefficients, i.e. $\eta_1, \ldots, \eta_6$, to zero one retrieves an isotropic yield function. For this special case we will discuss tension and compression yield behavior, shape of the yield function du to parameter variation and convexity. We will begin by noting, that when uneven powers of $\mathbf{N}_{\sigma'}$ are considered in the yield function, an asymmetry regarding tension and compression behavior is introduced [3]. This is sometimes also called $J_3$ theory, in contrast to the isotropic von Mises yield function, which is called $J_2$ theory. In this terminology $J_2$ and $J_3$ are the second and third principal invariants of the deviatoric stress tensor. The proposed yield function can easily be used to model such a behavior, by simply choosing $c_2 \neq 0$.

For further investigating the plastically incompressible isotropic yield function we use the two-dimensional $\pi$-plane [2]. Therefore a transformation from three-dimensional principal stress state to the $\pi$-plane is necessary, which is achieved with the transformation

$$\sigma_1' = -\frac{\sqrt{2}}{2}\left(x + \frac{\sqrt{3}}{3}y\right), \quad \sigma_2' = \frac{\sqrt{2}}{2}\left(x - \frac{\sqrt{3}}{3}y\right), \quad \sigma_3' = \sqrt{\frac{2}{3}}y. \tag{17}$$

In the $\pi$-plane the isotropic yield surface, the boundary of the yield function with $\varphi(\sigma') = \sigma_\mathrm{f}$, is implicitly defined as $y = y(x)$. In two dimensions the resulting yield function can be displayed graphically and convexity can be studied analytically and by visual inspection of the yield surface. A method [2] for studying convexity, where a vanishing curvature at given stress states is looked for, is used. The points where curvature vanishes are called convexity borders. However in the published manuscript some terms are missing, which has been reported [37]. In this paper we implemented the isotropic yield function in the commercial software tool MAPLE, differentiated symbolically and investigated vanishing curvature.

Due to the fact, that a purely isotropic yield function up to quartic terms is practically identical to the one up to cubic terms, we will limit this discussion to a yield function with quadratic and cubic isotropic terms. Shapes of the resulting yield function are displayed in Fig. 1 for three dimensional stress states and for a plane stress setting. The isotropic von Mises - Hill yield surface is included for comparison ($c_1 = \sqrt{3/2}$ as discussed in Subsec. 4.1) and different values for $c_2$ are used. The yield surface has been normalized to $\sigma_\mathrm{f}$.

This parameter study indicates, that $c_2$ can be used for a differentiation between tensile and compressive stress states. For $c_2 \leq 0$ yield stresses in tensile direction increase, whereas compressive yield strength decreases until a convexity border is reached. The opposite is true for $c_2 \geq 0$.

The convexity borders can be calculated along the lines $y = -\sqrt{3}x/3$ and $y = \sqrt{3}x/3$. They lie in the parameter range

$$-\frac{\sqrt{2}}{3\sqrt{3}} \leq \frac{c_2}{c_1} \leq \frac{\sqrt{2}}{3\sqrt{3}}. \tag{18}$$

## 5 | CONCLUSIONS

In this paper a micro-mechanically motivated quasi-phenomenological yield function for polycrystalline cubic metals is presented. The general form of the yield function follows after the assumptions of i) a correlation between crystallographic yield, ii) plastic incompressibility, iii) a polynomial form in powers of stress direction, iv) a positively homogeneous function of degree one in the absolute value of stress and v) a weakly pronounced crystallographic texture. By considering previously published group-theoretic results and the principle of material frame indifference we determine how the CODF, a one-point probability distribution in the form of its tensorial representation with Fourier coefficients, influences anisotropic yield behavior of cubic crystal aggregates. The tensorial Fourier coefficients, which are microstructural quantities accessible, e.g., through X-Ray diffraction measurement, are measures for the anisotropy in yield behavior.

The derived yield function covers plastically anisotropic and the special case of plastically isotropic material behavior in a single framework. It is shown, that the derived yield function can be considered as a generalization of the well known quadratic von Mises - Hill yield function. Further we present a simple way to identify material parameters of sheet metal for a three dimensional anisotropic yield behavior by experiments done in the sheet plane. After a discussion of the special isotropic case of the presented yield function we see, that a tension compression split in yield behavior can be easily introduced by including uneven powers of stresses into the yield function.

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