Arch. Mech., **56**, 6, pp. 425–445, Warszawa 2004

First published in:

The Voigt bound of the stress potential of isotropic viscoplastic FCC polycrystals[1)]

T. BÖHLKE

Otto-von-Guericke-Universität Magdeburg,
Institut für Mechanik, PSF 4120, D-39016 Magdeburg.
e-mail: boehlke@mb.uni-magdeburg.de

THE VOIGT BOUND of the stress potential of face-centered cubic (fcc) polycrystals without texture is numerically determined for all types of strain rate states. The numerical findings reveal the dependence of the stress potential on both the second and the third principal invariant of the strain rate deviator. The dependence on the determinant vanishes only for a linear viscoplastic behavior. Due to the dependence of the stress potential on the third principal invariant, the determinant, the viscoplastic flow is generally nonproportional to the stress deviator. A simple analytical expression is found, which reproduces the numerical findings over the full range of strain rate sensitivities.

1. Introduction

IN THE PRESENT WORK an old problem of solid mechanics is reconsidered: What is the relation between a (visco)plastic strain increment and the stress state in plastically incompressible and isotropic polycrystals? The problem of formulating a yield criterion for the aforementioned class of materials has been considered by TRESCA [38], GUEST [13], HUBER [18], MISES [23], and HENCKY [15]. Tresca and Guest formulated a flow criterion based on a critical value of the shear stress. Huber, Mises and Hencky postulated a flow criterion in terms of the norm of the stress deviator. In the case of an isotropic elastic law the Huber–Mises–Hencky criterion can be interpreted in terms of energy: Only a limited amount of distortional elastic energy can be stored by the material without plastic yielding. Experimental findings indicate that for most plastically isotropic and incompressible polycrystals the yield loci lie in between the Tresca–Guest criterion and the Huber–Mises–Hencky criterion. The Hershey–Davies criterion (HERSHEY [16], DAVIES [7]) contains the two aforementioned criteria as special cases. There are many other formulations of isotropic yield conditions, for example the Schmidt–Ishlinski–Hill (e.g., SCHMIDT [34]) criterion, which states

[1)] The paper has been presented at the International Symposium on Developments in Plasticity and Fracture, Centenary of M.T. HUBER Criterion, Kraków 2004.

that plastic yielding can occur if the extremal eigenvalue of the stress deviator reaches a critical magnitude. Mendelson [22] determines the bounds of convex yield loci of plastically isotropic and incompressible materials with symmetry in tension and compression. Karafillis and Boyce [20] formulated a one-parameter class of yield criteria, which contains the criteria by Tresca–Guest, Huber–Mises–Hencky, and Schmidt–Ishlinski–Hill as special cases. Phenomenological generalizations of the isotropic Huber–Mises–Hencky criterion for anisotropic materials have been formulated by Mises [24] and Hill [17]. For a formulation of micromechanically motivated yield criteria for textured polycrystals see, e.g., Gambin [11] and the references therein or Böhlke and Bertram [4] and Böhlke *et al.* [5].

In this paper the problem of determining a flow criterion is considered in the context of viscoplasticity. The advantage of a viscoplastic modeling is that on both the grain-scale and on the macro-scale, the constitutive equations are given by potential relations. The rate-independent behavior is obtained in the limit that a strain-rate sensitivity parameter approaches infinity. Furthermore, the methods of statistical continuum mechanics allow to bound the macroscopic potentials. In the most simple case, the one-point correlation function of crystal orientations is taken into account, which contains only the volume fraction information of the microstructural features. The corresponding bounds are called elementary bounds. In the present paper only the one-point correlation function of crystal orientations, i.e. the crystallite orientation distribution function (codf), is taken into account. Due to the high nonlinearity of the constitutive potential relations of fcc crystals at room temperature, it is a nontrivial task to estimate the effective potentials even in the isotropic case. Based on discrete sets of crystal orientations, Taylor [36], Hutchinson [19], and Dendievel *et al.* [9] calculated the Voigt bound of (visco)plastically isotropic fcc polycrystals for specific deformations. For the special case of a rate-independent behavior Nebozhyn *et al.* [25] computed the Voigt bound for different strain rate states.

The main result of this contribution is the numerical determination of the Voigt bound of viscoplastically isotropic polycrystals for *all* strain rate states over the whole range of strain rate sensitivities. Furthermore, a simple analytical expression is found, which reproduces the numerical findings over the full range of strain rate types and strain rate sensitivities and can be directly used in finite-element simulations. The Voigt bound is obtained by integrating the stress potential over the orientation space $SO(3)$. The numerical integration is performed based on an adaptive integration scheme. The orientation-dependent stress potential is given by a Legendre–Fenchel transformation of the strain rate potential, which is computed based on a conjugate gradient method. The numerical results reveal the dependence of the Voigt potential on the determinant of the strain rate deviator. This dependence implies that the viscoplastic flow

is generally not proportional to the stress deviator. Nevertheless, the isotropy makes stress and viscoplastic flow coaxial.

Notation. Throughout the text a direct tensor notation is preferred. The scalar product, the dyadic product, and the Frobenius norm are denoted by $\mathbf{A} \cdot \mathbf{B} = \mathrm{tr}(\mathbf{A}^\mathsf{T}\mathbf{B})$, $\mathbf{A} \otimes \mathbf{B}$, and $\|\mathbf{A}\| = (\mathbf{A} \cdot \mathbf{A})^{1/2}$, respectively. Symmetric and traceless tensors are designated by a prime, e.g., $\mathbf{A}'$. The symmetric and the skew part of a 2nd-order tensor $\mathbf{A}$ are denoted by $\mathrm{sym}(\mathbf{A})$ and $\mathrm{skw}(\mathbf{A})$, respectively. Volume and orientational averages are indicated by $\langle\cdot\rangle$.

2. The strain rate potential and the stress potential on the microscale

Flow rule and lattice spin. Elastic distortions are assumed to be negligible. Viscoplastic deformations are considered to result from inelastic deformations in slip systems and, hence, they are volume preserving. The slip rate is assumed to be driven by the resolved shear stress in the corresponding slip system. Therefore, it only depends on the deviatoric part of the stress tensor. The constitutive relation between the mass density and the hydrostatic pressure is not considered here, since only the isotropic viscoplastic behavior of an fcc polycrystal is of interest.

Distortions of viscoplastic single crystals can be modeled by the following set of equations:

$$\begin{aligned} 0 \;&=\; \mathbf{D}' \;-\; \mathbf{Q}\,\mathrm{sym}(\tilde{\mathbf{K}}(\mathbf{Q}^\mathsf{T}\boldsymbol{\tau}'\mathbf{Q}, \tau_\alpha^C))\mathbf{Q}^\mathsf{T}, \\ \dot{\mathbf{Q}}\mathbf{Q}^{-1} \;&=\; \mathbf{W} \;-\; \mathbf{Q}\,\mathrm{skw}(\tilde{\mathbf{K}}(\mathbf{Q}^\mathsf{T}\boldsymbol{\tau}'\mathbf{Q}, \tau_\alpha^C))\mathbf{Q}^\mathsf{T} \end{aligned} \tag{2.1}$$

(see, e.g., HUTCHINSON [19]). $\mathbf{D}$ and $\mathbf{W}$ are the symmetric and the skew-symmetric part of the velocity gradient $\mathbf{L} = \partial\mathbf{v}/\partial\mathbf{x}$. $\boldsymbol{\tau}$ denotes the Kirchhoff stress tensor, which is related to the Cauchy stress tensor $\boldsymbol{\sigma}$ by $\boldsymbol{\tau} = J\boldsymbol{\sigma}$, where $J = \varrho_0/\varrho$ is the determinant of the deformation gradient. The internal variables τ_α^C are the critical resolved shear stresses in the different slip systems. In the present work, fcc single crystals are considered. For this specific class of materials, it is a reasonable assumption that the slip systems harden in an isotropic manner, i.e. $\tau_\alpha^C = \tau^C$ (KOCKS and MECKING [21]).

The orientation of a crystallite is described by a proper orthogonal tensor $\mathbf{Q} = \mathbf{g}_i \otimes \mathbf{e}_i$, where $\mathbf{e}_i$ and $\mathbf{g}_i$ represent an orthonormal basis fixed to the sample and to the (orthonormal) lattice vectors of the crystal, respectively. For given strain rate tensor $\mathbf{D}'$ and crystal orientation $\mathbf{Q}$, Eq. $(2.1)_1$ is an implicit equation for the stress deviator $\boldsymbol{\tau}'$. For a given $\boldsymbol{\tau}'$, $\mathbf{W}$ and $\mathbf{Q}$, Eq. $(2.1)_2$ determines the spin $\dot{\mathbf{Q}}\mathbf{Q}^{-1}$ of the crystal lattice.

The function $\tilde{\mathbf{K}}$ is assumed to be given by

$$\begin{aligned} \tilde{\mathbf{K}}(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C) &= \sum_{\alpha}^{N} \dot{\gamma}_\alpha(\tau_\alpha, \tau^C)\tilde{\mathbf{M}}_\alpha, \\ \dot{\gamma}_\alpha(\tau_\alpha, \tau^C) &= \dot{\gamma}_0 \mathrm{sgn}\,(\tau_\alpha) \left| \frac{\tau_\alpha}{\tau^C} \right|^n, \\ \tau_\alpha &= (\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}) \cdot \tilde{\mathbf{M}}_\alpha \end{aligned} \tag{2.2}$$

(HUTCHINSON [19]). τ_α is the resolved shear stress in the slip system α. The material parameter n quantifies the strain rate sensitivity of the material. It is generally temperature-dependent and can be estimated by strain rate jump experiments. At room temperature n is usually in the range of 50–250. In the limit $n \to \infty$ a rate-independent behavior is obtained. The Schmid or slip system tensors $\tilde{\mathbf{M}}_\alpha = \tilde{\mathbf{d}}_\alpha \otimes \tilde{\mathbf{n}}^\alpha$ are rank-one tensors, which are defined in terms of the slip directions $\tilde{\mathbf{d}}_\alpha$ and the slip plane normals $\tilde{\mathbf{n}}^\alpha$. In the case of an fcc single crystal at room temperature, the octahedral slip systems $\{111\}\langle 110\rangle$ have to be taken into account ($N = 12$).

Strain rate potential. The specification of the flow rule in Eq. (2.2) implies the existence of a potential Ψ^τ for $\mathbf{D}'$

$$\mathbf{D}' = \mathbf{H}^\tau(\boldsymbol{\tau}', \mathbf{Q}, \tau^C) = \frac{\partial \Psi^\tau(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C)}{\partial \boldsymbol{\tau}'}, \tag{2.3}$$

where

$$\Psi^\tau(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C) = \frac{1}{n+1} \sum_{\alpha} \dot{\gamma}_0 \tau^C \left| \frac{(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}) \cdot \tilde{\mathbf{M}}_\alpha}{\tau^C} \right|^{n+1}. \tag{2.4}$$

The potential Ψ^τ is a convex function of the stress deviator $\boldsymbol{\tau}'$. Hence, there exists a one-to-one relation between $\boldsymbol{\tau}'$ and $\mathbf{D}'$. The functions $\mathbf{H}^\tau$ and Ψ^τ are homogeneous of degree n and $n+1$, respectively:

$$\mathbf{H}^\tau(\lambda\boldsymbol{\tau}', \mathbf{Q}, \tau^C) = \lambda^n \mathbf{H}^\tau(\boldsymbol{\tau}', \mathbf{Q}, \tau^C) \qquad \forall \lambda > 0, \tag{2.5}$$

$$\Psi^\tau(\lambda\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C) = \lambda^{n+1} \Psi^\tau(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C) \qquad \forall \lambda > 0. \tag{2.6}$$

Stress potential. The convexity of Ψ^τ implies the existence of a potential Ψ^D for $\boldsymbol{\tau}'$ such that

$$\boldsymbol{\tau}' = \mathbf{H}^D(\mathbf{D}', \mathbf{Q}, \tau^C) = \frac{\partial \Psi^{\mathrm{D}}(\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q}, \tau^C)}{\partial \mathbf{D}'}. \tag{2.7}$$

Ψ^τ and Ψ^D are dual potentials and Ψ^D can be determined by a Legendre–Fenchel transformation

$$\Psi^{\mathrm{D}}(\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q}, \tau^C) = \sup_{\boldsymbol{\tau}'}(\boldsymbol{\tau}' \cdot \mathbf{D}' - \Psi^\tau(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q}, \tau^C)). \tag{2.8}$$

The functions $\mathbf{H}^D$ and Ψ^D are homogeneous of degree $1/n$ and $(n+1)/n$, respectively

$$\mathbf{H}^D(\lambda\mathbf{D}', \mathbf{Q}, \tau^C) = \lambda^{1/n}\mathbf{H}^D(\mathbf{D}', \mathbf{Q}, \tau^C) \qquad \forall\lambda > 0, \tag{2.9}$$

$$\Psi^{\mathrm{D}}(\lambda\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q}, \tau^C) = \lambda^{(n+1)/n}\Psi^{\mathrm{D}}(\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q}, \tau^C) \qquad \forall\lambda > 0. \tag{2.10}$$

3. The strain rate potential and the stress potential on the macroscale

Macroscopic strain rate potential. In the following, a representative volume element (rve) in a statistically homogeneous fcc polycrystal is considered. An rve is a volume which is small enough to be macroscopically considered as a material point. Furthermore, an rve is large enough to contain a statistically representative volume fraction of the microstructure. The boundary of the rve and its outer normal vector are denoted by ∂v and $\mathbf{n}$, respectively. Both the velocity vector as well as the traction vector are assumed to be continuous on grain boundaries. Furthermore, the assumption of a homogeneous hardening state in the rve is adopted. In this section we shortly summarize the basic statements that are important in the context of the elementary bounds (see, e.g., WILLIS [40], PONTE CASTANEDA [27, 28], NEMAT-NASSER and HORI [26], PONTE CASTANEDA and SUQUET [30] TORQUATO [37]).

Let $\mathcal{B}_\tau$ be the class of trial stress fields $\check{\boldsymbol{\tau}}$ defined by the set

$$\mathcal{B}_\tau = \{\check{\boldsymbol{\tau}} : \check{\boldsymbol{\tau}}(\mathbf{x})\mathbf{n} = \bar{\boldsymbol{\tau}}\mathbf{n}\ \forall\mathbf{x} \in \partial v;\ \mathrm{div}\,(\check{\boldsymbol{\tau}}/J) = 0;\ \check{\boldsymbol{\tau}} = \check{\boldsymbol{\tau}}^{\mathsf{T}}\} \tag{3.1}$$

and let

$$\mathcal{F}_\tau(\check{\boldsymbol{\tau}}', \bar{\boldsymbol{\tau}}') = \langle\Psi^\tau(\mathbf{Q}^{\mathsf{T}}\check{\boldsymbol{\tau}}'\mathbf{Q}, \tau^C)\rangle \tag{3.2}$$

be the trial functional. Among all trial fields $\check{\boldsymbol{\tau}}$, the field $\boldsymbol{\tau}$ that makes the associated strain rate field compatible is the one that uniquely minimizes the trial functional $\mathcal{F}_\tau$

$$\mathcal{F}_\tau(\boldsymbol{\tau}', \bar{\boldsymbol{\tau}}') \leq \mathcal{F}_\tau(\check{\boldsymbol{\tau}}', \bar{\boldsymbol{\tau}}'), \tag{3.3}$$

$$\delta\mathcal{F}_\tau(\boldsymbol{\tau}', \bar{\boldsymbol{\tau}}') = 0, \qquad \delta^2\mathcal{F}_\tau(\boldsymbol{\tau}', \bar{\boldsymbol{\tau}}') = \left\langle \delta\boldsymbol{\tau}' \cdot \frac{\partial^2\Psi^\tau}{\partial\boldsymbol{\tau}'^2}[\delta\boldsymbol{\tau}'] \right\rangle \geq 0. \tag{3.4}$$

Furthermore, it can be shown that the average of Ψ^τ corresponding to the real field $\boldsymbol{\tau}'$

$$\bar{\Psi}^\tau(\bar{\boldsymbol{\tau}}') = \inf_{\check{\boldsymbol{\tau}}' \in \mathcal{B}_\tau} \langle \Psi^\tau(\mathbf{Q}^\mathsf{T} \check{\boldsymbol{\tau}}' \mathbf{Q}, \tau^C) \rangle \tag{3.5}$$

represents a potential for the average strain rate

$$\bar{\mathbf{D}}' = \frac{\partial \bar{\Psi}^\tau(\bar{\boldsymbol{\tau}}')}{\partial \bar{\boldsymbol{\tau}}'}. \tag{3.6}$$

Macroscopic stress potential. Let $\mathcal{B}_D$ be the class of trial strain rate fields $\check{\mathbf{D}}$ with associated velocity field $\check{\mathbf{v}}$ defined by the set

$$\mathcal{B}_D = \{\check{\mathbf{D}} : \check{\mathbf{v}}(\mathbf{x}) = \bar{\mathbf{D}}\mathbf{x} \, \forall \mathbf{x} \in \partial v \, , \check{\mathbf{D}} = (\operatorname{grad}(\check{\mathbf{v}}(\mathbf{x})) + \operatorname{grad}(\check{\mathbf{v}}(\mathbf{x}))^\mathsf{T})/2\} \tag{3.7}$$

and let

$$\mathcal{F}_D(\check{\mathbf{D}}', \bar{\mathbf{D}}') = \langle \Psi^D(\mathbf{Q}^\mathsf{T} \check{\mathbf{D}}' \mathbf{Q}, \tau^C) \rangle \tag{3.8}$$

be the trial functional. Among all trial fields $\check{\mathbf{D}}$, the field $\mathbf{D}$ that makes the associated stress field divergence-free and symmetric is the one that uniquely minimizes the trial functional $\mathcal{F}_D$

$$\mathcal{F}_D(\mathbf{D}', \bar{\mathbf{D}}') \leq \mathcal{F}_D(\check{\mathbf{D}}', \bar{\mathbf{D}}'), \tag{3.9}$$

$$\delta \mathcal{F}_D(\mathbf{D}', \bar{\mathbf{D}}') = 0, \qquad \delta^2 \mathcal{F}_D(\mathbf{D}', \bar{\mathbf{D}}') = \left\langle \delta \mathbf{D}' \cdot \frac{\partial^2 \Psi^D}{\partial \mathbf{D}'^2} [\delta \mathbf{D}'] \right\rangle \geq 0. \tag{3.10}$$

(HUTCHINSON [19]). Furthermore, it can be shown that the average of Ψ^D corresponding to the real field $\mathbf{D}'$

$$\bar{\Psi}^D(\bar{\mathbf{D}}') = \inf_{\check{\mathbf{D}}' \in \mathcal{B}_D} \langle \Psi^D(\mathbf{Q}^\mathsf{T} \check{\mathbf{D}}' \mathbf{Q}, \tau^C) \rangle \tag{3.11}$$

represents a potential for the average stress

$$\bar{\boldsymbol{\tau}}' = \frac{\partial \bar{\Psi}^D(\bar{\mathbf{D}}')}{\partial \bar{\mathbf{D}}'}. \tag{3.12}$$

The potentials $\bar{\Psi}^D(\bar{\mathbf{D}}')$ and $\bar{\Psi}^\tau(\bar{\boldsymbol{\tau}}')$ are not dual to each other in general, because the corresponding boundary conditions are different (WILLIS [40], PONTE CASTANEDA [27, 28]),

$$\bar{\Psi}^D(\bar{\mathbf{D}}') \geq \sup_{\bar{\boldsymbol{\tau}}'} \left(\bar{\boldsymbol{\tau}}' \cdot \bar{\mathbf{D}}' - \bar{\Psi}^\tau(\bar{\boldsymbol{\tau}}') \right). \tag{3.13}$$

Elementary bounds. The distribution of crystal orientations on the grain scale affects the mechanical as well as the nonmechanical properties of polycrystals. In statistical continuum mechanics the distribution of crystal orientations is described by n-point correlation functions (e.g., ETINGOF and ADAMS [10]). The one-point correlation function is called crystallite orientation distribution function (codf) in texture analysis. The codf specifies the volume fraction of crystals having a specific orientation and can be experimentally determined by e.g. the X-ray diffraction or neutron diffraction methods and pole figure inversion. If each crystal orientation occurs with the same probability, the codf is constant and equal to one. If the distribution of crystal orientations is inhomogeneous, the codf is nonconstant and the polycrystal is said to have a crystallographic texture. The morphology of the polycrystal on the grain scale is not described by the codf but by the two-point and the higher-order correlation functions of crystal orientations.

In the context of a viscoplastic material behavior it is possible to derive upper and lower bounds for the overall strain rate potential and the overall stress potential. The most simple estimates, the so-called elementary bounds, are based on the one-point statistics of the microstructure. The advantage of the elementary bounds is that they can be computed quite easily since no boundary-value problem has to be solved. These bounds are only accurate for small phase contrasts on the microscale. The incorporation of higher-order correlation functions allows to tighten the bounds. For the incorporation of higher-order bounds see for example DENDIEVEL *et al.* [9], WILLIS [41], and DE BOTTON and CASTANEDA [8], (see PONTE CASTANEDA and SUQUET [30] for a review). The methods developed in these works allow for the computation of bounds for viscoplastic polycrystals similar to the bounds derived by HASHIN and SHTRIKMAN [14] for linear elastic polycrystals. The bounds have been shown to tend to the Voigt bound in the rate-insensitive limit. In order to overcome this shortcoming, DE BOTTON and PONTE CASTANEDA [8] and PONTE CASTANEDA and NEBOZHYN [29] developed an alternative approach giving self-consistent estimates for nonlinear viscoplastic composites directly from the classical self-consistent estimates for linear elastic composites. It has been shown (NEBOZHYN *et al.* [25]) that for fcc and bcc polycrystals the new estimates are close to the Voigt bound, whereas for highly anisotropic grains with nearly deficient slip systems the distance to the elementary bounds is significant.

The Reuss bound. It immediately follows from Eq. (3.5) that the assumption of a homogeneous stress field (SACHS [33], REUSS [31]) gives a bound, called Reuss bound, for the strain rate potential

$$\bar{\Psi}^{\tau}(\bar{\boldsymbol{\tau}}') \leq \bar{\Psi}^{R}(\bar{\boldsymbol{\tau}}') = \langle \Psi^{\tau}(\mathbf{Q}^{\mathsf{T}}\bar{\boldsymbol{\tau}}'\mathbf{Q}, \tau^{C})\rangle. \tag{3.14}$$

The dual potential is obtained by a Legendre–Fenchel transformation

$$\bar{\Psi}^{R*}(\bar{\mathbf{D}}') = \sup_{\bar{\boldsymbol{\tau}}'} \left(\bar{\boldsymbol{\tau}}' \cdot \bar{\mathbf{D}}' - \bar{\Psi}^{R}(\bar{\boldsymbol{\tau}}') \right). \tag{3.15}$$

The Reuss bound predicts the following rate of deformation

$$\bar{\mathbf{D}}'^{R} = \frac{\partial \bar{\Psi}^{R}(\bar{\boldsymbol{\tau}}')}{\partial \bar{\boldsymbol{\tau}}'}. \tag{3.16}$$

The Voigt bound. Furthermore, it follows from Eq. (3.11) that the assumption of a homogeneous strain rate field (VOIGT [39], TAYLOR [36], BISHOP and HILL [3], HUTCHINSON [19]) gives a bound, called Voigt bound, for the stress potential

$$\bar{\Psi}^{D}(\bar{\mathbf{D}}') \le \bar{\Psi}^{V}(\bar{\mathbf{D}}') = \langle \Psi^{D}(\mathbf{Q}^{\mathsf{T}} \bar{\mathbf{D}}' \mathbf{Q}, \tau^{C}) \rangle. \tag{3.17}$$

The dual potential is obtained by a Legendre–Fenchel transformation

$$\bar{\Psi}^{V*}(\bar{\boldsymbol{\tau}}') = \sup_{\bar{\mathbf{D}}'} \left(\bar{\boldsymbol{\tau}}' \cdot \bar{\mathbf{D}}' - \bar{\Psi}^{V}(\bar{\mathbf{D}}') \right). \tag{3.18}$$

The Voigt bound predicts the following stress tensor:

$$\bar{\boldsymbol{\tau}}'^{V} = \frac{\partial \bar{\Psi}^{V}(\bar{\mathbf{D}}')}{\partial \bar{\mathbf{D}}'}. \tag{3.19}$$

The following relations hold for sufficiently large representative volume elements:

$$\bar{\Psi}^{V*}(\bar{\boldsymbol{\tau}}') \le \bar{\Psi}^{\tau}(\bar{\boldsymbol{\tau}}') \le \bar{\Psi}^{R}(\bar{\boldsymbol{\tau}}'), \tag{3.20}$$

$$\bar{\Psi}^{R*}(\bar{\mathbf{D}}') \le \bar{\Psi}^{D}(\bar{\mathbf{D}}') \le \bar{\Psi}^{V}(\bar{\mathbf{D}}'). \tag{3.21}$$

The Voigt estimate $\bar{\Psi}^{V}$ represents an upper bound whereas the Reuss estimate $\bar{\Psi}^{R*}$ is a lower bound for the stress potential $\bar{\Psi}^{D}$.

Orientational averages. The codf $f(\mathbf{Q})$ specifies the volume fraction dv/v of crystals having the orientation $\mathbf{Q}$ (BUNGE [6], ROE [32]), i.e.

$$\frac{dv}{v}(\mathbf{Q}) = f(\mathbf{Q})\, dQ. \tag{3.22}$$

dQ is the volume element in $SO(3)$ which ensures an invariant integration over $SO(3)$ (GEL'FAND *et al.* [12]), i.e.

$$\int_{SO(3)} f(\mathbf{Q})\, dQ = \int_{SO(3)} f(\mathbf{Q}\mathbf{Q}_0)\, dQ \qquad \forall \mathbf{Q}_0 \in SO(3). \tag{3.23}$$

If $SO(3)$ is parameterized by Euler angles, the volume element dQ is given by

$$dQ = \frac{\sin(\Phi)}{8\pi^2}\, d\varphi_1\, d\Phi\, d\varphi_2. \tag{3.24}$$

The function $f(\mathbf{Q})$ is nonnegative and normalized such that

$$f(\mathbf{Q}) \geq 0 \qquad \forall \mathbf{Q} \in SO(3), \qquad \int\limits_{SO(3)} f(\mathbf{Q})\, dQ = 1. \tag{3.25}$$

The orientation distribution function $f(\mathbf{Q})$ reflects both the symmetry of the crystallites forming the aggregate and the sample symmetry, which results from the processing history (ZHENG and FU [42]). The crystal symmetry implies the following symmetry relation for $f(\mathbf{Q})$:

$$f(\mathbf{Q}) = f(\mathbf{Q}\mathbf{H}^C) \qquad \forall \mathbf{H}^C \in S^C \subseteq SO(3). \tag{3.26}$$

S^C denotes the symmetry group of the crystallite. The sample symmetry implies the following symmetry relation for $f(\mathbf{Q})$

$$f(\mathbf{Q}) = f(\mathbf{H}^S\mathbf{Q}) \qquad \forall \mathbf{H}^S \in S^S \subseteq SO(3). \tag{3.27}$$

S^S denotes the symmetry group of the sample.

Let $\psi(\mathbf{Q}(\mathbf{x}))$ be a mechanical quantity of a crystallite which depends on the position vector only by its dependence on the orientation $\mathbf{Q}$. Volume averages of such a quantity can be transformed by Eq. (3.22) into averages over $SO(3)$

$$\bar{\psi} = \langle\psi\rangle = \frac{1}{v}\int\limits_v \psi(\mathbf{Q}(\mathbf{x}))\, dv = \int\limits_{SO(3)} f(\mathbf{Q})\psi(\mathbf{Q})\, dQ. \tag{3.28}$$

4. Numerical approximation of the isotropic Voigt bound

Parameterization of the strain rate tensor. The deviatoric strain rate tensor $\bar{\mathbf{D}}'$ generally can be decomposed into

$$\bar{\mathbf{D}}' = \|\bar{\mathbf{D}}'\|\bar{\mathbf{N}}'_D = \|\bar{\mathbf{D}}'\|\mathbf{Q}_D\bar{\mathbf{N}}'_0\mathbf{Q}_D^{\mathsf{T}}, \tag{4.1}$$

where $\|\bar{\mathbf{D}}'\|$ is the magnitude of $\bar{\mathbf{D}}'$. $\mathbf{Q}_D$ is an orthogonal tensor that maps an arbitrary orthonormal reference bases $\mathbf{e}_i$ onto the eigenvectors of $\bar{\mathbf{D}}'$. The eigenvectors of the symmetric tensor $\bar{\mathbf{N}}'_0$ are $\mathbf{e}_i$ and the eigenvalues n_α of $\bar{\mathbf{N}}'_0$ are equal to those of $\bar{\mathbf{D}}'$ divided by $\|\bar{\mathbf{D}}'\|$. The restrictions $\mathrm{tr}(\bar{\mathbf{N}}'_0) = 0$ and $\|\bar{\mathbf{N}}'_0\| = 1$ hold. As a result, the eigenvalues n_α are constrained by $n_1 + n_2 + n_3 = 0$ and

$n_1^2+n_2^2+n_3^2=1$, respectively. These constraints are identically fulfilled by the following parameterization of $\bar{\mathbf{N}}_0'$:

$$\bar{\mathbf{N}}_0'(\xi)=\sum_{\alpha=1}^{3} n_\alpha \mathbf{e}_\alpha\otimes\mathbf{e}_\alpha,\qquad n_{1,3}=-\frac{\sqrt{6}}{6}\xi\pm\frac{\sqrt{2}}{2}\sqrt{1-\xi^2},\qquad n_2=\frac{\sqrt{6}}{3}\xi, \tag{4.2}$$

$\xi\in[-1/2,+1/2]$. The principal invariants of $\bar{\mathbf{D}}'$ are

$$I=0,\qquad II=-\frac{1}{2}\|\bar{\mathbf{D}}'\|^2,\qquad III=\frac{\sqrt{6}}{6}\|\bar{\mathbf{D}}'\|^3\xi\left(\frac{4}{3}\xi^2-1\right). \tag{4.3}$$

The principal invariants of $\bar{\mathbf{N}}_0'$ are

$$I^*=0,\qquad II^*=-\frac{1}{2},\qquad III^*=\frac{\sqrt{6}}{6}\xi\left(\frac{4}{3}\xi^2-1\right)\in\left[-\frac{\sqrt{6}}{18},+\frac{\sqrt{6}}{18}\right]. \tag{4.4}$$

Inspection of (4.4) shows that there exists a one-to-one relation of III^* and ξ. The derivative of III^* with respect to $\bar{\mathbf{D}}$ has the following form

$$\frac{\partial III^*}{\partial\bar{\mathbf{D}}'}=\frac{1}{\|\bar{\mathbf{D}}'\|}\left(\frac{\bar{\mathbf{D}}'^{2\prime}}{\|\bar{\mathbf{D}}'\|}-3III^*\frac{\bar{\mathbf{D}}'}{\|\bar{\mathbf{D}}'\|}\right). \tag{4.5}$$

The ξ-values $-1/2$, 0, and $+1/2$ belong to the strain rate states corresponding to uniaxial elongation, plane strain compression, and simple compression, respectively.

The isotropic Voigt bound of the stress potential. On the basis of Eqs. (2.8), (3.17), and (3.28), it can be concluded that the Voigt bound is given by

$$\bar{\Psi}^V(\bar{\mathbf{D}}')=\int_{SO(3)} f(\mathbf{Q})\sup_{\boldsymbol{\tau}'}(\boldsymbol{\tau}'\cdot\bar{\mathbf{D}}'-\Psi^\tau(\mathbf{Q}^{\mathsf{T}}\boldsymbol{\tau}'\mathbf{Q},\tau^C))dQ. \tag{4.6}$$

After exploiting the homogeneity properties of the stress potential (see (2.10)) and some elementary rearrangements, one obtains the following equivalent form of the Voigt bound

$$\bar{\Psi}^V(\bar{\mathbf{D}}')=\tau^C\dot{\gamma}_0\left\|\frac{\bar{\mathbf{D}}'}{\dot{\gamma}_0}\right\|^{(n+1)/n}\Gamma^V(\bar{\mathbf{N}}_D',n), \tag{4.7}$$

where

$$\Gamma^V(\bar{\mathbf{N}}_D',n)=\int_{SO(3)} f(\mathbf{Q})\sup_{\mathbf{A}'}(\mathbf{A}'\cdot\bar{\mathbf{N}}_D'-\Psi^{\tau*}(\mathbf{Q}^{\mathsf{T}}\mathbf{A}'\mathbf{Q},n))dQ \tag{4.8}$$

and

$$\Psi^{\tau*}(\mathbf{Q}^{\mathsf{T}}\mathbf{A}'\mathbf{Q}, n) = \frac{1}{n+1}\sum_{\alpha}\left|\,(\mathbf{Q}^{\mathsf{T}}\mathbf{A}'\mathbf{Q})\cdot\tilde{\mathbf{M}}_{\alpha}\,\right|^{n+1}. \tag{4.9}$$

Here, $\mathbf{A}'$ is a dimensionless, symmetric and traceless tensor. Both Γ^V and $\Psi^{\tau*}$ are solely formulated in terms of dimensionless variables.

For an isotropic distribution of crystal orientations $f(\mathbf{Q}) = 1$ holds. As a result, the Voigt bound is isotropic, i.e. Γ^V is an isotropic tensor function. Due to the resulting isotropy of the bound, $\mathbf{Q}_D$ can be assumed to be equal to the unit tensor without loss of generality. Then the bound is given by

$$\boxed{\bar{\Psi}^{VI}(\bar{\mathbf{D}}') = \tau^C\dot{\gamma}_0\left\|\frac{\bar{\mathbf{D}}'}{\dot{\gamma}_0}\right\|^{(n+1)/n}\Gamma^{VI}(III^*, n),} \tag{4.10}$$

where

$$\boxed{\Gamma^{VI}(III^*, n) = \int\limits_{SO(3)}\sup_{\mathbf{A}'}(\mathbf{A}'\cdot\bar{\mathbf{N}}'_{\mathbf{0}}(III^*) - \Psi^{\tau*}(\mathbf{Q}^{\mathsf{T}}\mathbf{A}'\mathbf{Q}, n))\,dQ.} \tag{4.11}$$

Equations (4.10) and (4.11) show that for a computation of the isotropic Voigt bound for all strain rate states only the function Γ^{VI} is needed, which depends on two parameters.

The flow rule in the isotropic case. The combination of the potential relation (3.19) and the homogeneity property (2.9) gives

$$\bar{\boldsymbol{\tau}}'^V = \frac{\partial\bar{\Psi}^V(\bar{\mathbf{D}}')}{\partial\bar{\mathbf{D}}'} = \tau^C\boldsymbol{\Gamma}^V(\bar{\mathbf{D}}'/\dot{\gamma}_0, n) = \tau^C\|\bar{\mathbf{D}}'/\dot{\gamma}_0\|^{1/n}\boldsymbol{\Gamma}^V(\bar{\mathbf{N}}'_D, n) \tag{4.12}$$

with

$$\boldsymbol{\Gamma}^V(\bar{\mathbf{N}}'_D, n) = \frac{\partial\Gamma^V(\bar{\mathbf{N}}'_D, n)}{\partial\bar{\mathbf{N}}'_D}. \tag{4.13}$$

For an isotropic codf, $\bar{\Psi}^{VI}$ depends only on the norm of $\bar{\mathbf{D}}'$ and its determinant. Hence the potential relation can be simplified to

$$\begin{aligned}\bar{\boldsymbol{\tau}}'^{VI} = \frac{\partial\bar{\Psi}^{VI}(\|\bar{\mathbf{D}}'\|, \det(\bar{\mathbf{D}}'))}{\partial\bar{\mathbf{D}}'} &= \frac{\partial\bar{\Psi}^{VI}(\|\bar{\mathbf{D}}'\|, \det(\bar{\mathbf{D}}'))}{\partial\|\bar{\mathbf{D}}'\|}\frac{\bar{\mathbf{D}}'}{\|\bar{\mathbf{D}}'\|}\\ &\quad + \frac{\partial\bar{\Psi}^{VI}(\|\bar{\mathbf{D}}'\|, \det(\bar{\mathbf{D}}'))}{\partial\det(\bar{\mathbf{D}}')}\bar{\mathbf{D}}'^{2\prime},\end{aligned} \tag{4.14}$$

where the following relations have been taken into account:

$$\frac{\partial\|\bar{\mathbf{D}}'\|}{\partial\bar{\mathbf{D}}'}=\frac{\bar{\mathbf{D}}'}{\|\bar{\mathbf{D}}'\|},\qquad\qquad\frac{\partial\det(\bar{\mathbf{D}}')}{\partial\bar{\mathbf{D}}'}=\bar{\mathbf{D}}'^{2\prime}. \tag{4.15}$$

In Huber–Mises–Hencky flow theories $\bar{\boldsymbol{\tau}}'$ and $\bar{\mathbf{D}}'$ are not only coaxial due to the assumed isotropy but also proportional. In such theories the proportionality holds because the flow potential is independent of III^*.

The Taylor factor. If the deformation field and the hardening state are homogeneous in the aggregate, then the Taylor factor can be used to relate the microscopic and macroscopic flow stresses. On the microscale, the (viscoplastic) dissipation is given by

$$\boldsymbol{\tau}'\cdot\mathbf{D}'=\frac{\partial\Psi^D(\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q},\tau^C)}{\partial\mathbf{D}'}\cdot\mathbf{D}'=\frac{n+1}{n}\Psi^D(\mathbf{Q}^{\mathsf{T}}\mathbf{D}'\mathbf{Q},\tau^C). \tag{4.16}$$

The upper bound approach predicts the following macroscopic dissipation:

$$\langle\boldsymbol{\tau}'\cdot\mathbf{D}'\rangle^V=\langle\boldsymbol{\tau}'\rangle\cdot\bar{\mathbf{D}}'=\frac{n+1}{n}\bar{\Psi}^V(\bar{\mathbf{D}}'). \tag{4.17}$$

In the context of a rate-dependent modeling, the mean Taylor factor $\bar{M}$ can be introduced in the following manner:

$$\langle\boldsymbol{\tau}'\cdot\mathbf{D}'\rangle^V=\tau^C\dot{\gamma}_0\bar{M}\dot{\bar{\varepsilon}}^{*(n+1)/n}, \tag{4.18}$$

where the dimensionless equivalent strain rate $\dot{\bar{\varepsilon}}^*$ is defined by

$$\dot{\bar{\varepsilon}}^*=\sqrt{\frac{2}{3}}\|\bar{\mathbf{D}}'/\dot{\gamma}_0\|^{(n+1)/n}. \tag{4.19}$$

As a result, the Taylor factor can be determined by the equation

$$\bar{M}(\bar{\mathbf{N}}'_D,n)=\frac{n+1}{n}\left(\sqrt{\frac{3}{2}}\right)^{(n+1)/n}\Gamma^V(\bar{\mathbf{N}}'_D,n). \tag{4.20}$$

An isotropy of the aggregate implies that $\bar{M}$ is given by the simplified form

$$\bar{M}(III^*,n)=\frac{n+1}{n}\left(\sqrt{\frac{3}{2}}\right)^{(n+1)/n}\Gamma^{VI}(III^*,n). \tag{4.21}$$

As an example, the tensile deformation of a generally anisotropic aggregate is considered. Based on the equation

$$\langle\boldsymbol{\tau}'\cdot\mathbf{D}'\rangle^V=\bar{\sigma}\dot{\bar{\varepsilon}}, \tag{4.22}$$

where the equivalent quantities are defined by

$$\bar{\sigma} = \sqrt{\frac{3}{2}}\|\bar{\boldsymbol{\tau}}'\|, \qquad \dot{\bar{\varepsilon}} = \sqrt{\frac{2}{3}}\|\bar{\mathbf{D}}'\|, \tag{4.23}$$

and (4.18), it can be seen that the ratio of the macroscopic flow stress $\bar{\sigma}$ and the microscopic critical resolved shear stress τ^C is bounded by

$$\frac{\bar{\sigma}}{\tau^C} \leq \bar{M}(\bar{\mathbf{N}}'_D, n)\left(\frac{\dot{\bar{\varepsilon}}}{\dot{\gamma}_0}\right)^{1/n}. \tag{4.24}$$

The Voigt bound in the rate-independent limit. A rate-independent flow behavior can be described by the material model as a special case. The distortions of the material are rigid-plastically modeled if the strain rate sensitivity parameter n approaches infinity. In this case the bound of the stress potential reduces to

$$\begin{aligned} \bar{\Psi}^V_\infty(\bar{\mathbf{D}}') &= \tau^C\dot{\gamma}_0\|\bar{\mathbf{D}}'/\dot{\gamma}_0\|\ \mathit{\Gamma}^V_\infty(\bar{\mathbf{N}}'_D), \\ \mathit{\Gamma}^V_\infty(\bar{\mathbf{N}}'_D) &= \lim_{n\to\infty} \mathit{\Gamma}^V(\bar{\mathbf{N}}'_D, n). \end{aligned} \tag{4.25}$$

In the isotropic case one obtains

$$\begin{aligned} \bar{\Psi}^{VI}_\infty(\bar{\mathbf{D}}') &= \tau^C\dot{\gamma}_0\|\bar{\mathbf{D}}'/\dot{\gamma}_0\|\ \mathit{\Gamma}^{VI}_\infty(\mathit{III}^*), \\ \mathit{\Gamma}^{VI}_\infty(\mathit{III}^*) &= \lim_{n\to\infty} \mathit{\Gamma}^{VI}(\bar{\mathbf{N}}'_D, n). \end{aligned} \tag{4.26}$$

Furthermore, the rate-independence implies that the stress deviator is homogeneous of degree zero in the strain rate deviator

$$\bar{\boldsymbol{\tau}}'^V_\infty = \frac{\partial\bar{\Psi}^V_\infty(\bar{\mathbf{D}}')}{\partial\bar{\mathbf{D}}'} = \tau^C\boldsymbol{\Gamma}^V_\infty(\bar{\mathbf{D}}'/\dot{\gamma}_0, n) = \tau^C\|\bar{\mathbf{D}}'/\dot{\gamma}_0\|\boldsymbol{\Gamma}^V_\infty(\bar{\mathbf{N}}'_D) \tag{4.27}$$

with

$$\boldsymbol{\Gamma}^V_\infty(\bar{\mathbf{N}}'_D) = \lim_{n\to\infty}\frac{\partial\mathit{\Gamma}^V(\bar{\mathbf{N}}'_D, n)}{\partial\bar{\mathbf{N}}'_D}. \tag{4.28}$$

For $n \to \infty$ the classical definition of the Taylor factor is reestablished

$$\langle\boldsymbol{\tau}'\cdot\mathbf{D}'\rangle^V_\infty = \lim_{n\to\infty}\langle\boldsymbol{\tau}'\cdot\mathbf{D}'\rangle^V = \tau^C\dot{\gamma}_0\bar{M}_\infty\dot{\bar{\varepsilon}}^* = \tau^C\bar{M}_\infty\dot{\bar{\varepsilon}} \tag{4.29}$$

or equivalently

$$\bar{M}_\infty(\bar{\mathbf{N}}'_D) = \lim_{n\to\infty}\bar{M}(\bar{\mathbf{N}}'_D, n) = \sqrt{\frac{3}{2}}\mathit{\Gamma}^V_\infty(\bar{\mathbf{N}}'). \tag{4.30}$$

It can be seen that in both the rate-dependent case and in the rate-independent case, the Taylor factor depends only on the direction of the macroscopic strain rate deviator. Equation (4.24), which holds for the tensile deformation of a polycrystal, can now be simplified

$$\frac{\bar{\sigma}}{\tau^C} \leq \bar{M}(\bar{\mathbf{N}}'_D, n). \tag{4.31}$$

Numerical computation of $\bar{\Psi}^{VI}(\bar{\mathbf{D}}')$. The crucial point for the determination of the isotropic Voigt bound for all strain rate states is the numerical computation of the function Γ^{VI} which depends on the two parameters III^* and n. The numerical method which has been applied for the computation of Γ^{VI} consists essentially of two parts: i) an integration scheme and ii) an algorithm for the computation of the Legendre–Fenchel transform. The numerical integration over $SO(3)$ has been performed by means of the adaptive integration scheme by BERNTSEN and ESPELID [1, 2]. The Legendre–Fenchel transformation is computed by the conjugate gradient method by SHANNO and PHUA [35].

The numerical results for Γ^{VI} versus III^* are shown in Figs. 1 and 2. Figure 1 shows the results for the linearly viscous behavior, which is obtained for $m = n + 1 = 2$ and values of m in the range $10, \ldots, 48$. Figure 2 shows Γ^{VI} for values of m up to 190. It can be seen that only in the linearly viscous case Γ^{VI} is independent of III^*, which implies that $\bar{\boldsymbol{\tau}}'$ and $\bar{\mathbf{D}}'$ are proportional. For increasing values of m the dependence on III^* becomes significant. The curve for $m = 190$ is close to the limiting case $m \to \infty$. The symbols ■ represent the numerical results. The solid line corresponds to an approximation of the isotropic Voigt bound by an ansatz function discussed in the next subsection.

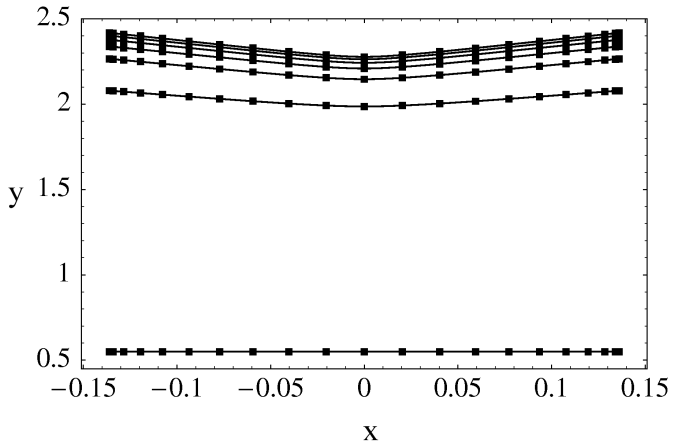

FIG. 1. Γ^{VI} vs. III^* for different values of m (from the bottom up: $m = 2, 10, 18, 24, 32, 40, 48$).

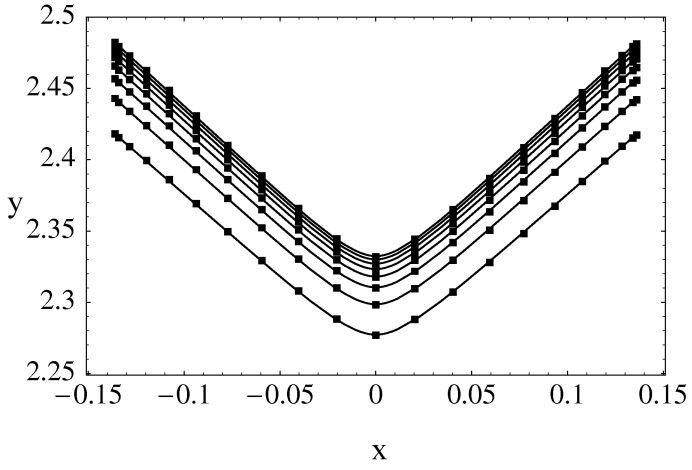

FIG. 2. Γ^{VI} vs. III^* for different values of m (from the bottom up: $m = 50, 70, 90, 110, 130, 150, 170, 190$).

HUTCHINSON [19] determined the Voigt bound for uniaxial tension and pure shear. A tensile deformation is specified by $\xi = -1/2$, or equivalently, by $III^* = -\sqrt{6}/18$. In the case of uniaxial tension he defined a function $f(n)$ which is related to Γ^{VI} by

$$f(n) = \left(\sqrt{\frac{2}{3}}\right)^{-(n+1)/n} \frac{n+1}{n} \Gamma^{VI}(-\sqrt{6}/18, n). \tag{4.32}$$

For the linearly viscous and the rate-independent behavior one obtains

$$f(1) = 3\Gamma^{VI}(-\sqrt{6}/18, 1), \qquad f(\infty) = \sqrt{\frac{3}{2}}\Gamma^{VI}(-\sqrt{6}/18, n \to \infty). \tag{4.33}$$

From Figs. 1 and 2 it can be concluded that $f(1) = 1.65$ and $f(\infty) \approx 3.06$. These numerical results correspond to Taylor's and Hutchinson's findings. The constant value of $\Gamma^{VI}(III^*, 1) = 11/10$ can also be computed analytically.

A pure shear deformation is specified by $\xi = 0$, or equivalently, by $III^* = 0$. In the context of pure shear, Hutchinson defined a function $g(n)$ which is related to Γ^{VI} by

$$g(n) = \left(\sqrt{2}\right)^{(1-n)/n} \frac{n+1}{n} \Gamma^{VI}(0, n). \tag{4.34}$$

For the linearly viscous and the rate-independent behavior one obtains

$$g(1) = 2\Gamma^{VI}(0, 1), \qquad g(\infty) = \frac{1}{\sqrt{2}}\Gamma^{VI}(0, n \to \infty). \tag{4.35}$$

From Figs. 1 and 2 it can be concluded that $g(1) = 1.1$ and $g(\infty) \approx 1.65$. These values again correspond to Hutchinson's numerical results.

Approximation of the numerical results. In this subsection a simple ansatz for $\mathit{\Gamma}^{VI}$ is presented, which is motivated by the numerical findings and reproduces the numerical results over the full range of strain rate sensitivities. Figures 1 and 2 indicate that the function $\mathit{\Gamma}^{VI}$ depends only on the magnitude of III^*. Furthermore, it is almost linear for $|\,\mathit{III}^*\,| > 0.025$. The minimum value of $\mathit{\Gamma}^{VI}$ depends on n. The following ansatz seems to be suitable for an approximation

$$\mathit{\Gamma}(\mathit{III}^*, n) = A + B\,(C\,|\,\mathit{III}^*\,| + \exp(-C\,|\,\mathit{III}^*\,|) - 1)\,, \tag{4.36}$$

which has the properties

$$\mathit{\Gamma}(\mathit{III}^* = 0, n) = A(n), \qquad \frac{\partial \mathit{\Gamma}(\mathit{III}^*, n)}{\partial \mathit{III}^*}\Big|_{\mathit{III}^*=0} = 0. \tag{4.37}$$

It contains the three parameters A, B, and C, which are assumed to depend on $m = n + 1$. For each curve of $\mathit{\Gamma}^{VI}$ with fixed m, the Levenberg–Marquardt algorithm is applied in order to determine the optimal values of A, B, and C, respectively. The results are shown in the Figs. 3, 4, and 5. It can be seen that the simple ansatz allows to reproduce the numerical findings. For large values of m the values of A, B, and C, saturate at values $A_\infty \approx 2.33$, $B_\infty \approx 0.018$, and $C_\infty \approx 70.0$ describing the rate-independent case. Finally it can be concluded that the isotropic Voigt potential can be approximated by

$$\begin{aligned} \bar{\mathit{\Psi}}^{VI}(\bar{\mathbf{D}}') &= \tau^C \dot{\gamma}_0 \left\| \frac{\bar{\mathbf{D}}'}{\dot{\gamma}_0} \right\|^{(n+1)/n} \mathit{\Gamma}^{VI}(\mathit{III}^*, n), \\ \mathit{\Gamma}^{VI}(\mathit{III}^*, n) &\approx A + B\,(C\,|\,\mathit{III}^*\,| + \exp(-C\,|\,\mathit{III}^*\,|) - 1)\,. \end{aligned} \tag{4.38}$$

In the rate-independent case one obtains

$$\begin{aligned} \bar{\mathit{\Psi}}^{VI}_\infty(\bar{\mathbf{D}}') &\approx \tau^C \dot{\gamma}_0 \|\bar{\mathbf{D}}'/\dot{\gamma}_0\| \mathit{\Gamma}^{VI}_\infty(\mathit{III}^*), \\ \mathit{\Gamma}^{VI}_\infty(\mathit{III}^*) &\approx A_\infty + B_\infty\,(C_\infty\,|\,\mathit{III}^*\,| + \exp(-C_\infty\,|\,\mathit{III}^*\,|) - 1)\,. \end{aligned} \tag{4.39}$$

In Fig. 6 the contour lines of $\mathit{\Psi}^{VI}$ are shown for the linearly viscous case (left) and the rate-independent case (middle). Figure 6 (right) shows that also a regularized version of the Tresca–Guest criterion can be described by the ansatz (4.36). Note that in the strain rate space the hexagon is oriented differently compared to its representation in the stress space.

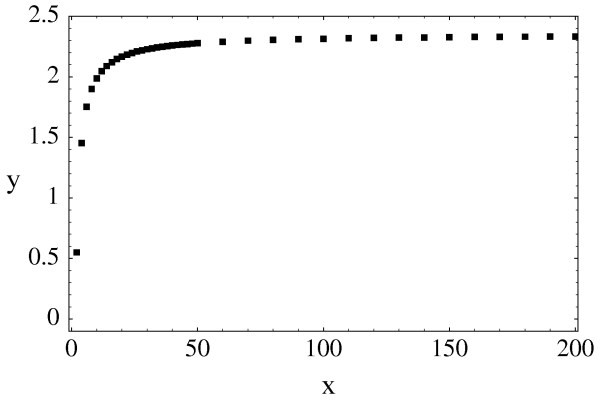

FIG. 3. Parameter A vs. m (see Eq. (4.36)) obtained by the Levenberg–Marquardt algorithm.

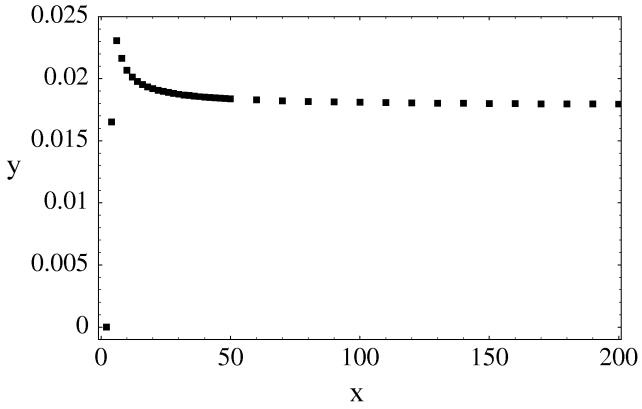

FIG. 4. Parameter B vs. m (see Eq. (4.36)) obtained by the Levenberg–Marquardt algorithm.

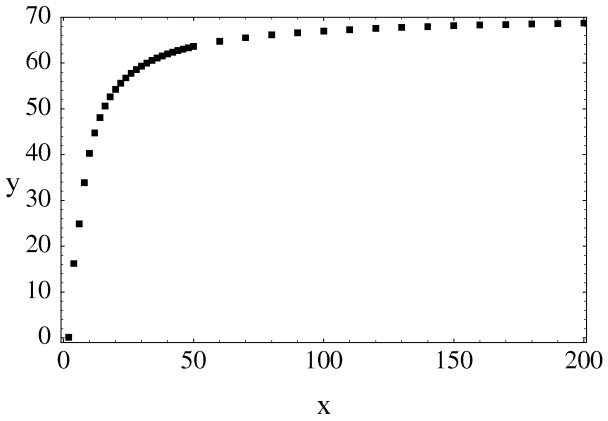

FIG. 5. Parameter C vs. m (see Eq. (4.36)) obtained by the Levenberg–Marquardt algorithm.

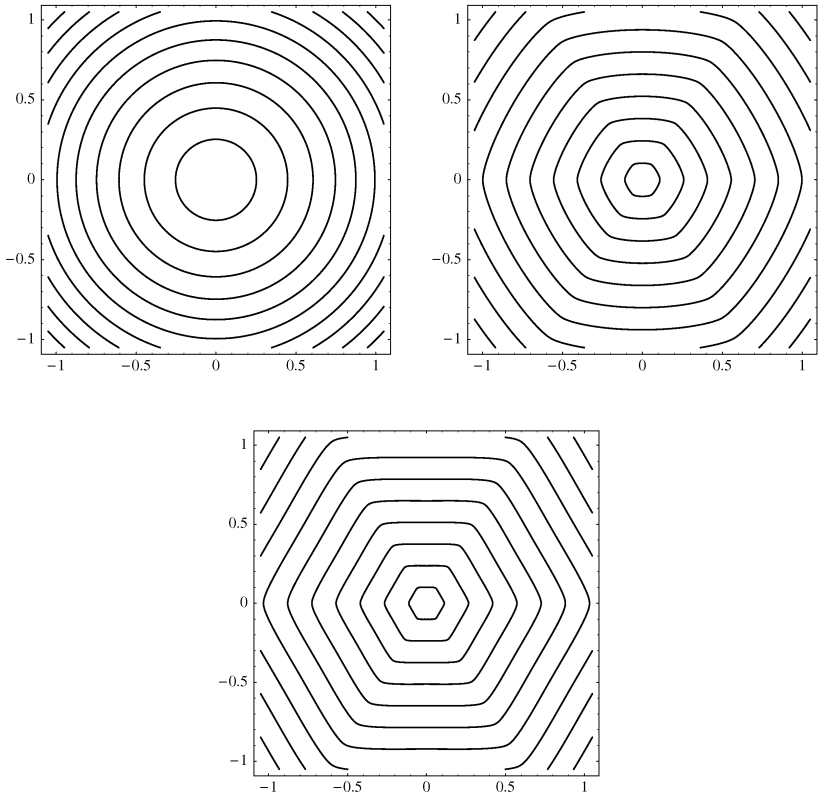

FIG. 6. Contour lines of Ψ^{VI} (see Eq. (4.38)) in the π-plane of the strain rate space (left: $m = 2$, middle: $m = 200$, right: $A = 1.0$, $B = 0.013$, $C = 75.0$).

Based on the ansatz function for the isotropic Voigt potential (4.36), the stress deviator can be specified by (see also (4.5))

$$\bar{\boldsymbol{\tau}}' = \frac{\partial \bar{\Psi}^{VI}(\bar{\mathbf{D}}')}{\partial \bar{\mathbf{D}}'} = \tau^C \left\| \frac{\bar{\mathbf{D}}'}{\dot{\gamma}_0} \right\|^{1/n} \tag{4.40}$$
$$\times \left(\left(\Gamma^{VI}(III^*, n) - 3III^* \frac{\partial \Gamma^{VI}(III^*, n)}{\partial III^*} \right) \frac{\bar{\mathbf{D}}'}{\|\bar{\mathbf{D}}'\|} - \frac{\partial \Gamma^{VI}(III^*, n)}{\partial III^*} \frac{\bar{\mathbf{D}}'^{2\prime}}{\|\bar{\mathbf{D}}'\|} \right)$$

where

$$\frac{\partial \Gamma^{VI}(III^*, n)}{\partial III^*} = B\, C\, \operatorname{sgn}(III^*) \left(1 - \exp(-C\,|\,III^*\,|)\right). \tag{4.41}$$

5. Summary

It has been shown that the isotropic Voigt bound of the stress potential shows a significant dependence on the determinant of the strain rate deviator. This dependence implies that the viscoplastic flow is not proportional to the stress deviator. A simple analytical expression is found which allows for reproducing the numerical findings over the full range of strain rate sensitivities. The fact that for fcc polycrystals the variational self-consistent estimates are close to the Voigt bound, NEBOZHYN *et al.* [25], seems to justify the derivation of quasi-analytical expressions for the macroscopic flow potential based on a numerical analysis of the Voigt bound. Such an analytical expression for the stress potential can be used for finite-element simulations in order to specify the Taylor factor and the flow direction of viscoplastically isotropic polycrystals. It contains the Huber–Mises–Hencky yield criterion as a special case.

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Received February 3, 2004; revised version June 14, 2004.