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An energy-based yield criterion for solids of cubic elasticity and orthotropic limit state

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THE AIM OF THE PAPER is to formulate a particular case of the J. Rychlewski yield condition for anisotropic linear elastic solids with Hooke's law and the limit tensor representing elastic range in the Mises yield condition under the assumption that different symmetry of elasticity tensors and the limit tensor appears. The elasticity tensor **C** is assumed to have cubic symmetry. The yield condition is based on the concept of stored elastic energy density, the theory of proper elastic states and energy orthogonal stress states developed by J. RYCHLEWSKI [1–3]. Three possible specifications of energy-based yield condition for cubic crystals are considered: the criterion based on the total distortion energy, the criterion based on the energy accumulated in the three proper states pertinent to cubic symmetry and the energy based criterion for cubic symmetry in elastic range and orthotropic symmetry in the limit state. Physical motivation, comparison with available experimental results and possible applications in mechanics of anisotropic solids as well as in nanomechanics are discussed.

1. Introduction

THE AIM OF THE PAPER is to study some particular cases of the RYCHLEWSKI yield condition [2, 3] for anisotropic linear elastic solids with Hooke's law

$$\boldsymbol{\sigma} = \mathbf{S} \cdot \boldsymbol{\varepsilon} \leftrightarrow \sigma_{ij} = S_{ijkl}\varepsilon_{kl}\,, \quad \boldsymbol{\varepsilon} = \mathbf{C} \cdot \boldsymbol{\sigma} \leftrightarrow \varepsilon_{mn} = C_{mnij}\sigma_{ij} \tag{1.1}$$

such that

$$\mathbf{C} \circ \mathbf{S} = \mathbf{S} \circ \mathbf{C} = \mathbf{I}_S \leftrightarrow S_{ijkl}C_{klmn} = \frac{1}{2}\left(\delta_{im}\delta_{jn} + \delta_{in}\delta_{jm}\right) \tag{1.2}$$

and the limit tensor **H** representing elastic range in the Mises yield condition

$$\boldsymbol{\sigma} \cdot \mathbf{H} \cdot \boldsymbol{\sigma} = H_{ijkl}\sigma_{ij}\sigma_{kl} \leq 1, \tag{1.3}$$

under the assumption that different symmetry of elasticity tensors of stiffness **S** and compliance **C** vis-à-vis the limit tensor **H** appears. The elasticity tensor **C** is assumed to have cubic symmetry, while at the limit the state material becomes cubic or tetragonal or in general orthotropic. Three possible formulations of the energy-based yield condition are considered.

In the simplest case, the energy of distortion, which can be separated from the total elastic energy density, is taken as a measure of material effort. This is a direct extension of the approach proposed independently by J. C. MAXWELL [4], M. T. HUBER [5] and H. HENCKY [6] for isotropic solids, which is based on the assumption that only a part of the density of elastic energy – energy of distortion – is responsible for reaching a limit state. In this case, only one critical value of the limit state exists, e.g. yield strength. Such an approach can be applied only for solids of isotropic or cubic symmetry because only in such a case the part of elastic energy related with volumetric change corresponds to proper elastic state and the assumption of material incompressibility is admissible. For other symmetries, a volumetric change does not correspond to proper elastic state and W. BURZYŃSKI condition [7] should be assumed in order to extract the density of elastic energy related with spherical part of stress from the total one. This confines the considerations to the class of solids with volumetric (spherical) isotropy and enables introduction of the simplifying constraint of incompressibility (cf. [8]).

The second case is related with the elastic energy densities corresponding to three proper elastic states, as derived in [9, 10]. In such a case three critical values of limit state (e.g. yield constants) can appear in the limit condition. Under incompressibility assumption the number of critical values reduces to two. The advantage of J. RYCHLEWSKI approach [2, 3] lays in the possibility of consideration of different symmetries of a solid body in the elastic range and in the limit state. This enriches the spectrum of possible applications. Therefore, in the third case, the energy-based yield criterion is derived for the situation when a body is of cubic symmetry in elastic range and becomes orthotropic in the limit state. Physical motivation is presented and possible experimental verification of the proposed energy based criteria is discussed.

2. Physical motivation

The well-known examples of solids with cubic symmetry are metal single crystals of FCC and BCC lattice. Since early investigations of E. SCHMID [11, 12], the assumption that single crystal starts to yield, if the shear stress resolved onto the crystallographically defined slip plane and in the slip direction reached a critical value, is commonly used in plasticity of single crystals and polycrystalline aggregates. Such a criterion, known as the Schmid rule, can be expressed in the case of a single crystal subjected to tensile load P in the form:

$$\frac{P}{A}\cos\varphi\cos\lambda = \tau_{\mathrm{cr}}, \tag{2.1}$$

where φ and λ are, respectively, the inclination angle of the normal to the slip plane $\mathbf{n}$ with respect to the tensile axis and the inclination angle of the slip direction $\mathbf{b}$ with respect to the tensile axis, while τ_{cr} denotes critical value of shear stress once plastic glide starts to operate. In general, for arbitrary Cauchy stress tensor $\boldsymbol{\sigma}$ the criterion reads

$$\mathbf{b}\boldsymbol{\sigma}\mathbf{n} = \tau_{\mathrm{cr}}. \tag{2.2}$$

The experimental investigations reveal a good confirmation of this criterion for HCP and FCC single crystals in situations, when only a single slip system operates. Remarkable deviations have been observed, however, in cases when multiple slip occurs, e.g. for the orientations of tensile axis lying near to the corners of the fundamental triangle of stereographic projection. The plastic yield in BCC single crystals also does not conform to the Schmid criterion. These facts have been already reported in [12, 13]. The studies concerning localization of plastic deformation in single crystals [14, 15] also show that modification of the Schmid condition accounting for other components of stress tensor provides better prediction of localization phenomena. The atomistic study based on molecular dynamics simulations and examining the effect of crystal orientation on the stress-strain relationship of Ni single crystal shows large deviations from the Schmid criterion [16]. The recent investigations of [17, 18] related with atomistic calculations of the behaviour of dislocation core and the so-called non-Schmid effects in the plastic yielding of BCC single crystals led the authors to the yield criterion including non-glide components of stress. Although the mentioned applications of molecular dynamics simulations provide deeper insight into the phenomenon of the onset of plastic glide and the core structure of a dislocation in BCC metals, the criterion accounting for non-glide components bears an empirical character. Therefore, such an approach cannot be generalized for other situations, which might be related with other crystalline structures, e.g.: nanostructures, thin layers or interfaces. In the case of nanocrystals the difference in the interatomic distances, with resulting change of symmetry of the bulk material and strained surface layer becomes essential (cf. e.g. [19]). The strained surface layer is often a site, where a limit state can appear first. Under the limit state, we can understand in such a situation breaking of atomic bonds, which may lead to formation of a point defect or a dislocation. Evaluation of the critical energy of breaking of atomic bonds with application of a quantum-mechanical model of an ideal Cu crystal was presented in [20]. The question arises then, how to formulate the limit criteria for solids exhibiting different symmetry in elastic range and in limit state.

The problem was studied afresh in [21], where a new approach has been proposed. It is based on the fundamental concept of density of elastic energy of distortion accumulated in a strained solid, anticipated in 1856 by J. C. Maxwell in his private letter to W. Thompson [4] and discovered, independently, by M. T. Huber [5]. This pivotal idea, proposed originally for isotropic solids, was further extended for elastic anisotropic solids in the studies of W. BURZYŃSKI [7], W. OLSZAK, W. URBANOWSKI [22], W. OLSZAK, J. OSTROWSKA-MACIEJEWSKA [23] J. OSTROWSKA-MACIEJEWSKA, J. RYCHLEWSKI [9] and J. RYCHLEWSKI [2].

3. Formulation of the problem

The yield conditions are based on the concept of stored elastic energy, the theory of proper elastic states and energy orthogonal stress states developed by J. RYCHLEWSKI [1–3], who proved that the Mises limit criterion bounds the weighted sum of stored elastic energies of uniquely defined, energy orthogonal states of stress

$$\boldsymbol{\sigma} \cdot \mathbf{H} \cdot \boldsymbol{\sigma} = \frac{1}{h_1} \Phi(\boldsymbol{\sigma}_1) + \cdots + \frac{1}{h_p} \Phi(\boldsymbol{\sigma}_p), \qquad p \le 6, \tag{3.1}$$

where $\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \cdots + \boldsymbol{\sigma}_p$ is the unique decomposition of stress tensor $\boldsymbol{\sigma}$ into energy orthogonal states, $\boldsymbol{\sigma}_k \cdot \mathbf{C} \cdot \boldsymbol{\sigma}_l = 0$ for $k \ne l$, and $h_1, \ldots, h_p$ are the pertinent energy limits of elasticity, which we called in [20] the Rychlewski moduli.

If the compliance tensor $\mathbf{C}$ possesses cubic symmetry, three elastic proper states exist. The spectral decomposition of the compliance tensor for cubic symmetry has the form [9, 10]:

$$\mathbf{C} = \frac{1}{\lambda_{\mathrm{I}}} \mathbf{P}_{\mathrm{I}} + \frac{1}{\lambda_{\mathrm{II}}} \mathbf{P}_{\mathrm{II}} + \frac{1}{\lambda_{\mathrm{III}}} \mathbf{P}_{\mathrm{III}}, \tag{3.2}$$

where the projectors $\mathbf{P}_K$, $K = \mathrm{I}$, II, III are given by

$$\begin{aligned} \mathbf{P}_{\mathrm{I}} &= \frac{1}{3} \mathbf{1} \otimes \mathbf{1}, \\ \mathbf{P}_{\mathrm{II}} &= \left(\mathbf{K} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \right), \\ \mathbf{P}_{\mathrm{III}} &= (\mathbf{I}_S - \mathbf{K}) \end{aligned} \tag{3.3}$$

and λ_{I}, λ_{II} and λ_{III} are the Kelvin moduli, which can be expressed by elasticity constants representing the components of stiffness tensor (cf. [24], where the opposite notation for the tensors of compliance – $\mathbf{S}$ and stiffness – $\mathbf{C}$ in comparison with our work was assumed):

$$\begin{aligned} \lambda_{\mathrm{I}} &= \lambda_1 = S_{1111} + 2S_{1122}, \\ \lambda_{\mathrm{II}} &= \lambda_2 = \lambda_3 = \lambda_4 = S_{1111} - S_{1122}, \\ \lambda_{\mathrm{III}} &= \lambda_5 = \lambda_6 = 2S_{2323}, \end{aligned} \tag{3.4}$$

whereas the fourth-order tensor $\mathbf{K}$ is defined by unit vectors lying along the edges of the elementary cube $(\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$

$$\mathbf{K} = \mathbf{m}_1 \otimes \mathbf{m}_1 \otimes \mathbf{m}_1 \otimes \mathbf{m}_1 + \mathbf{m}_2 \otimes \mathbf{m}_2 \otimes \mathbf{m}_2 \otimes \mathbf{m}_2 + \mathbf{m}_3 \otimes \mathbf{m}_3 \otimes \mathbf{m}_3 \otimes \mathbf{m}_3. \tag{3.5}$$

The stored elastic energy for unit volume is composed in such a case of three parts [9, 10]

$$\begin{aligned} \Phi(\boldsymbol{\sigma}) &= \frac{1}{2}\boldsymbol{\sigma} \cdot \mathbf{C} \cdot \boldsymbol{\sigma} = \Phi_v^{\mathrm{I}}(\boldsymbol{\sigma}) + \Phi_f^{\mathrm{II}}(\boldsymbol{\sigma}) + \Phi_f^{\mathrm{III}}(\boldsymbol{\sigma}) \\ &= \frac{1}{6}\frac{1}{\lambda_{\mathrm{I}}}(\mathrm{tr}\boldsymbol{\sigma})^2 + \frac{1}{2\lambda_{\mathrm{II}}}\left[\boldsymbol{\sigma} \cdot \mathbf{K} \cdot \boldsymbol{\sigma} - \frac{1}{3}(\mathrm{tr}\boldsymbol{\sigma})^2\right] + \frac{1}{2\lambda_{\mathrm{III}}}\left(\mathrm{tr}\boldsymbol{\sigma}^2 - \boldsymbol{\sigma} \cdot \mathbf{K} \cdot \boldsymbol{\sigma}\right), \end{aligned} \tag{3.6}$$

the energy of hydrostatic states $\Phi_v^{\mathrm{I}}(\boldsymbol{\sigma})$ and the energy of distortion $\Phi_f(\boldsymbol{\sigma}) = \Phi_f^{\mathrm{II}}(\boldsymbol{\sigma}) + \Phi_f^{\mathrm{III}}(\boldsymbol{\sigma})$ related with two deviatoric states, respectively.

4. Criterion based on the energy of distortion

In the first approach, the energy of distortion $\Phi_f(\boldsymbol{\sigma})$ that can be separated from the total elastic energy density is taken as a measure of material effort:

$$\begin{aligned} \Phi_f(\boldsymbol{\sigma}) &= \Phi_f^{\mathrm{II}}(\boldsymbol{\sigma}) + \Phi_f^{\mathrm{III}}(\boldsymbol{\sigma}) \\ &= \frac{(\mathbf{m}_1\boldsymbol{\sigma}\mathbf{m}_1)^2 + (\mathbf{m}_2\boldsymbol{\sigma}\mathbf{m}_2)^2 + (\mathbf{m}_3\boldsymbol{\sigma}\mathbf{m}_3)^2 - \frac{1}{3}(\mathrm{tr}\boldsymbol{\sigma})^2}{2\lambda_{\mathrm{II}}} \\ &\quad + \frac{\boldsymbol{\sigma} \cdot \boldsymbol{\sigma} - (\mathbf{m}_1\boldsymbol{\sigma}\mathbf{m}_1)^2 + (\mathbf{m}_2\boldsymbol{\sigma}\mathbf{m}_2)^2 + (\mathbf{m}_3\boldsymbol{\sigma}\mathbf{m}_3)^2}{2\lambda_{\mathrm{III}}}. \end{aligned} \tag{4.1}$$

The criterion of energy of distortion for solids of cubic symmetry, in particular for crystals of cubic lattice, can be stated as follows [21]:

The yield condition is satisfied, if the density of energy of distortion accumulated in a body of cubic symmetry attains certain critical value Φ_{cr}

$$\Phi_f(\boldsymbol{\sigma}) = \Phi_{\mathrm{cr}}. \tag{4.2}$$

The critical value of energy of distortion can be determined experimentally in a tensile test of a single crystal along the direction of unit vector $\mathbf{n} = l\mathbf{m}_1 + m\mathbf{m}_2 + n\mathbf{m}_3$ with stress $\boldsymbol{\sigma} = \sigma_n \mathbf{n} \otimes \mathbf{n}$. The energy of distortion takes in such a case the form [10]:

$$(4.3)\qquad \Phi_f(\sigma_n, \mathbf{n}) = \frac{1}{2\lambda_{II}}\sigma_n^2\left(l^4+m^4+n^4-\frac{1}{3}\right)+\frac{1}{2\lambda_{III}}\sigma_n^2\left(1-\left(l^4+m^4+n^4\right)\right)$$
$$= \sigma_n^2\left[\left(\frac{1}{2\lambda_{II}}-\frac{1}{2\lambda_{III}}\right)\left(l^4+m^4+n^4\right)+\frac{1}{2\lambda_{III}}-\frac{1}{6\lambda_{II}}\right].$$

Let us observe that there are two initial orientations of the crystal subjected to tension, for which the formula (4.3) obtains a particularly simple form [21]:

- Initial orientation chosen for one of the edges of elementary cube, i.e. [100], [010] or [001].
- Initial orientation taken along the normal to the octahedral plane [111].

For the orientations [100], [010] or [001] we have, respectively, $l=1$, $m=n=0$, $m=1$, $l=n=0$, or $n=1$, $l=m=0$ and the energy of distortion can be expressed by means of tensile stress along one of the cube edges:

$$(4.4)\qquad \Phi_f^{II}\left(\sigma_{[100]}\right)=\frac{1}{3}\frac{1}{\lambda_{II}}\sigma_{[100]}^2=\frac{1}{3}\frac{1}{\lambda_{II}}\sigma_{[010]}^2=\frac{1}{3}\frac{1}{\lambda_{II}}\sigma_{[001]}^2,\qquad \Phi_{cr}=\frac{1}{3}\frac{1}{\lambda_{II}}Y_2^2,$$

while

$$(4.5)\qquad \Phi_f^{III}\left(\sigma_{[100]}\right)=\Phi_f^{III}\left(\sigma_{[010]}\right)=\Phi_f^{III}\left(\sigma_{[001]}\right)=0.$$

On the other hand, for the initial orientation [111] the distortion energy takes the form

$$(4.6)\qquad \Phi_f^{III}\left(\sigma_{[111]}\right)=\frac{1}{3}\frac{1}{\lambda_{III}}\sigma_{[111]}^2,\qquad \Phi_{cr}=\frac{1}{3}\frac{1}{\lambda_{III}}Y_3^2,$$

while

$$(4.7)\qquad \Phi_f^{II}\left(\sigma_{[111]}\right)=0.$$

It means that in the limit state the ratio of two critical values of tensile stress at yield is determined by Kelvin moduli λ_{II} and λ_{III}

$$(4.8)\qquad \frac{Y_2}{Y_3}=\sqrt{\frac{\lambda_{II}}{\lambda_{III}}}.$$

Then, the tensile tests of a single crystal along one of the edges of elementary cube and along the initial orientation [111] lead to two deviatoric states, which are energy orthogonal. It can be also proved that these directions correspond to the extremal values of Young modulus (cf. [10]). Due to this we can use one of these tests to measure the yield stress and the other one to verify by means of (4.6) the proposed criterion of energy of distortion.

5. Specification of the criterion for cubic crystals for spectral decomposition of the elasticity tensor C

The second case of possible formulations of energy-based yield condition is related with the elastic energy densities corresponding to three proper elastic states (3.3), as derived in [9, 10]. It is the specification of general criterion (3.1) that was obtained originally by J. Rychlewski from the main energy orthogonal decomposition for cubic symmetry. According to [9] it takes form:

$$\frac{\sigma_1^2}{k_1^2} + \frac{\sigma_2^2}{k_2^2} + \frac{\sigma_3^2}{k_3^2} \leq 1, \tag{5.1}$$

where $\sigma_i^2 = \boldsymbol{\sigma}_i \cdot \boldsymbol{\sigma}_i$, $k_i^2 \equiv 2h_i\lambda_i$, $i = 1, 2, 3$ – no summation for i. In such a case three critical values of limit state (e.g. yield constants) can appear in the limit condition. If $k_i \to \infty$, we say that the i-th state is safe for any state of stress. In the theory of plasticity of isotropic metallic solids it is often assumed that the spherical parts of stress tensors are safe. Such an assumption can be also extended to bulk metallic solids of cubic symmetry, since the hydrostatic state is a proper elastic state. Therefore, sometimes a body of cubic symmetry is called, if we abstract from its crystallographic features, a body of cubic isotropy. It should be mentioned however that for other types of symmetry (anisotropy) the hydrostatic state is not a proper elastic state. If we assume for certain reasons, for simplicity or having experimental justification, that the material is pressure insensitive, we confine at the same time our considerations to certain class of bodies with constraints, which are volumetrically isotropic (cf. [2, 8]). It is also worthwhile to observe that the limit condition (5.1) can be obtained also if we assume that the limit tensor **H** possesses the same symmetry as the compliance tensor **C** (they are coaxial, i.e. they have the same proper subspaces but different proper values).

If the hydrostatic state of stress is safe, we have $k_1 \to \infty$ and the quadratic limit condition (5.1) can be expressed only for two deviatoric states

$$\frac{\sigma_2^2}{k_2^2} + \frac{\sigma_3^2}{k_3^2} = \frac{(\mathbf{m}_1\boldsymbol{\sigma}\mathbf{m}_1)^2 + (\mathbf{m}_2\boldsymbol{\sigma}\mathbf{m}_2)^2 + (\mathbf{m}_3\boldsymbol{\sigma}\mathbf{m}_3)^2 - \dfrac{1}{3}(\mathrm{tr}\boldsymbol{\sigma})^2}{k_2^2} + \frac{\boldsymbol{\sigma}\cdot\boldsymbol{\sigma} - \left[(\mathbf{m}_1\boldsymbol{\sigma}\mathbf{m}_1)^2 + (\mathbf{m}_2\boldsymbol{\sigma}\mathbf{m}_2)^2 + (\mathbf{m}_3\boldsymbol{\sigma}\mathbf{m}_3)^2\right]}{k_2^2} \leq 1, \tag{5.2}$$

where $k_2^2 \equiv 2h_2\lambda_{\mathrm{II}}$, $k_3^2 \equiv 2h_3\lambda_{\mathrm{III}}$ are the limit constants, which should be determined experimentally, e.g. in tensile tests. The tensile tests for single FCC crystals with different initial orientations have been proposed in [20] to verify experimentally the new yield criterion. Accordingly, the yield stress in tension along the direction $\mathbf{n} = l\mathbf{m}_1 + m\mathbf{m}_2 + n\mathbf{m}_3$, while the elasticity tensor $\mathbf{C}$ and the limit tensor $\mathbf{H}$ are coaxial for single cubic crystals, was calculated under the assumption that $k_1 \to \infty$

$$Y = \left[-\frac{1}{3k_2^2} + \frac{1}{k_3^2} + \left(\frac{1}{k_2^2} - \frac{1}{k_3^2} \right) \left(l^4 + m^4 + n^4 \right) \right]^{-1/2}. \tag{5.3}$$

Two limit constants k_2 and k_3 can be determined in the independent tensile tests for a single crystal with initial orientation chosen along one of the edges of elementary cube [100], [010] or [001], what gives $\sigma_{[100]} = \sigma_{[010]} = \sigma_{[001]} = Y_2 = \sqrt{\frac{3}{2}} k_2$, and along the direction $\mathbf{n} = \frac{1}{\sqrt{3}}[111]$, what leads to $\sigma_{[111]} = Y_3 = \sqrt{\frac{3}{2}} k_3$.

6. Specification of the Rychlewski approach for materials of cubic elasticity and orthotropic limit state

In the foregoing discussion there was not necessary to specify the limit tensor $\mathbf{H}$. The limit conditions were derived on the basis of the elasticity tensor $\mathbf{S}$ and compliance tensor $\mathbf{C}$. If we assume that $\mathbf{H}$ is coaxial with $\mathbf{C}$, then the criterion of the form (5.1) can be also obtained

$$\frac{\Phi(\boldsymbol{\sigma}_1)}{h_1} + \frac{\Phi(\boldsymbol{\sigma}_2)}{h_2} + \frac{\Phi(\boldsymbol{\sigma}_3)}{h_3} \leq 1, \tag{6.1}$$

where the Rychlewski moduli $h_i = \Phi_{\mathrm{cr}}(\boldsymbol{\sigma}_i)$, $i = 1, 2, 3$ correspond to critical energy of pertinent proper state.

In the general approach of J. RYCHLEWSKI [2] tensors $\mathbf{C}$ and $\mathbf{H}$ are not interrelated and can possess arbitrary symmetry. In the third case of energy-based limit condition, cubic symmetry of elasticity tensor $\mathbf{C}$ and orthotropy of limit tensor $\mathbf{H}$ is studied. As an example, we can consider a single crystal with the lattice of cubic symmetry in a natural state. According to the Cauchy–Born hypothesis, which says that the lattice vectors deform like "material filaments", an extension along one of the edges of the cell with cubic lattice transforms it into the cell of tetragonal lattice. Such a situation appears also if we consider nanocrystals, where the difference in the interatomic distances in bulk material and strained surface layer results in the change of symmetry from cubic to tetragonal. Similar situation appears in the case of heterostructures composed of layers of cubic symmetry and strained interface of tetragonal symmetry. Therefore, in the elastic regime the bulk material remains cubic and the limit state can appear first in the surface layer or interface, which is of tetragonal symmetry. This is a special case of an orthotropic limit state. In further considerations, we assume that the symmetry axes of the material in elastic range and limit state coincide.

As it was observed in [25], for orthotropy the spherical tensor is not a proper elastic state. However, for the additional constraints $\mathbf{H} \cdot \mathbf{1} = \mathbf{0}$, it becomes the proper state with the eigenvalue equal 0. Such an assumption is often made in order to eliminate the influence of spherical part of stress on plastic yield. In such a case, it can be shown that spectral decomposition of the limit tensor $\mathbf{H}$ takes the form [26]:

$$\mathbf{H} = \frac{1}{K_1}\mathbf{\Gamma}_1 + \ldots + \frac{1}{K_6}\mathbf{\Gamma}_6, \tag{6.2}$$

where $\mathbf{\Gamma}_1, \ldots, \mathbf{\Gamma}_6$, are the orthogonal projectors for $\mathbf{H}$. The orthogonal projectors $\mathbf{\Gamma}_i$ are defined by proper states χ_i corresponding to the different eigenvalues K_i of the limit tensor $\mathbf{H}$ that is:

$$\mathbf{\Gamma}_1 = \chi_1 \otimes \chi_1, \quad \cdots, \quad \mathbf{\Gamma}_6 = \chi_6 \otimes \chi_6. \tag{6.3}$$

Proper states χ_i of the tensor $\mathbf{H}$ can be expressed as follows

$$\begin{aligned}
\chi_1 &= \frac{1}{\sqrt{3}}\mathbf{I},\\
\chi_2 &= \cos\psi \mathbf{a}_{\mathrm{II}} + \sin\psi \mathbf{a}_{\mathrm{III}},\\
\chi_3 &= -\sin\psi \mathbf{a}_{\mathrm{II}} + \cos\psi \mathbf{a}_{\mathrm{III}},\\
\chi_4 &= \frac{1}{\sqrt{2}}\left(\mathbf{m}_2 \otimes \chi_3 + \mathbf{m}_3 \otimes \mathbf{m}_2\right),\\
\chi_5 &= \frac{1}{\sqrt{2}}\left(\mathbf{m}_1 \otimes \chi_3 + \mathbf{m}_3 \otimes \mathbf{m}_1\right),\\
\chi_6 &= \frac{1}{\sqrt{2}},
\end{aligned} \tag{6.4}$$

where $(\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3)$ denote the unit vectors lying along the edges of the elementary cube, whereas the tensors $\mathbf{a}_{\mathrm{II}}$ and $\mathbf{a}_{\mathrm{III}}$ are defined by the formulae

$$\begin{aligned}
\mathbf{a}_{\mathrm{II}} &= \frac{1}{\sqrt{2}}\left(\mathbf{m}_1 \otimes \mathbf{m}_1 - \mathbf{m}_2 \otimes \mathbf{m}_2\right),\\
\mathbf{a}_{\mathrm{III}} &= \frac{1}{\sqrt{6}}\left(\mathbf{m}_1 \otimes \mathbf{m}_1 + \mathbf{m}_2 \otimes \mathbf{m}_2 - 2\mathbf{m}_3 \otimes \mathbf{m}_3\right)
\end{aligned} \tag{6.5}$$

and ψ is the strength distributor that depends on the components of the limit tensor $\mathbf{H}$.

From (3.3) and (6.3) it follows that

$$\mathbf{\Gamma}_1 = \mathbf{P}_{\mathrm{I}}, \qquad \mathbf{\Gamma}_2 + \mathbf{\Gamma}_3 = \mathbf{P}_{\mathrm{II}}, \qquad \mathbf{\Gamma}_4 + \mathbf{\Gamma}_5 + \mathbf{\Gamma}_6 = \mathbf{P}_{\mathrm{III}}, \tag{6.6}$$

what results from (3. 2) in

$$\mathbf{C} = \frac{1}{\lambda_{\mathrm{I}}}\mathbf{\Gamma}_1 + \frac{1}{\lambda_{\mathrm{II}}}(\mathbf{\Gamma}_2 + \mathbf{\Gamma}_3) + \frac{1}{\lambda_{\mathrm{III}}}(\mathbf{\Gamma}_4 + \mathbf{\Gamma}_5 + \mathbf{\Gamma}_6). \tag{6.7}$$

By comparing (6.2) with (6.7) one comes to the conclusion that, in the considered case, the limit tensor **H** is *partially coaxial* with the compliance tensor **C**, that is *all the proper states of* **H** *are the proper states of* **C** (but not opposite). It means that the symmetry group of **H** is contained in the symmetry group of **C**.

Let us formulate the Mises-type condition (1.3) for the assumed tensor **H** given by (6.2) in the energy-based form (3.1). In order to obtain this form, according to [2], the following eigenvalue problem is to be solved

$$\left(\mathbf{H} - \frac{1}{2h}\mathbf{C}\right) \cdot \boldsymbol{\kappa} = \mathbf{0}. \tag{6.8}$$

Substituting (6.2) and (6.7) into the above formula it is found that

$$\det\left(\mathbf{H} - \frac{1}{2h}\mathbf{C}\right) = 0$$
$$\Updownarrow$$
$$h_1 = \frac{K_1}{2\lambda_{\mathrm{I}}} \to \infty, \quad h_2 = \frac{K_2}{2\lambda_{\mathrm{II}}}, \quad h_3 = \frac{K_3}{2\lambda_{\mathrm{II}}},$$
$$h_4 = \frac{K_4}{2\lambda_{\mathrm{III}}}, \quad h_5 = \frac{K_5}{2\lambda_{\mathrm{III}}}, \quad h_6 = \frac{K_6}{2\lambda_{\mathrm{III}}} \tag{6.9}$$

and $\boldsymbol{\kappa}_i = \boldsymbol{\chi}_i$ (i = 1,...,6) given in (6. 4), so in this case the energy proper states $\boldsymbol{\kappa}_i$ are equal to the proper states of the tensor **H**. The energy orthogonal stresses $\boldsymbol{\sigma}_i$ are then calculated as

$$\boldsymbol{\sigma}_i = \mathbf{\Gamma}_i \cdot \boldsymbol{\sigma} \qquad \text{and} \qquad \boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 + \ldots + \boldsymbol{\sigma}_6. \tag{6.10}$$

Graphical illustration of the above stress state decomposition for the analysed case of material symmetry is presented in Fig. 1, where the following notation is used:

$$r = \frac{1}{3}(\sigma_{11} + \sigma_{22} + \sigma_{33}),$$
$$s = \frac{1}{2(3+\gamma^2)}[\sigma_{11} + \sigma_{22} - 2\sigma_{33} - \gamma(\sigma_{11} - \sigma_{22})],$$
$$u = \frac{1}{2(3+\gamma^2)}[3(\sigma_{11} - \sigma_{22}) + \gamma(\sigma_{11} + \sigma_{22} - 2\sigma_{33})], \tag{6.11}$$
$$p = \sigma_{13}, \qquad q = \sigma_{23}, \qquad v = \sigma_{12}, \qquad \gamma = -\sqrt{3}\cot\psi.$$

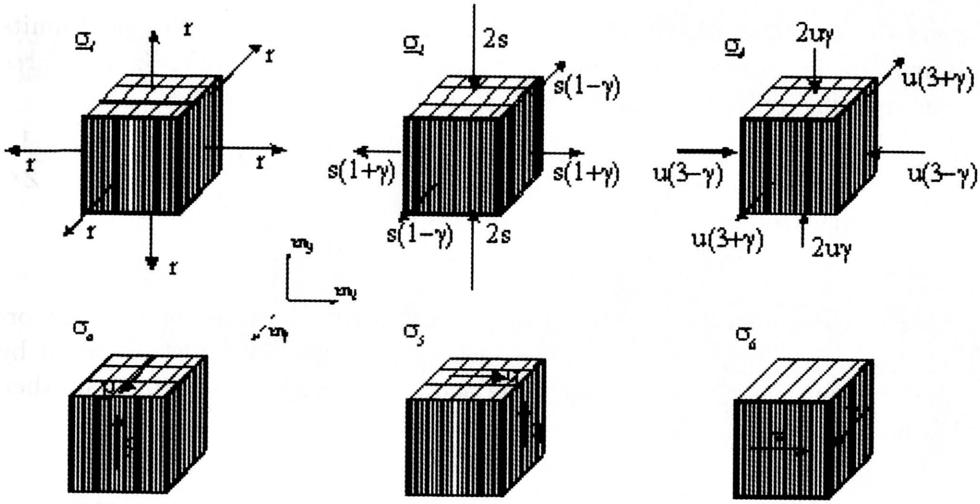

FIG. 1. The energy-orthogonal decomposition of the stress state for the material that has cubic symmetry in the elastic range and becomes orthotropic in the limit state.

Energy-based formulation of the limit criterion for the considered case is therefore due to (3.1) and (6.9) as follows:

$$\boldsymbol{\sigma}\cdot\mathbf{H}\cdot\boldsymbol{\sigma}=\frac{2\lambda_{\mathrm{II}}}{K_2}\Phi(\boldsymbol{\sigma}_2)+\frac{2\lambda_{\mathrm{II}}}{K_3}\Phi(\boldsymbol{\sigma}_3)+\frac{2\lambda_{\mathrm{III}}}{K_4}\Phi(\boldsymbol{\sigma}_4)+\frac{2\lambda_{\mathrm{III}}}{K_5}\Phi(\boldsymbol{\sigma}_5)+\frac{2\lambda_{\mathrm{III}}}{K_6}\Phi(\boldsymbol{\sigma}_6)=1. \tag{6.12}$$

It should be noted that from (3.6), (4.1) and (6.12) it transpires that

$$\Phi_f^{\mathrm{II}}=\Phi(\boldsymbol{\sigma}_2)+\Phi(\boldsymbol{\sigma}_3)\qquad\text{and}\qquad\Phi_f^{\mathrm{III}}=\Phi(\boldsymbol{\sigma}_4)+\Phi(\boldsymbol{\sigma}_5)+\Phi(\boldsymbol{\sigma}_6). \tag{6.13}$$

7. An energy interpretation of the Hill yield condition for orthotropic solids

The equation (6. 9) enables an energy-based interpretation of the Hill yield condition for plastically incompressible orthotropic solids that exhibit cubic symmetry in the elastic regime. The Hill yield condition for the orthotropic solids is given by the formula [27]:

$$F(\sigma_{22}-\sigma_{33})^2+G(\sigma_{33}-\sigma_{11})^2+H(\sigma_{11}-\sigma_{22})^2+2N\sigma_{12}^2+2M\sigma_{13}^2+2L\sigma_{23}^2=1, \tag{7.1}$$

where the constants F, G, H, N, M, L can be expressed by the yield limits obtained in three tensile tests along the orthotropy axes, X, Y, Z and three shear tests in the planes of orthotropy R, S, T:

$$(7.2)\qquad \begin{gathered} 2F = \frac{1}{Y^2} + \frac{1}{Z^2} - \frac{1}{X^2}, \quad 2G = \frac{1}{Z^2} + \frac{1}{X^2} - \frac{1}{Y^2}, \quad 2H = \frac{1}{X^2} + \frac{1}{Y^2} - \frac{1}{Z^2}, \\ 2L = \frac{1}{R^2}, \quad 2M = \frac{1}{S^2}, \quad 2N = \frac{1}{T^2}. \end{gathered}$$

Stress components σ_{ij} are the components of the stress tensor $\boldsymbol{\sigma}$ in the orthotropy axes. This equation can be rewritten in the form (1.3) proposed by Mises. Eigenvalues of the limit tensor $\mathbf{H}$ and the strength distributor ψ are then obtained as [26]:

$$(7.3)\qquad \begin{gathered} K_2 = \frac{1}{F+G+H+\frac{1}{2}\sqrt{\Delta_H}}, \qquad K_3 = \frac{1}{F+G+H-\frac{1}{2}\sqrt{\Delta_H}}, \\ K_4 = \frac{1}{L}, \qquad K_5 = \frac{1}{M}, \qquad K_6 = \frac{1}{N}, \\ \tan\psi = \frac{F+G-2H-\sqrt{\Delta_H}}{\sqrt{3}\,(F-G)}, \\ \Delta_H = 2\left[(H-F)^2 + (H-G)^2 + (F-G)^2\right] \geq 0. \end{gathered}$$

Equivalently, due to (7.2) and (7.3) we have

$$(7.4)\qquad \begin{aligned} \frac{1}{K_2} &= \frac{1}{2}\left(\frac{1}{X^2} + \frac{1}{Y^2} + \frac{1}{Z^2}\right) \\ &\quad + \frac{1}{2}\left[\left(\frac{1}{X^2} - \frac{1}{Z^2}\right)^2 + \left(\frac{1}{Y^2} - \frac{1}{Z^2}\right)^2 + \left(\frac{1}{Y^2} - \frac{1}{X^2}\right)^2\right]^{1/2}, \\ \frac{1}{K_3} &= \frac{1}{2}\left(\frac{1}{X^2} + \frac{1}{Y^2} + \frac{1}{Z^2}\right) \\ &\quad - \frac{1}{2}\left[\left(\frac{1}{X^2} - \frac{1}{Z^2}\right)^2 + \left(\frac{1}{Y^2} - \frac{1}{Z^2}\right)^2 + \left(\frac{1}{Y^2} - \frac{1}{X^2}\right)^2\right]^{1/2}, \\ K_4 &= 2R^2, \qquad K_5 = 2S^2, \qquad K_6 = 2T^2, \end{aligned}$$

(7.4)
[cont.]

$$\tan\psi = \frac{-\left[2\left[\left(\frac{1}{X^2}-\frac{1}{Z^2}\right)^2+\left(\frac{1}{Y^2}-\frac{1}{Z^2}\right)^2+\left(\frac{1}{Y^2}-\frac{1}{X^2}\right)^2\right]\right]^{1/2}}{\sqrt{3}\left(\frac{1}{Y^2}-\frac{1}{X^2}\right)} - \frac{\frac{1}{Y^2}-\frac{1}{X^2}+\frac{2}{Z^2}}{\sqrt{3}\left(\frac{1}{Y^2}-\frac{1}{X^2}\right)}.$$

The particular case of orthotropy with the additional symmetry of rotations of the angle $\pi/2$ about the axis parallel to $\mathbf{m}_3$ was considered. The results are applied for the analysis of a single cubic crystal which, due to the finite extension along the one of cubic directions, changes symmetry and becomes tetragonal. In such a case we have $F = G$ and $L = M$, or equivalently $X = Y$ and $R = S$, therefore

$$\psi = \frac{\pi}{2}, \quad K_2 = \frac{1}{F+2H}, \quad K_3 = \frac{1}{3F}, \quad K_4 = \frac{1}{L}, \quad K_5 = \frac{1}{N}, \tag{7.5}$$

$$\begin{aligned} \frac{1}{K_2} &= \frac{2+\sqrt{2}}{2}\frac{1}{X^2} + \frac{1-\sqrt{2}}{2}\frac{1}{Z^2}, \\ \frac{1}{K_3} &= \frac{2-\sqrt{2}}{2}\frac{1}{X^2} + \frac{1+\sqrt{2}}{2}\frac{1}{Z^2}, \\ K_4 &= K_5 = 2S^2, \qquad K_6 = 2T^2. \end{aligned} \tag{7.6}$$

Still tensor $\mathbf{H}$ is partially coaxial with the tensor $\mathbf{C}$, but in this case we have only five uniquely defined energy-orthogonal projectors $\mathbf{\Gamma}'_i$.

$$\mathbf{\Gamma}'_i = \mathbf{\Gamma}_i \quad \text{for} \quad \mathrm{i} = 1, ..., 3 \quad \text{and} \quad \mathbf{\Gamma}'_4 = \mathbf{\Gamma}_4 + \mathbf{\Gamma}_5, \quad \mathbf{\Gamma}'_5 = \mathbf{\Gamma}_6. \tag{7.7}$$

The form of energy-orthogonal decomposition (6.10) of the stress state σ for this special case of material symmetry (tetragonal) is shown in Fig. 2. The following notation is used (see (6.11)) for $\gamma = 0$:

$$\begin{gathered} r = \frac{1}{3}(\sigma_{11}+\sigma_{22}+\sigma_{33}), \quad s = \frac{1}{6}(\sigma_{11}+\sigma_{22}-2\sigma_{33}), \quad u = \frac{1}{2}(\sigma_{11}-\sigma_{22}), \\ p = \sigma_{13}, \qquad q = \sigma_{23}, \qquad v = \sigma_{12}. \end{gathered} \tag{7.8}$$

According to (6.2) and (7.6), the limit condition for the material of cubic symmetry in elastic range and tetragonal in limit state can be expressed as follows:

$$\lambda_{II}\frac{(2+\sqrt{2})Z^2+(1-\sqrt{2})X^2}{X^2Z^2}\Phi(\sigma_2) + \lambda_{II}\frac{(2-\sqrt{2})Z^2+(1+\sqrt{2})X^2}{X^2Z^2}\Phi(\sigma_3) + \frac{\lambda_{III}}{S^2}\Phi(\sigma_4) + \frac{\lambda_{III}}{T^2}\Phi(\sigma_5)=1, \tag{7.9}$$

where, besides the Kelvin elastic moduli λ_{II} and λ_{III}, four limit values are to be determined; in two tensile tests along the edges of the tetragonal unit cell and two shear tests changing the right angles between the edges.

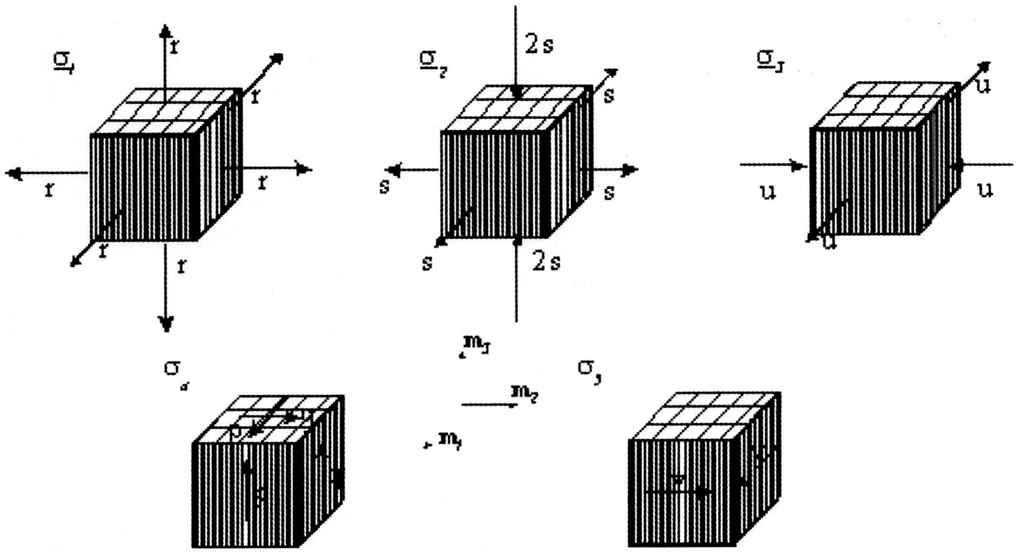

FIG. 2. Energy-orthogonal decomposition of the stress state for the material that has cubic symmetry in the elastic state and becomes tetragonal in the limit state.

8. Discussion of possible experimental verification and conclusions

From the geometry of slip in a FCC single crystal which is subjected to tension in the direction [100], it appears that eight potential slip systems can operate. In such a case we have

$$\sigma_{[100]} = Y_2 = \sqrt{6}\tau_{\mathrm{cr}}. \tag{8.1}$$

Similar relation holds for tension in the direction [110] corresponding to activation of four potential slip systems, $\sigma_{[110]} = \sqrt{6}\tau_{\mathrm{cr}}$. In the case of tension in the [111] direction, six potential slip systems exist and the critical stress at yield reads

$$\sigma_{[111]} = Y_3 = \frac{3\sqrt{6}}{2}\tau_{cr}. \tag{8.2}$$

Comparison of the discussed energy-based limit conditions on the example of Cu single crystal leads to the following relations:

- Schmid criterion – $\dfrac{Y_2}{Y_3} = \dfrac{2}{3} \cong 0.67\,, \quad \tau_{cr} = \text{const}.$
- Hypothesis of elastic energy of distortion – $\dfrac{Y_2}{Y_3} = 0.56.$
- Energy-based quadratic condition – $\dfrac{Y_2}{Y_3} = \dfrac{k_2}{k_3}.$

These relations should be verified experimentally. The results of J. DIEHL [28] can be applied to make at least an approximate assessment of the ratio Y_2/Y_3 for Cu single crystals. In [28] (Fig. 12, p. 335) the values of critical resolved shear stress τ_{cr} for different initial orientations of single crystals subjected to tension were given. We calculated the average values of τ_{cr} taken from the neighborhoods of the orientations corresponding to the corners of fundamental triangle of stereographic projection: $(\tau_{cr})^{[001]}_{aver} = 106.67$ [g/mm^2] for [001], $(\tau_{cr})^{[111]}_{aver} = 127.20$ [g/mm^2] for [111] and $(\tau_{cr})^{[110]}_{aver} = 110.25$ [g/mm^2] for [110]. The resulting values of tensile yield strengths are: $Y_2 = \sqrt{6}\,(\tau_{cr})^{[001]}_{aver} = 261.29$ [g/mm^2], $Y_3 = \dfrac{3\sqrt{6}}{2}\,(\tau_{cr})^{[111]}_{aver} = 467.36$ [g/mm^2] and $\sigma_{[110]} = \sqrt{6}\,(\tau_{cr})^{[110]}_{aver} = 270.06$ [g/mm^2], respectively. It is visible that the resulting ratio $Y_2/Y_3 = 0.56$ is close to the value obtained from the hypothesis of elastic energy of distortion. The equality within two digits of accuracy is rather coincidental because the assessment of experimental data is very rough. Nevertheless, rather large discrepancy with the prediction of the ratio $Y_2/Y_3 \cong 0.67$ calculated according to the Schmid criterion should be noted. The test for the direction [110] does not provide so good confirmation. We can observe that due to (4.3) and (4.4), with an account of Kelvin moduli for Cu single crystals $\lambda_{II} = 47\,[\text{GPa}]\,,\ \lambda_{III} = 150\,[\text{GPa}]$, the theoretical prediction of the ratio $Y_2/\sigma_{[110]} = 1.39$ and the discussed above experimental data provide $Y_2/\sigma_{[110]} = 0.97$. The program of systematic experimental tests is necessary to verify the proposed criteria. The main difficulty lies in accuracy of measurement of yield limit for single crystals.

The proposed energy-based criteria can be applied in mechanics of anisotropic solids, e.g. formulation of yield criteria for metals subjected to shaping operations as well as for polymers and composites. For example, it could provide deeper insight into the description of elastic and plastic anisotropy in sheet metals presented in [29]. The application of spectral decomposition of elasticity tensor and energy orthogonal stress states proposed by J. Rychlewski for transversely isotropic material, representing fiber reinforced composites, was studied in [30]. Also in the field of nanomechanics the proposed approach can appear helpful filling the gap between the atomistic calculations and continuum mechanics modelling of the behaviour of different kinds of crystalline nanostructures. In such a case the pertinent limit values of elastic energy should be determined from the first principles with use of quantum mechanical theory of the strength of atomic bonds.

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