Arch. Mech., **63**, 3, pp. 287–310, Warszawa 2011

Selective symmetrization of the slip-system interaction matrix in crystal plasticity

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The symmetry issue of the interaction matrix between multiple slip-systems in the theory of crystal plasticity at finite deformation is revisited. By appealing to possibly non-uniform distribution of slip-system activity in a representative space-time element of a crystal, symmetry of the slip-system interaction matrix for the representative element is derived under assumptions that have a physical meaning. This conclusion refers to active slip-systems only. Accordingly, for any given hardening law, a new symmetrization rule is proposed that is restricted to active slip-systems and leaves the latent hardening of inactive slip-systems unchanged. Advantages of the proposal in comparison with full symmetrization are illustrated by a simple example of uniaxial tension.

Key words: finite deformation; metal crystal; plasticity; hardening; symmetry.

1. Introduction

The constitutive framework for a metal crystal undergoing plastic deformation by shearing on multiple crystallographic slip-systems is a classical topic. A rigorous finite-deformation theory of plastically deforming crystals has been established by R. Hill and J. R. Rice [1–3], and subsequently applied and extended by many authors. Comprehensive reviews are available, cf. [4–8]. An overview of recent extensions to strain-gradient and size effects – which are not addressed here – can be found in [8, 9].

In any version of the crystal plasticity theory, an adequate description of slip-system interactive hardening plays a central role. It affects strongly the stress-strain characteristics and represents a long-standing and vital problem. There exists a vast literature on experimental investigations of hardening of metal single crystals, cf. the surveys in [5, 6, 10] and the references therein.

The manner of incorporating experimental observations into the theoretical description represents itself a problem. We address here the question of possible dependence of the instantaneous slip-system hardening moduli matrix on the current set of active slip-systems. We do it in the framework of the classical finite-deformation theory of single crystal plasticity, intentionally disregarding other effects (like non-Schmid or strain-gradient effects). In particular, the issue of symmetrization of the slip-system interaction matrix, (g_{KL}), is revisited. Components of this matrix specify the relationship, at a given strain-rate, between a shear-rate on the L-th slip-system and a rate of the K-th yield function. The latter one is defined as the difference between the actual (τ_K) and critical $(\tau_K^{\rm cr})$ values of the generalized, resolved shear stress on the K-th system. Frequently, a symmetric matrix of physical hardening moduli is assumed in the evolution equation for $\tau_K^{\rm cr}$. Then, the geometric effect of rotation of the material with respect to the crystallographic lattice on the rate of τ_K renders the matrix (g_{KL}) non-symmetric in general, cf. [4].

There are specific advantages of having the matrix (g_{KL}) symmetric as it leads to a variational structure of the incremental problem, cf. [11, 6, 12]. Recognizing such advantages, attempts were made in the past to symmetrize the matrix (g_{KL}) in advance by adjusting the hardening matrix appropriately [13, 4]. That procedure requires latent hardening of inactive slip-systems to be affected by terms proportional to the actual stress. Such extra terms have not found a common acceptance in the literature. For instance, in the last years the symmetrization of the slip-system interaction matrix was addressed only occasionally, e.g. in [14].

The considerations in this paper may lead to re-assessment of the postulate of symmetry of the slip-system interaction matrix in a representative space-time element of a crystal. The lack of symmetry of the interaction matrix (g_{KL}) mentioned above is a consequence of geometric interaction between the slip-systems at a material point and at a time instant as assumed in earlier papers. In that treatment, active slip-systems are identified with simultaneous and spatially uniform plastic shearing in a homogeneous and uniformly deforming crystal. However, slip-system activity represents a macroscopic idealization of the real effect of motion of a large number of individual dislocations, the motion that is strongly non-uniform both in space and time. Therefore, what is called an instantaneous slip at a material point, must be understood in an averaged sense adopted for a certain representative element of a crystal, representative both in space and time. The assumption of uniform activity of slip-systems within such a four-dimensional representative element, from which the conclusion about non-symmetry of the interaction matrix is drawn, may be an oversimplification. This may be especially true if a constitutive law for that element is to be used for a grain in a mean-field homogenization schemes for a polycrystal. If this uniformity assumption is abandoned then geometric interactions between slip-systems, and thus the conclusion about non-symmetry of the effective matrix of their interaction in the representative element, are to be revisited, which is done in this paper.

Such considerations lead to a novel and milder version of symmetrization of the slip-system interaction matrix (g_{KL}), namely, restricted to its subset that corresponds to *active slip-systems only.* In Sec. 3, such symmetry is studied with special reference to the incremental behaviour of a crystal with non-uniform distribution of slip-system activity, within a representative volume element or a representative time interval. In Sec. 4, a new selective symmetrization rule is proposed that is restricted to active slip-systems and therefore does not affect latent hardening of inactive slip-systems. Essential differences between consequences of applying the previous full symmetrization of matrix (g_{KL}) and the proposed selective symmetrization are illustrated in Sec. 5 by an example of simulation of a uniaxial tension test.

2. Constitutive framework

We apply the classical rate-independent theory of elastic-plastic crystals at finite deformation developed in [1–3]. The formulation of the theory as given later in [4, 5] is commonly known, therefore only a brief account is given below. We begin with quoting in Subsec. 2.1 and 2.2 some basic relationships of the finite-strain crystal plasticity from the papers cited above. The relationships provided in a transformed form in Subsec. 2.3 are found to be more convenient for discussing the symmetry issue of slip-system interactions. The essence of a novel proposal is in formula (2.19) specified further in Sec. 4.

The following notation is used. Bold-face letters denote vectors (in $\mathbf{R}^3$) or second-order tensors, and doublestruck capitals like $\mathbb{L}$ stand for fourth-order tensors. Direct juxtaposition of two tensors denotes simple contraction, a central dot means double contraction, and the symbol $\otimes$ denotes a tensor product. A superimposed -1, T or $-$T over a tensor symbol denotes an inverse, transpose or transposed inverse, respectively. Occasionally, components on a fixed orthonormal basis are used which are denoted by lower case Latin subscripts with the summation convention adopted for repeated subscripts (e.g., $\mathbf{A}\cdot\mathbf{B} = A_{ij}B_{ij}$). No implicit summation is used for repeated *upper* case Latin subscripts that denote slip-system indices.

2.1. Kinematics

Consider a material point that, in a more refined scale, is viewed as a representative volume element of a metal crystal deformed plastically by shearing on a number N of slip-systems. It is assumed that the plastic slips leave the crystallographic lattice at a material point unchanged. The lattice deformation gradient, taken relative to a fixed, local, stress-free reference configuration of the lattice, is denoted by $\mathbf{F}^*$; it encompasses both (arbitrarily large) rotations and (typically small) elastic strains of the lattice.

The reference configuration of the material is, for convenience, identified with some stress-free configuration. The plastic slip enforces the material to flow through the lattice, so that the coincidence of the reference configurations of the material and lattice is only momentary in general.

Multiplicative decomposition of the deformation gradient $\mathbf{F}$ taken relative to the fixed (stress-free) reference configuration yields

$$\mathbf{F} = \mathbf{F}^*\mathbf{F}^{\mathrm{p}}, \qquad \det \mathbf{F}^{\mathrm{p}} = 1, \qquad \det \mathbf{F}^* \equiv J^* > 0, \tag{2.1}$$

where $\mathbf{F}^{\mathrm{p}}$ is the plastic deformation gradient from the reference configuration to a locally unstressed, intermediate configuration. The plastic deformation due to activity of multiple slip-systems is described incrementally as follows:

$$\dot{\mathbf{F}}^{\mathrm{p}}\overset{-1}{\mathbf{F}^{\mathrm{p}}} = \sum_K \mathbf{s}_K \overset{\circ}{\gamma}_K, \qquad \mathbf{s}_K = \mathbf{m}_K \otimes \mathbf{n}_K, \qquad \mathbf{m}_K \cdot \mathbf{n}_K = 0. \tag{2.2}$$

The material time derivative (rate) is denoted by a superimposed dot. The plastic multiplier $\overset{\circ}{\gamma}_K$ represents the rate of plastic simple shear on the K-th slip-system defined by a pair of orthogonal unit vectors, $\mathbf{m}_K$ – the slip direction and $\mathbf{n}_K$ – the slip-plane normal, both in the stress-free configuration of the lattice. A circle rather than a dot over γ_K is used to indicate that $\overset{\circ}{\gamma}_K$ itself is *not* identified with the rate of any internal state variable. On using $\mathbf{F}^* = \mathbf{F}\overset{-1}{\mathbf{F}^{\mathrm{p}}}$ and

$$\dot{\mathbf{F}}^* = \dot{\mathbf{F}}\overset{-1}{\mathbf{F}^{\mathrm{p}}} - \mathbf{F}\overset{-1}{\mathbf{F}^{\mathrm{p}}}\dot{\mathbf{F}}^{\mathrm{p}}\overset{-1}{\mathbf{F}^{\mathrm{p}}}, \tag{2.3}$$

in the current configuration we obtain

$$\dot{\mathbf{F}}^*\overset{-1}{\mathbf{F}^*} = \dot{\mathbf{F}}\overset{-1}{\mathbf{F}} - \sum_K \mathbf{s}^*_K \overset{\circ}{\gamma}_K, \qquad \mathbf{s}^*_K = \mathbf{F}^*\mathbf{s}_K\overset{-1}{\mathbf{F}^*}. \tag{2.4}$$

The terms above can be classically decomposed into symmetric and antisymmetric (skew) parts, denoted by sym( ) and skew( ), respectively.

2.2. Constitutive relationships

The basic rate-independent rule of slip-system activity reads

$$\overset{\circ}{\gamma}_K \geq 0, \qquad f_K \leq 0, \qquad f_K\overset{\circ}{\gamma}_K = 0 \quad (\text{no sum over } K), \tag{2.5}$$

where f_K is the yield function for K-th slip-system, defined by

$$f_K = \tau_K - \tau_K^{\rm cr}. \tag{2.6}$$

τ_K denotes the (generalized) resolved shear stress on the K-th slip-system, and $\tau_K^{\rm cr}$ is its current critical value determined from a hardening rule with a moduli matrix (h^*_{KL}), cf. Subsec. 2.4 below. In accord with the normality flow rule, τ_K is defined as the projection of the (symmetric) Kirchhoff stress $\boldsymbol{\tau}$, taken with respect to the stress-free configuration,

$$\boldsymbol{\tau} = J^*\boldsymbol{\sigma}, \qquad (\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\rm T} = \text{Cauchy stress}),$$

on the dyad $\mathbf{s}^*_K$ defined in Eq. (2.4)[1],

$$\tau_K = \boldsymbol{\tau} \cdot \mathbf{s}^*_K. \tag{2.7}$$

The set of assumptions is completed by introducing the elastic constitutive law for the lattice. It can be written down in various equivalent versions; for instance, in the frequently used, objective form in the current configuration,

$$\overset{\nabla}{\boldsymbol{\tau}} = \mathbb{L}^* \cdot \mathbf{d} \qquad \text{if all } \overset{\circ}{\gamma}_K \equiv 0, \tag{2.8}$$

which in the case of purely elastic straining relates the Zaremba-Jaumann flux of Kirchhoff stress $\boldsymbol{\tau}$ to the Eulerian strain-rate $\mathbf{d}$ by a diagonally symmetric fourth-order tensor $\mathbb{L}^*$[2], where

$$\overset{\nabla}{\boldsymbol{\tau}} = \dot{\boldsymbol{\tau}} + \boldsymbol{\tau}\mathbf{w} - \mathbf{w}\boldsymbol{\tau},$$
$$\mathbf{w} = \mathsf{skew}(\dot{\mathbf{F}}\overset{-1}{\mathbf{F}}),$$
$$\mathbf{d} = \mathsf{sym}(\dot{\mathbf{F}}\overset{-1}{\mathbf{F}}).$$

The resulting set of constitutive rate-equations and inequalities for an elastic-plastic crystal with multiple slip-systems, is widely known and is summarized in Table 1 for convenience. However, most of these equations will *not* be used in this paper since equivalent expressions given in Subsec. 2.3 are found to be more convenient for the present purposes.

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[1] For metals under ordinary pressures, the elastic strains (but *not* rotations) of the crystallographic lattice are negligible, and τ_K differs only slightly from the classical Schmid stress defined as the projection of the Cauchy stress on a normalized dyad $\propto \mathbf{s}^*_K$.

[2] If other stress-rate or strain-rate measures are used, then the elastic moduli tensor $\mathbb{L}^*$ is to be modified accordingly, cf. [11].

Table 1. Summary of constitutive rate-equations and inequalities for an elastic-plastic crystal with multiple slip-systems.

Consistency conditions	
$\dot f_K \le 0, \quad \dot f_K \overset{\circ}{\gamma}_K = 0 \quad \text{for} \quad K \in \mathcal{P} = \{L : f_L = 0\} \supseteq \mathcal{A} = \{L : \overset{\circ}{\gamma}_L > 0\}$	
Constitutive rate equations (with normality structure)	
$\overset{\triangledown}{\boldsymbol\tau} = \mathbb{L}^* \cdot \mathbf{d} - \sum_K \boldsymbol\lambda_K \overset{\circ}{\gamma}_K$ $\dot f_K = \boldsymbol\lambda_K \cdot \mathbf{d} - \sum_L g_{KL} \overset{\circ}{\gamma}_L$	$\mathbf{d} = \overset{-1}{\mathbb{L}^*} \cdot \overset{\triangledown}{\boldsymbol\tau} + \sum_K \boldsymbol\mu_K \overset{\circ}{\gamma}_K$ $\dot f_K = \boldsymbol\mu_K \cdot \overset{\triangledown}{\boldsymbol\tau} - \sum_L h_{KL} \overset{\circ}{\gamma}_L$
Yield-surface normals	
$\boldsymbol\lambda_K = \mathbb{L}^* \cdot \mathbf{p}^*_K + \boldsymbol\beta^*_K \qquad \boldsymbol\lambda_K = \mathbb{L}^* \cdot \boldsymbol\mu_K \qquad \boldsymbol\mu_K = \mathbf{p}^*_K + \overset{-1}{\mathbb{L}^*} \cdot \boldsymbol\beta^*_K$	
Slip-system interaction moduli	
$g_{KL} = \boldsymbol\lambda_K \cdot \mathbf{p}^*_L + h^*_{KL} = \boldsymbol\mu_K \cdot \boldsymbol\lambda_L + h_{KL}$	
Auxiliary tensors	
$\mathbf{p}^*_K = \mathsf{sym}(\mathbf{s}^*_K) \qquad \boldsymbol\beta^*_K = \mathbf{w}^*_K \boldsymbol\tau - \boldsymbol\tau\, \mathbf{w}^*_K \qquad \mathbf{w}^*_K = \mathsf{skew}(\mathbf{s}^*_K)$	

2.3. Transformation to non-symmetric variables

The (unsymmetric) Piola stress[3)] tensor $\mathbf{S}$, and the (symmetric) Kirchhoff stress tensor $\boldsymbol\tau$, and their material time derivatives, are well-known to be related through

$$\mathbf{S} = \boldsymbol\tau \overset{-\mathrm{T}}{\mathbf{F}}, \qquad \dot{\mathbf{S}} = \dot{\boldsymbol\tau} \overset{-\mathrm{T}}{\mathbf{F}} - \boldsymbol\tau \overset{-\mathrm{T}}{\mathbf{F}} \dot{\mathbf{F}}^{\mathrm{T}} \overset{-\mathrm{T}}{\mathbf{F}}. \tag{2.9}$$

The values of f_K and $\overset{\circ}{\gamma}_L$ are assumed to be invariant under transformation to the non-symmetric variables. Accordingly, the constitutive rate-equations from Table 1 are transformed to their equivalent form

$$\dot{\mathbf{S}} = \mathbb{C}^{\mathrm{e}} \cdot \dot{\mathbf{F}} - \sum_K \boldsymbol\Lambda_K \overset{\circ}{\gamma}_K, \tag{2.10}$$

$$\dot f_K = \boldsymbol\Lambda_K \cdot \dot{\mathbf{F}} - \sum_L g_{KL} \overset{\circ}{\gamma}_L\,, \tag{2.11}$$

where

$$\boldsymbol\Lambda_K = \boldsymbol\lambda_K \overset{-\mathrm{T}}{\mathbf{F}} \tag{2.12}$$

[3)]For brevity we call it the Piola stress rather than the first Piola–Kirchhoff stress, although the latter name is more popular.

is the yield-surface normal in $\mathbf{F}$-space. The relationship between $\mathbf{\Lambda}_K$ and $\boldsymbol{\lambda}_K$ is easily demonstrated by substituting $\dot{\mathbf{F}} = \mathbf{0}$ into the equation for $\dot{\mathbf{S}}$, or alternatively, $\overset{\circ}{\gamma}_L \equiv 0$ into the equation for $\dot{f}_K$, cf. [15]. Note that the matrix (g_{KL}) remains invariant under transformation to the non-symmetric variables. Details of the standard transformation from the elastic moduli tensor $\mathbb{L}^*$ to $\mathbb{C}^{\mathrm{e}} = \partial\mathbf{S}/\partial\mathbf{F}$ can be found in [11]; in indicial notation with the use of the Kronecker symbol δ_{ij}, the known relationship reads

$$F_{ip}F_{kq}C^{\mathrm{e}}_{jplq} = L^*_{ijkl} - \frac{1}{2}(\tau_{jl}\delta_{ik} + \tau_{jk}\delta_{il} + \tau_{il}\delta_{jk} - \tau_{ik}\delta_{jl}), \tag{2.13}$$

implying $C^{\mathrm{e}}_{ijkl} = C^{\mathrm{e}}_{klij}$ on account of $L^*_{ijkl} = L^*_{klij}$. The expression for τ_K is conveniently transformed by using other non-symmetric stress measures, the Piola stress $\mathbf{S}^*$ taken with respect to the intermediate configuration and the Mandel stress $\mathbf{M}$ [16],

$$\mathbf{M} = \overset{\mathrm{T}}{\mathbf{F}^*}\boldsymbol{\tau}\overset{-\mathrm{T}}{\mathbf{F}^*} = \overset{\mathrm{T}}{\mathbf{F}^*}\mathbf{S}^*, \qquad \mathbf{S}^* = \boldsymbol{\tau}\overset{-\mathrm{T}}{\mathbf{F}^*} = \mathbf{S}\overset{\mathrm{T}}{\mathbf{F}^{\mathrm{p}}}. \tag{2.14}$$

The projection of $\mathbf{M}$ on a *fixed* dyad $\mathbf{s}_K$ for the K-th slip-system in a stress-free configuration coincides with the expression in Eq. (2.7), i.e.

$$\tau_K = \mathbf{M}\cdot\mathbf{s}_K = \mathbf{S}^*\cdot\mathbf{F}^*\mathbf{s}_K. \tag{2.15}$$

The rate of the (generalized) resolved shear stress τ_K thus reads

$$\dot{\tau}_K = \dot{\mathbf{M}}\cdot\mathbf{s}_K = \dot{\mathbf{S}}^*\cdot\mathbf{F}^*\mathbf{s}_K + \mathbf{S}^*\cdot\dot{\mathbf{F}}^*\mathbf{s}_K. \tag{2.16}$$

$\dot{\mathbf{S}}^*$ is related to $\dot{\mathbf{F}}^*$ by the (diagonally-symmetric) elastic moduli tensor $\mathbb{C}^* = \partial\mathbf{S}^*/\partial\mathbf{F}^*$ taken relative to the intermediate configuration, of components given by Eq. (2.13) when substituting $\mathbf{F}^{\mathrm{p}} = \mathbf{I}$. Hence, after rearranging the formula (2.16), we arrive at

$$\dot{\tau}_K = \dot{\mathbf{F}}^*\cdot\mathbb{C}^*\cdot\mathbf{F}^*\mathbf{s}_K + \mathbf{M}\cdot\overset{-1}{\mathbf{F}^*}\dot{\mathbf{F}}^*\mathbf{s}_K. \tag{2.17}$$

This formula is particularly useful for deriving a concise expression for the *geometric interaction moduli* discussed in Subsection 3.1.

2.4. Hardening moduli

The slip-system hardening moduli h^*_{KL} relate the rate of critical resolved shear stress τ^{cr}_K on the K-th slip-system to shear-rate $\overset{\circ}{\gamma}_L$ on the same $(L = K)$ and any other $(L \neq K)$ slip-systems,

$$\dot{\tau}^{\mathrm{cr}}_K = \sum_L h^*_{KL}\,\overset{\circ}{\gamma}_L. \tag{2.18}$$

Moduli h^*_{KL} were commonly assumed to depend only on the prior history of $\overset{\circ}{\gamma}_L$'s, that is, on the current state of the material. It meant the lack of dependence of the hardening moduli on how many slip-systems are currently active. That assumption is relaxed in this paper. In fact, there is *a priori* no reason why the relationship between $\dot{\tau}^{\rm cr}_K$ and $\overset{\circ}{\gamma}_L$ should be precisely the same for an active and inactive K-th system.

A study of physical mechanisms of mutual interactions between mobile and sessile dislocations is beyond the scope of this paper. The considerations below are limited to the macroscopic level of a representative volume element of a plastically deforming crystal, and also to incremental effects corresponding to a representative time increment. Strain and stress refer to quantities obtained upon appropriate averaging over a representative volume, and their rates are understood in an average sense of a difference quotient taken with respect to a representative time increment. Slip rates and hardening moduli are analogously understood in an average sense for a representative space-time domain.

We propose to split the slip-system hardening moduli in Eq. (2.18) into two parts as follows:

$$h^*_{KL} = H_{KL} + h^{\mathcal{A}}_{KL}, \qquad h^{\mathcal{A}}_{KL} = 0 \ \text{ if } \ \overset{\circ}{\gamma}_K = 0. \tag{2.19}$$

Hardening moduli H_{KL} depend on the prior history of $\overset{\circ}{\gamma}_L$'s, that is, on the current state of the material, in a manner analogous to that assumed so far in the literature. Moduli H_{KL} are usually taken to be symmetric in modelling, $H_{KL} = H_{LK}$, and we adopt that assumption here for simplicity, although arguments can be found for non-symmetric H_{KL} [17]. Moduli H_{KL} are frequently assumed in the following two-parameter form

$$H_{KL} = \big(q + (1-q)\delta_{KL}\big)h. \tag{2.20}$$

Here, parameter h depends on the history of slipping on all slip-systems in a manner relevant to the actual material hardening, and δ_{KL} is the Kronecker symbol. Parameter q denotes the ratio of latent hardening to self-hardening and is usually taken from the range $1 \le q \le 1.4$ as suggested by experiments [18]. If a more accurate description of crystal hardening is needed then a more complex form of H_{KL} can be adopted, for instance, by introducing changes in the value of q along a deformation path, cf. [19], or distinguishing five different latent hardening mechanisms in the crystal, cf. [20]. For a more recent review of other proposals, cf. [21, 22].

The novelty of the second term $h^{\mathcal{A}}_{KL}$ lies in its relevance to active slip-systems ($K, L \in \mathcal{A}$) only; note that we can take $h^{\mathcal{A}}_{KL} = 0$ for $\overset{\circ}{\gamma}_L = 0$ without any loss of generality. $h^{\mathcal{A}}_{KL}$ can undergo discontinuous changes when the set $\mathcal{A}$ of active slip-systems changes along a loading path, which is allowed here. In the next section, arguments are given for taking $h^{\mathcal{A}}_{KL}$ such that the resulting subset $(g^{\mathcal{A}}_{KL})$ of the interaction matrix (g_{KL}) for *active* slip-systems in a representative crystal element is symmetric.

3. The symmetry issue of slip-system interaction moduli revisited

3.1. Geometric interaction between slip-systems

Crystallographic slipping on some L-th slip-system of a crystal influences the rate of generalized resolved shear stress τ_K on the K-th slip-system. This interaction is of geometric nature as it is independent of physical latent hardening. When examined for a homogeneous and uniformly deforming crystal, the moduli of geometric interaction between slip-systems are expressed in the following form:

$$g^{\text{geom}}_{KL} \equiv -\frac{\partial \dot{\tau}_K}{\partial \overset{\circ}{\gamma}_L}\bigg|_{\dot{\mathbf{F}}} = \mathbf{F}^*\mathbf{s}_K \cdot \mathbb{C}^* \cdot \mathbf{F}^*\mathbf{s}_L + \mathbf{M} \cdot \mathbf{s}_L\mathbf{s}_K. \tag{3.1}$$

The *Proof* is immediate when using the expression (2.17) for $\dot{\tau}_K$ derived in Subsection 2.3. By differentiating it with respect to $\overset{\circ}{\gamma}_L$ and substituting the formula $\partial\dot{\mathbf{F}}^*/\partial\overset{\circ}{\gamma}_L|_{\dot{\mathbf{F}}} = -\mathbf{F}^*\mathbf{s}_L$ implied by Eq. (2.4), the result (3.1) follows.

The matrix (g^{geom}_{KL}) added to the hardening matrix (h^*_{KL}) yields (g_{KL}), viz.

$$g_{KL} = g^{\text{geom}}_{KL} + h^*_{KL}, \tag{3.2}$$

which is easily verified by combining Eqs. (3.1), (2.18), (2.6) and (2.11).

The first term on the right-hand side in Eq. (3.1) is symmetric and the second one is generally non-symmetric with respect to interchange of slip-system indices $K \leftrightarrow L$. However, the latter term vanishes for coplanar ($\mathbf{n}_K = \mathbf{n}_L$) or collinear ($\mathbf{m}_K = \pm\mathbf{m}_L$) slip-systems, for which $\mathbf{n}_L \cdot \mathbf{m}_K = \mathbf{n}_K \cdot \mathbf{m}_L = 0$ and $\mathbf{s}_L\mathbf{s}_K = \mathbf{s}_K\mathbf{s}_L = \mathbf{0}$, so that $g^{\text{geom}}_{KL} = g^{\text{geom}}_{LK}$ in those cases.

The latter conclusion is less obvious when the geometric part is equivalently expressed in the usual way as $g^{\text{geom}}_{KL} = \boldsymbol{\lambda}_K \cdot \mathbf{p}^*_L$, cf. Table 1. A direct transformation of that expression to Eq. (3.1) is somewhat lengthy and is omitted here as the derivation given above is more transparent. The authors were unable to find formula (3.1) in the literature.

As a special case, consider a perfectly plastic crystal for which $\tau^{\text{cr}}_K = \text{const}$ by assumption. Then we have $h^*_{KL} \equiv 0$ while geometric hardening/softening is still present, $g_{KL} = g^{\text{geom}}_{KL}$, i.e. the slip-system interaction moduli matrix is of purely geometric type. The non-symmetry of g^{geom}_{KL} transmits thus unaltered to g_{KL}.

This conclusion is immediately extended to any hardening rule with a *symmetric* hardening moduli matrix, viz.

$$g_{KL} - g_{LK} = \mathbf{M} \cdot (\mathbf{s}_L \mathbf{s}_K - \mathbf{s}_K \mathbf{s}_L) \qquad \text{if } h^*_{KL} = h^*_{LK}, \tag{3.3}$$

which is the case when h^*_{KL} is assumed to reduce to $H_{KL} = H_{LK}$.

However, the situation is different when the term $h^{\mathcal{A}}_{KL}$ in Eq. (2.19) is present and not symmetric, so that the resultant matrix g_{KL} *may* be symmetric whenever restricted to the set of indices of active slip-systems. Certain arguments in favour of that assumption are discussed below.

3.2. Symmetry of tangent stiffness moduli

The set of constitutive rate-equations and inequalities, see Table 1 or the counterparts for non-symmetric variables in Subsection 2.3, need not have a unique solution even if $\dot{\mathbf{F}}$ is fully prescribed in a given state of the crystal. A condition sufficient for existence and uniqueness of a solution $\overset{\circ}{\gamma}_K \geq 0$ for any given $\dot{\mathbf{F}}$ is that all principal minors of the matrix (g_{KL}) with $K, L \in \mathcal{P}$ are positive, which is also necessary for the uniqueness if the potentially active slip-systems (of indices from set $\mathcal{P}$), are linearly independent [15].

Suppose that this condition sufficient for uniqueness is satisfied. The set of indices of the active mechanisms ($\overset{\circ}{\gamma}_K > 0$) is denoted by $\mathcal{A} \subseteq \mathcal{P}$ and is uniquely determined by $\dot{\mathbf{F}}$, although not specified explicitly in general. Denote the respective principal submatrix of (g_{KL}) with $K, L \in \mathcal{A}$ by $(g^{\mathcal{A}}_{KL})$ and components of its inverse by $(g^{\mathcal{A}})^{-1}_{KL}$. From the consistency condition $\dot{f}_K = 0$ if $\overset{\circ}{\gamma}_K > 0$ and Eq. (2.11), we obtain

$$\overset{\circ}{\gamma}_K = \sum_{L \in \mathcal{A}} (g^{\mathcal{A}})^{-1}_{KL} \, \mathbf{\Lambda}_L \cdot \dot{\mathbf{F}} > 0 \quad \text{for } K \in \mathcal{A}, \qquad \overset{\circ}{\gamma}_K = 0 \quad \text{for } K \notin \mathcal{A}, \tag{3.4}$$

so that, from Eq. (2.10), the following known formula is obtained:

$$\dot{\mathbf{S}} = \mathbb{C}^{\mathcal{A}} \cdot \dot{\mathbf{F}}, \qquad \mathbb{C}^{\mathcal{A}} = \mathbb{C}^{\mathrm{e}} - \sum_{K,L \in \mathcal{A}} (g^{\mathcal{A}})^{-1}_{KL} \, \mathbf{\Lambda}_K \otimes \mathbf{\Lambda}_L. \tag{3.5}$$

From diagonal symmetry of the elastic moduli tensor, $\mathbb{C}^{\mathrm{e}} = \overset{\mathrm{T}}{\mathbb{C}}{}^{\mathrm{e}}$, we have

$$\mathbb{C}^{\mathcal{A}} - \overset{\mathrm{T}}{\mathbb{C}}{}^{\mathcal{A}} = \sum_{K,L \in \mathcal{A}} ((g^{\mathcal{A}})^{-1}_{LK} - (g^{\mathcal{A}})^{-1}_{KL}) \mathbf{\Lambda}_K \otimes \mathbf{\Lambda}_L.$$

It follows that diagonal symmetry of the tangent stiffness moduli tensor $\mathbb{C}^{\mathcal{A}}$ is implied by symmetry of the slip-system interaction matrix $(g^{\mathcal{A}}_{KL})$ *restricted to active slip-systems.* Hence, for $\mathbb{C}^{\mathcal{A}} = \overset{\mathrm{T}}{\mathbb{C}}{}^{\mathcal{A}}$ it is sufficient that

$$g_{KL} - g_{LK} = 0 \qquad \text{if } \overset{\circ}{\gamma}_K > 0, \overset{\circ}{\gamma}_L > 0. \tag{3.6}$$

If the active slip-systems are linearly independent then condition (3.6) can be shown to be both sufficient and necessary for $\mathbb{C}^{\mathcal{A}} = \overset{\mathrm{T}}{\mathbb{C}}{}^{\mathcal{A}}$.

The diagonal symmetry of the tangent stiffness moduli tensor is known to be a convenient property, strictly related to the variational structure which is useful analytically [11], and to the symmetry of a global tangent stiffness matrix useful in numerical applications to a discretized problem. This motivated in the past the attempts to symmetrize the slip-system interaction matrix (g_{KL}), cf. the references listed in Introduction. However, as demonstrated above, with the same purpose in mind, it suffices to restrict symmetrization of the slip-system interaction matrix *to active slip-systems only.*

3.3. Spatial averaging

In the derivation of Eq. (3.1), activity of both slip-systems K and L was uniformly distributed within the whole crystal under consideration, or equivalently, examined at the material point level. The geometric interaction matrix takes another form if activity of slip-systems K and L takes place in *different* subdomains of the crystal. Throughout this subsection, the crystal is no longer assumed to be uniformly deforming, so that the approach is analogous to that of micromechanics of heterogeneous materials.

Consider the *macroscopic* deformation gradient $\bar{\mathbf{F}}$ and macroscopic Piola stress $\bar{\mathbf{S}}$ for a non-uniformly deforming crystal. Under the assumptions of continuity of displacements and equilibrium of stresses, $\bar{\mathbf{F}}$ and $\bar{\mathbf{S}}$ are defined as unweighted averages of their local counterparts, $\mathbf{F}$ and $\mathbf{S}$, respectively, over the volume V of the crystal in the reference configuration [23]. Moreover, to treat $\dot{\bar{\mathbf{F}}}$ and $\dot{\bar{\mathbf{S}}}$ as constitutive rate-variables for the crystal as a whole, we assume that the Hill lemma holds [23]

$$\overset{\vartriangle}{\bar{\mathbf{S}}} \cdot \dot{\bar{\mathbf{F}}} = \frac{1}{V} \int_V \overset{\vartriangle}{\mathbf{S}} \cdot \dot{\mathbf{F}} \, dV, \tag{3.7}$$

where both the superimposed dot and triangle denote rates which need not be related to each other. Equality (3.7) requires the assumptions of continuity of velocities and equilibrium of stress-rates within V, and imposes restrictions on the boundary data (for instance, they may be periodic) over the crystal boundary.

The quantity called "Hill's bilinear invariant" is of special interest [23]. On using the constitutive relationship (2.10) for each solution pair $(\dot{\mathbf{S}}, \dot{\mathbf{F}})$ and $(\overset{\vartriangle}{\mathbf{F}}, \overset{\vartriangle}{\mathbf{S}})$ separately, in a given material state it reads:

$$\dot{\mathbf{S}} \cdot \overset{\vartriangle}{\mathbf{F}} - \overset{\vartriangle}{\mathbf{S}} \cdot \dot{\mathbf{F}} = (\overset{\vartriangle}{\mathbf{F}} \cdot \mathbb{C}^{\mathrm{e}} \cdot \dot{\mathbf{F}} - \dot{\mathbf{F}} \cdot \mathbb{C}^{\mathrm{e}} \cdot \overset{\vartriangle}{\mathbf{F}}) - \overset{\vartriangle}{\mathbf{F}} \cdot \sum_L \mathbf{\Lambda}_L \overset{\circ}{\gamma}_L + \dot{\mathbf{F}} \cdot \sum_K \mathbf{\Lambda}_K \overset{\vartriangle}{\gamma}_K. \tag{3.8}$$

The term in parentheses above vanishes on account of diagonal symmetry of the elastic moduli tensor $\mathbb{C}^{\mathrm{e}}$.

From the constitutive relationship (2.11), we have

$$\dot{f}_K \overset{\vartriangle}{\gamma}_K = \Big(\mathbf{\Lambda}_K \cdot \dot{\mathbf{F}} - \sum_L g_{KL} \mathring{\gamma}_L\Big) \overset{\vartriangle}{\gamma}_K \tag{3.9}$$

and analogously

$$\overset{\vartriangle}{f}_L \mathring{\gamma}_L = \Big(\mathbf{\Lambda}_L \cdot \overset{\vartriangle}{\mathbf{F}} - \sum_K g_{LK} \overset{\vartriangle}{\gamma}_K\Big) \mathring{\gamma}_L. \tag{3.10}$$

Consider two pairs $(\dot{\mathbf{F}}, \mathring{\gamma}_K)$, $(\overset{\vartriangle}{\mathbf{F}}, \overset{\vartriangle}{\gamma}_L)$ sufficiently close to each other, so that they correspond to *the same* set $\mathcal{A}$ of active slip-systems. Then, from the consistency conditions $\dot{f}_K = 0$ and $\overset{\vartriangle}{f}_L = 0$ if $K, L \in \mathcal{A}$, it follows that

$$\dot{f}_K \overset{\vartriangle}{\gamma}_K = 0 \qquad \text{and} \qquad \overset{\vartriangle}{f}_L \mathring{\gamma}_L = 0 \qquad \text{if} \quad K, L \in \mathcal{A}. \tag{3.11}$$

Hence, from Eqs. (3.8)–(3.11) we obtain

$$\dot{\mathbf{S}} \cdot \overset{\vartriangle}{\mathbf{F}} - \overset{\vartriangle}{\mathbf{S}} \cdot \dot{\mathbf{F}} = \sum_{K,L \in \mathcal{A}} (g_{KL} - g_{LK}) \overset{\vartriangle}{\gamma}_K \mathring{\gamma}_L \qquad \text{if } \mathcal{A} = \{K \mid \mathring{\gamma}_K > 0\} = \{L \mid \overset{\vartriangle}{\gamma}_L > 0\}. \tag{3.12}$$

Assuming the same structure of macroscopic constitutive relations for the non-uniformly deforming crystal and for its material point, and in terms of the average slip-rates for the crystal,

$$\bar{\overset{\vartriangle}{\gamma}}_K = \frac{1}{V} \int_V \overset{\vartriangle}{\gamma}_K \, dV, \qquad \bar{\mathring{\gamma}}_L = \frac{1}{V} \int_V \mathring{\gamma}_L \, dV,$$

we can analogously write

$$\dot{\bar{\mathbf{S}}} \cdot \bar{\overset{\vartriangle}{\mathbf{F}}} - \bar{\overset{\vartriangle}{\mathbf{S}}} \cdot \dot{\bar{\mathbf{F}}} = \sum_{K,L \in \bar{\mathcal{A}}} (\bar{g}_{KL} - \bar{g}_{LK}) \bar{\overset{\vartriangle}{\gamma}}_K \bar{\mathring{\gamma}}_L \qquad \text{if } \bar{\mathcal{A}} = \{K \mid \bar{\mathring{\gamma}}_K > 0\} = \{L \mid \bar{\overset{\vartriangle}{\gamma}}_L > 0\}. \tag{3.13}$$

The overall (effective) slip-system interaction moduli matrix $(\bar{g}_{KL})$ remains unspecified. However, from Hill's lemma (3.7) applied to the left-hand products in Eqs. (3.12) and (3.13), we have

$$\dot{\bar{\mathbf{S}}} \cdot \bar{\overset{\vartriangle}{\mathbf{F}}} - \bar{\overset{\vartriangle}{\mathbf{S}}} \cdot \dot{\bar{\mathbf{F}}} = \frac{1}{V} \int_V (\dot{\mathbf{S}} \cdot \overset{\vartriangle}{\mathbf{F}} - \overset{\vartriangle}{\mathbf{S}} \cdot \dot{\mathbf{F}}) \, dV.$$

This provides the relationship, valid under the assumptions indicated in Eqs. (3.12) and (3.13),

$$\sum_{K,L\in\bar{\mathcal{A}}} (\bar{g}_{KL} - \bar{g}_{LK})\bar{\overset{\triangle}{\gamma}}_K \bar{\overset{\circ}{\gamma}}_L = \frac{1}{V}\int_V \sum_{K,L\in\mathcal{A}} (g_{KL} - g_{LK})\overset{\triangle}{\gamma}_K \overset{\circ}{\gamma}_L \, dV \tag{3.14}$$

from which some conclusions about symmetry of $(\bar{g}_{KL})$ for active slip-systems can be drawn.

The major conclusion is as follows: for symmetry of the interaction matrix $(\bar{g}_{KL})$ between *active* slip-systems in a non-uniformly deforming crystal, it is sufficient but *not* necessary that the local matrix (g_{KL}) be symmetric. On the contrary, for an *arbitrary* matrix (g_{KL}), the integrand of the right-hand integral in (3.14) vanishes identically if the crystal is split into domains in which only single slip operates (or none), in general on different slip-systems in different domains. Then, the left-hand expression in (3.14) must vanish identically, and it is concluded that the following symmetry property holds:

$$\bar{g}_{KL} - \bar{g}_{LK} = 0 \qquad \text{if } \bar{\overset{\triangle}{\gamma}}_K > 0, \bar{\overset{\circ}{\gamma}}_L > 0. \tag{3.15}$$

The argument can be extended by appealing to the special cases of double slip discussed in Subsection 3.1, when $h^*_{KL} = h^*_{LK}$ implies $g_{KL} = g_{LK}$ on account of vanishing of the terms in parentheses in Eq. (3.3). On substituting this into the right-hand side integral in Eq. (3.14), analogously as above we arrive at the following conclusion: *property* (3.15) *is obtained if either no slip or a single slip or double slip on coplanar or collinear system operates at each material point of the crystal* (provided $h^*_{KL} = h^*_{LK}$ for that double slip).

It is emphasized that the derived symmetry of the macroscopic slip-system interaction matrix $(\bar{g}_{KL})$ *refers to the active slip-systems only*, under the assumptions specified.

The above derivation of the symmetry property (3.15) with the explicit reference to non-uniform slip-system activity in a crystal appears to be new. It may be added that the result obtained is not unexpected, in view of transmissibility of the symmetry of the tangent stiffness moduli tensor (3.5), and of certain other constitutive properties, from the micro to macro level, cf. [23, 24].

3.4. Time averaging

In the preceding subsection, the overall (effective) slip-system interaction moduli for a crystal were examined in the case of crystal subdivision, at a single instant of time, into subdomains of single slip or of double slip on coplanar or collinear systems. The crystal was regarded as a representative *volume* element deforming non-uniformly in space, while variations of slip-rates and strain-rate in time have not been analyzed.

In this subsection, we consider an opposite problem, namely, the rates are understood as unweighted averages over a representative *time* interval at a material point, while variations of strain-rate in space are not analyzed.

Consider a short path in deformation-gradient space, accompanied by variations of slip-rates such that the constitutive rate equations and inequalities given in Section 2 are satisfied at each instant along the path. The path length $\Delta\theta = \int_t^{t+\Delta t} \dot{\theta}\, dt$, where $\dot{\theta} = (\dot{\mathbf{F}} \cdot \dot{\mathbf{F}})^{1/2} + \sum_K \overset{\circ}{\gamma}_K$, say, serves as a small parameter. We examine the deformation work calculated up to the second-order terms with respect to $\Delta\theta$. Following [25], we use the concept of the second-order work defined on arbitrarily circuitous *indirect* paths whose complexity can be preserved as their length tends to zero. On integrating over a time increment the expression $\dot{w} = \mathbf{S} \cdot \dot{\mathbf{F}}$ for the rate of deformation work per unit volume in the reference configuration, substituting the constitutive relationships, and displaying the first- and second-order terms only, we obtain (cf. [25], Eq. (3.9))

$$\Delta w = \mathbf{S} \cdot \Delta\mathbf{F} + \frac{1}{2}\Delta\mathbf{F} \cdot \mathbb{C}^{\mathrm{e}} \cdot \Delta\mathbf{F} - \int_0^{\Delta\theta} \sum_{K,L} (\dot{f}_K + g_{KL}\overset{\circ}{\gamma}_L)\gamma_K(\theta)\, d\theta + o((\Delta\theta)^2). \tag{3.16}$$

A superimposed dot (or circle in $\overset{\circ}{\gamma}_L$) denotes here the rate taken with respect to θ as a time variable, Δ indicates an increment such that $\Delta\psi = \int_0^{\Delta\theta} \dot{\psi}\, d\theta$, while $\gamma_K(\theta) = \int_0^{\theta} \overset{\circ}{\gamma}_K(\theta')\, d\theta'$. The values of $\mathbf{S}$, $\mathbb{C}^{\mathrm{e}}$ and g_{KL}, that are assumed to vary continuously with θ, are taken at $\theta = 0$. Integration by parts (of a *half* of the second integrand) yields

$$\Delta w = \mathbf{S} \cdot \Delta\mathbf{F} + \frac{1}{2}\Delta\mathbf{F} \cdot \mathbb{C}^{\mathrm{e}} \cdot \Delta\mathbf{F} - \frac{1}{2}\sum_{K,L} g_{KL}\Delta\gamma_K\Delta\gamma_L - \sum_K \Delta f_K \Delta\gamma_K - \frac{1}{2}\int_0^{\Delta\theta} \sum_{K,L} (g_{KL} - g_{LK})\overset{\circ}{\gamma}_L\gamma_K(\theta)\, d\theta + o((\Delta\theta)^2), \tag{3.17}$$

where the complementarity condition $f_K\overset{\circ}{\gamma}_K = 0$ has been used, with the implication that $f_K = 0$ at $\theta = 0$ if $\Delta\gamma_K \neq 0$ for $\Delta\theta$ arbitrarily small.

The value of Δw is path-dependent in general, although all the terms displayed, except the last integral, depend only on final increments $\Delta\mathbf{F}$ and $\Delta\gamma_K$. Suppose that those final increments from a given state of the material are given, and search a path $\gamma_K(\theta)$ that minimizes the respective deformation work Δw to second order[4)], that is, maximizes the integral in Eq. (3.17). The corresponding Euler–Lagrange equation of the calculus of variation implies that along the extremal path we must have

$$g_{KL} - g_{LK} = 0 \qquad \text{if } \overset{\circ}{\gamma}_K > 0,\ \overset{\circ}{\gamma}_L > 0. \tag{3.18}$$

It is pointed out that, due to the unilateral constraint $\overset{\circ}{\gamma}_K \geq 0$, the extremum condition $g_{KL} - g_{LK} = 0$ need *not* be satisfied if $\overset{\circ}{\gamma}_K \overset{\circ}{\gamma}_L = 0$ at each instant along the minimum work path. For instance, consider an example of double slip on systems K, L with arbitrary $g_{KL} - g_{LK} > 0$. A minimum of the second-order work is readily attained on a path consisting of two consecutive segments such that $\overset{\circ}{\gamma}_K > 0, \overset{\circ}{\gamma}_L = 0$ along the first one is followed by $\overset{\circ}{\gamma}_K = 0, \overset{\circ}{\gamma}_L > 0$ along the second one. In general, we can define a lower bound $\Delta w^{\min}$ such that $\Delta w^{\min} \leq \Delta w$ (to second order) for all paths.

In turn, consider a *direct path* along which, by definition, the *rates* $\dot{\mathbf{F}}$ and $\overset{\circ}{\gamma}_K$ are constant or deviate from constant values by a distance of order of $\Delta\theta$. Then the last two terms in Eq. (3.17) vanish (to second order), and substitution of the constitutive law (2.10) in the incremental form shows that Eq. (3.17) reduces to the usual formula [23, 25]

$$\Delta w^{\text{direct}} = \mathbf{S} \cdot \Delta\mathbf{F} + \frac{1}{2}\Delta\mathbf{S} \cdot \Delta\mathbf{F} + o((\Delta\theta)^2). \tag{3.19}$$

The final argument is as follows. If the rates are understood as averages over a representative interval $(0, \Delta\theta)$, then formula (3.19) should be applicable when adopting a certain representative matrix (g_{KL}). If the symmetry condition (3.18), with $\overset{\circ}{\gamma}_M$ interpreted now as $\Delta\gamma_M/\Delta\theta$, does not hold for that matrix then, as shown above, a lower value of Δw can be attained on a non-direct path. Therefore, if formula (3.19) is intended to correspond to the lower bound $\Delta w^{\min}$ then the symmetry condition (3.18) should be imposed on the representative matrix. This provides an argument in favour of using a slip-system interaction matrix that satisfies condition (3.18), which is based on a more physical hypothesis of minimization of the incremental deformation work.

A similar conclusion has been drawn from a postulate of minimum incremental dissipation attained on a direct path [12]. That derivation of Eq. (3.18) required operations on a dissipation function of (unspecified) internal state variables and their rates. The present derivation of the symmetry condition (3.18) from the postulate of minimum incremental deformation work is independent of thermodynamic analysis.

[4)] It is assumed that the side condition $f_K(\theta)\overset{\circ}{\gamma}_K(\theta) = 0$ can be satisfied by suitably adjusting the path $\mathbf{F}(\theta)$.

4. Selective symmetrization

Let us summarize the conclusions obtained above regarding symmetry of the slip-system interaction matrix (g_{KL}) for a representative space-time element of a crystal. The geometric interaction part of that matrix, if determined by using the uniformity assumptions that lead to Eq. (3.1), disturbs the symmetry of (g_{KL}) in general. All the arguments presented in the preceding section in favour of symmetry of a representative matrix (g_{KL}) (of course, without proving it unconditionally) have referred to *active slip-systems only*, $K, L \in \mathcal{A}$. To obtain such symmetry, the non-symmetric part of geometric interaction matrix (g_{KL}^{geom}) may be compensated by adjusting the novel term $h_{KL}^{\mathcal{A}}$ in formula (2.19) that takes into account the differences between mutual interactions of active slip-systems and latent hardening of an inactive K-th slip-system. As the value of $h_{KL}^{\mathcal{A}}$ is immaterial for $L \notin \mathcal{A}$, the compensating term refers to active slip-systems only, $K, L \in \mathcal{A}$, precisely as the arguments for symmetry of g_{KL} do.

The present proposal of *the selective symmetrization* of the slip-system interaction moduli matrix, in case $H_{KL} = H_{LK}$[5)], is to define the term $h_{KL}^{\mathcal{A}}$ as follows:

$$
h_{KL}^{\mathcal{A}} = \begin{cases} \mathbf{M} \cdot \big(r\, \mathbf{s}_K \mathbf{s}_L - (1-r)\, \mathbf{s}_L \mathbf{s}_K\big) & \text{if } K, L \in \mathcal{A}, \\ 0 & \text{otherwise}, \end{cases} \tag{4.1}
$$

where r is a free scalar parameter. In general, r may depend on the actual state of the material as well as on a pair (K, L) to which it applies. The simplest way is to take r as a constant from the interval $0 \le r \le 1$; for instance, $r = \frac{1}{2}$. Note that self-hardening moduli are not influenced by the proposed selective symmetrization since $h_{KK}^{\mathcal{A}} \equiv 0$ on account of $\mathbf{s}_K \mathbf{s}_K = \mathbf{0}$.

On using relationships $(2.14)_1$ and $(2.4)_2$, the expression for $h_{KL}^{\mathcal{A}}$ is given an equivalent form,

$$
\mathbf{M} \cdot \big(r\, \mathbf{s}_K \mathbf{s}_L - (1-r)\, \mathbf{s}_L \mathbf{s}_K\big) = \boldsymbol{\tau} \cdot \big(r\, \mathbf{s}_K^* \mathbf{s}_L^* - (1-r)\, \mathbf{s}_L^* \mathbf{s}_K^*\big). \tag{4.2}
$$

The expressions for g_{KL}, following Eqs. (3.2), (2.19), (3.1) and (4.1), are now summarized as follows:

$$
\begin{aligned}
g_{KL} &= g_{KL}^{\mathrm{geom}} + H_{KL} + h_{KL}^{\mathcal{A}}, \qquad H_{KL} = H_{LK}, \\
g_{KL} &= g_{KL}^{\mathrm{geom}} + H_{KL} \qquad \text{if } K \notin \mathcal{A},
\end{aligned}
$$

[5)] The selective symmetrization can be easily extended to non-symmetric H_{KL} by adding to $h_{KL}^{\mathcal{A}}$ another term $(rH_{LK} - (1-r)H_{KL})$ for $K, L \in \mathcal{A}$, or by symmetrizing analogously only the sum $(g_{KL}^{\mathrm{geom}} + H_{KL})$. The essence of the *selective* symmetrization is again in restricting it to the set of *active* slip-systems.

$$g_{KL} = \mathbf{F}^*\mathbf{s}_K \cdot \mathbb{C}^* \cdot \mathbf{F}^*\mathbf{s}_L + H_{KL} + r\mathbf{M} \cdot \big(\mathbf{s}_K\mathbf{s}_L + \mathbf{s}_L\mathbf{s}_K\big) \qquad \text{if } K, L \in \mathcal{A},$$
$$g_{KL} = g_{LK} \qquad \text{if } K, L \in \mathcal{A}.$$

In the special case $r = \frac{1}{2}$ we have $h^{\mathcal{A}}_{KL} = -h^{\mathcal{A}}_{LK}$, and the selective symmetrization reduces simply to replacing *the subset* $(g^{\mathcal{A}}_{KL}) = (g_{KL})|_{K,L\in\mathcal{A}}$ of an original slip-system interaction moduli matrix (g_{KL}) by its symmetric part $\frac{1}{2}(g^{\mathcal{A}}_{KL} + g^{\mathcal{A}}_{LK})$. In spite of formal resemblance, the effect is substantially different from the P.A.N. rule [4] where the matrix g_{KL} was symmetrized without any restriction placed on (K, L). In result, the P.A.N. rule has affected latent hardening of inactive slip-systems in contrast to the present proposal.

The procedure of exploiting the selective symmetrization rule in a computational algorithm will be discussed in a separate paper.

5. Example: effect of symmetrization rule on simulation of uniaxial tension

A simple example of uniaxial tension of an f.c.c. crystal is used to illustrate the differences between the proposed selective symmetrization of the slip-system interaction moduli matrix (g_{KL}), restricted to the set of active slip-systems, and the earlier proposals to symmetrize the matrix (g_{KL}) without this restriction. The hardening moduli matrix is assumed in the form (2.20). Hardening parameter h is taken to depend on $\gamma = \int \sum_K \overset{\circ}{\gamma}_K \, dt$ through $h(\gamma) = h_0\big(\frac{h_0\,\gamma}{n\,\tau_0} + 1\big)^{n-1}$ as in [4], where we use $n = 0.16$, and the latent hardening ratio $q = 1.4$. Other parameters correspond to those adopted in [26] for Cu single crystal: the initial plasticity parameters are $h_0 = 180$ MPa, $\tau_0 = 16$ MPa, standard elasticity moduli for cubic symmetry are $C^{\mathrm{E}}_{11} = 170$ GPa, $C^{\mathrm{E}}_{12} = 124$ GPa, $C^{\mathrm{E}}_{44} = 75$ GPa, and the tensile axis is oriented initially along the $[\bar{2}\,3\,6]$ direction.

The material response has been simulated by using three symmetrization rules:

(i) The present selective symmetrization rule, with $r = \frac{1}{2}$,

$$h^*_{KL} = \begin{cases} H_{KL} + \dfrac{1}{2}\mathbf{M} \cdot \big(\mathbf{s}_K\mathbf{s}_L - \mathbf{s}_L\mathbf{s}_K\big) & \text{if } K, L \in \mathcal{A}, \\ H_{KL} & \text{otherwise.} \end{cases} \tag{5.1}$$

(ii) The P.A.N. symmetrization rule [4]

$$h^*_{KL} = H_{KL} + \frac{1}{2}(\mathbf{p}^*_K \cdot \boldsymbol{\beta}^*_L - \mathbf{p}^*_L \cdot \boldsymbol{\beta}^*_K) \qquad \text{for all } K, L. \tag{5.2}$$

(iii) The H.S. symmetrization rule [13]

$$h^*_{KL} = H'_{KL} + \mathbf{p}^*_K \cdot \boldsymbol{\beta}^*_L \qquad \text{for all } K, L. \tag{5.3}$$

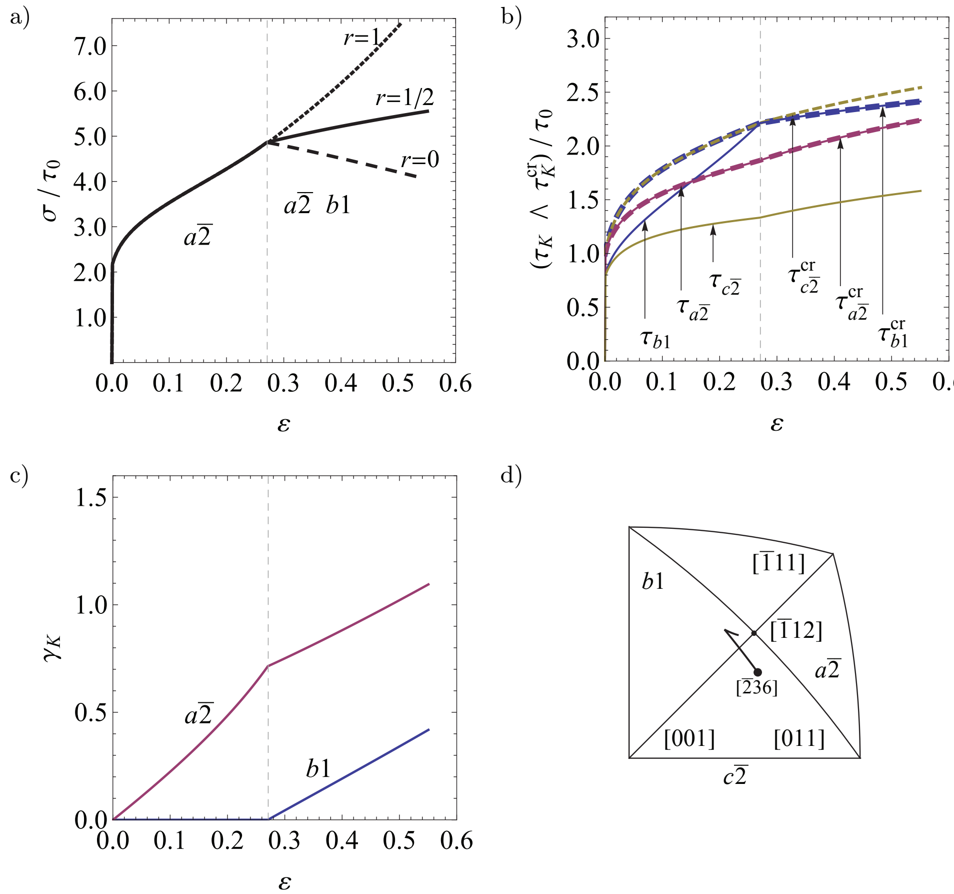

Fig. 1. Simulation of uniaxial tension using the selective symmetrization rule: a) tensile stress-strain curve, b) resolved τ_K (solid lines) and critical $\tau_K^{\rm cr}$ (dashed lines) shear stresses on systems $\{b1,\ a\bar{2},\ c\bar{2}\}$, c) cumulative shears on activated slip-systems, d) rotation of the tensile axis with respect to the crystallographic lattice in the stereographic projection.

The symbols $\mathbf{p}_K^*$ and $\boldsymbol{\beta}_L^*$ are defined in Table 1; a difference between H'_{KL} and H_{KL} is discussed below.

The results of simulation of the material response under uniaxial tension in the above three cases are shown in Figs. 1–3, respectively. The stress-strain curves are presented in Figs. 1a–3a, and changes of cumulative shears on activated slip-systems are given in Figs. 1c–3c. The respective hardening or softening of relevant slip-systems is shown in more detail in Figs. 1b–3b. The corresponding rotation of the tensile axis with respect to the crystallographic lattice is visualized in Figs. 1d–3d using the stereographic projection. The labeling of the relevant slip-systems, planes and directions is as follows: $b1 = (\bar{1}\bar{1}1)[011]$, $a\bar{2} = (111)[\bar{1}01]$, $c\bar{2} = (\bar{1}11)[101]$.

Early stages of plastic flow like stage I (easy glide) and a linear stage II are disregarded in the example as they are inessential for activation of the conjugate slip that takes place here later in the nonlinear regime, after overshooting the symmetry line. Also any secondary slip accompanying the dominant slip in the basic stereographic triangle is disregarded by the theory where latent hardening is greater than self-hardening. These simplifications are independent of the symmetrization and do not affect the present comparison of the effects of different symmetrization rules. It is worth mentioning that the solid line in Fig. 1a is similar in shape to that obtained in [4] without symmetrization. The initial curves up to true strain 0.27 are insensitive to the symmetrization since only a single slip operates in this range. For the same reason, the material behaviour in this range (and in the whole range in case (iii)) is independent of the value of $q > 1$.

In all cases, the primary slip-system activated is $a\bar{2}$. Increase in the true strain $\varepsilon = \ln(l/l_0)$ and tensile Cauchy stress σ (Figs. 1a–3a) is associated with rotation of the lattice and relative rotation of the tensile axis from the initial orientation $[\bar{2}\,3\,6]$ marked as $\bullet$ in Figs. 1d–3d.

In case (i), activation of the conjugate slip-system $b1$ takes place after a certain overshoot of the lattice symmetry line $[001]$–$[\bar{1}11]$ by the tensile direction and causes a change in the crystallographic lattice rotation. Subsequently, the tensile direction goes backwards to the line $[001]$–$[\bar{1}11]$ and towards the lattice direction $[\bar{1}12]$. The onset of the second stage of the deformation process, when two slip-systems $\{b1, a\bar{2}\}$ become active, is associated with discontinuous change of slope of the hardening curves. The effect of adopting different values of parameter r is only illustrated in Fig. 1a, while the remaining results shown have been obtained for $r = 1/2$. Activation of slip-system $b1$ is explained in Fig. 1b and starts at the point where the solid curve of resolved shear stress τ_{b1} reaches the dashed curve of critical resolved shear stress $\tau_{b1}^{\rm cr}$. The resolved ($\tau_{a\bar{2}}$) and critical ($\tau_{a\bar{2}}^{\rm cr}$) shear stress curves for the primary slip-system $a\bar{2}$ overlap in the whole plastic range of the deformation process calculated.

In case (ii), shortly after activating the conjugate slip-system $b1$, the third stage of the deformation process starts with sudden decrease of the stress σ, Fig. 2a. The sudden change in the material response results from unloading of both slip-systems $\{b1, a\bar{2}\}$ and activation of slip-system $c\bar{2}$, Fig. 2c. Activation of system $c\bar{2}$ causes an untypical rotation of the tensile axis with respect to the lattice, cf. Fig. 2d, which is experimentally not observed in such circumstances. The reason for the activation of the slip-system $c\bar{2}$ lies in the softening of critical resolved shear stress $\tau_{c\bar{2}}^{\rm cr}$ on the inactive slip-system $c\bar{2}$ that is induced by the P.A.N. rule, Fig. 2b. In result, the resolved shear stress $\tau_{c\bar{2}}$ reaches its critical value $\tau_{c\bar{2}}^{\rm cr}$ at $\varepsilon = 0.442$.

In case (iii), the stress-strain curve depends on how the moduli H'_{KL} in formula (5.3) are defined. If a straightforward substitution $H'_{KL} = H_{KL}$ is used

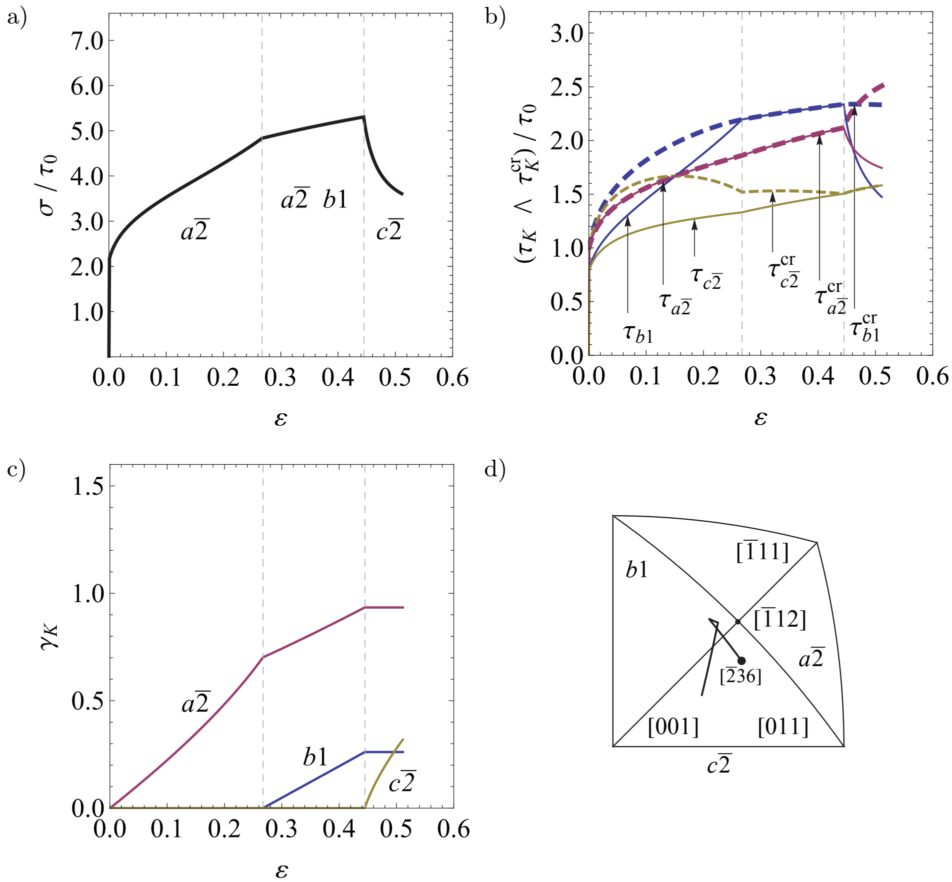

FIG. 2. Simulation of uniaxial tension using the P.A.N. symmetrization rule. The description as in Fig. 1.

then tensile stress σ increases initially, but as deformation and lattice rotation develop, a significant softening is generated, Fig. 3a, although only the primary slip-system $a\bar{2}$ remains active. The reason for this behaviour, at a first glance unexpected, lies in the presence of a negative self-hardening term $\mathbf{p}^*_{a\bar{2}} \cdot \boldsymbol{\beta}^*_{a\bar{2}}$ in formula (5.3). The use of $H'_{KL} = h$ yields the same result since $q > 1$ has no effect in this case.

Therefore, it is more reasonable to adjust H'_{KL} such that the stress-strain curve coincides with those obtained in cases (i) and (ii) in the range of activity of the single slip-system $a\bar{2}$. Moreover, in the 'simple theory' proposed by HAVNER and SHALABY [13], only one parameter is used, say $H'_{KL} = h'$. We adopt this and, to adjust the stress-strain curve as mentioned above, take $h' = h - \mathbf{p}^*_{a\bar{2}} \cdot \boldsymbol{\beta}^*_{a\bar{2}}$.

This change in moduli H'_{KL} corresponds to the change of the stress-strain curve shown in Fig. 3a, while Figs. 3c and 3d are unaffected by that change.

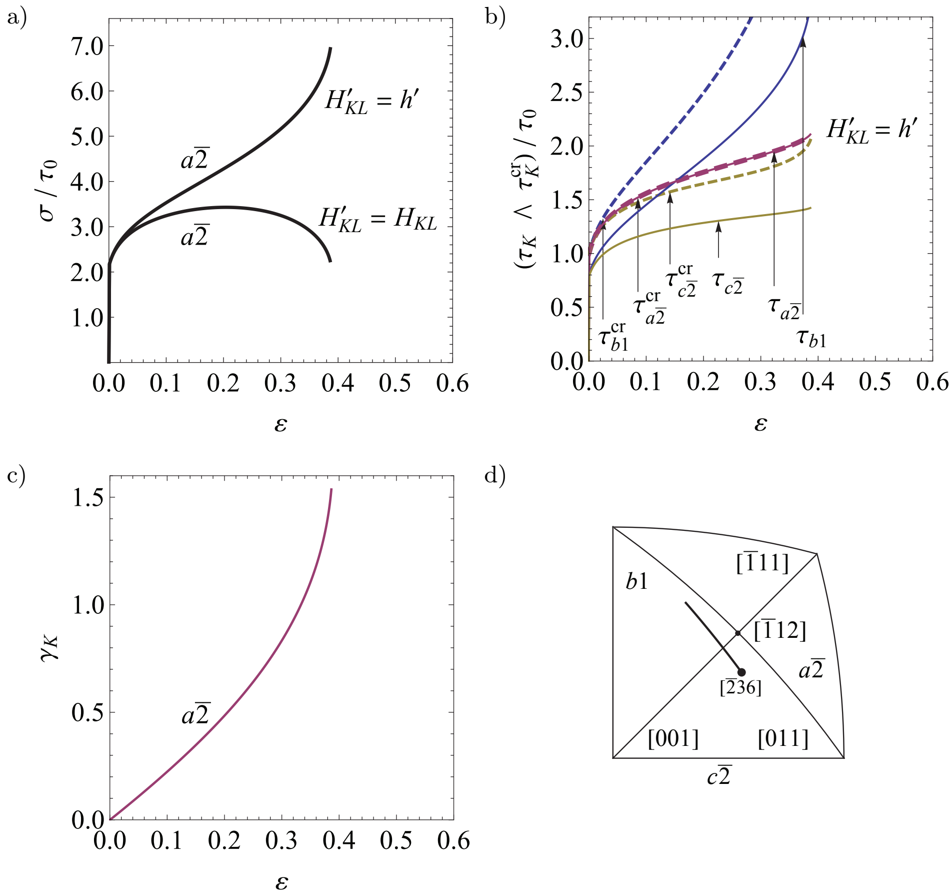

FIG. 3. Simulation of uniaxial tension using the H.S. symmetrization rule. The description as in Fig. 1; moduli H'_{KL} are discussed in the text.

The geometrical terms in the H.S. rule have significantly different effects on critical resolved shear stresses $\tau_K^{\rm cr}$ on different slip-systems, which can be seen in Fig. 3b. During the whole deformation process examined only one $a\bar{2}$ slip-system is active, Fig. 3c, also far beyond overshooting the symmetry line [001]–[$\bar{1}$11]. The deformation proceeds without changes in the tendency of lattice rotation, Fig. 3d, and with increasing hardening rate, Fig. 3a and 3b. The H.S. rule in this case does not predict activation of a conjugate slip-system even after considerable overshooting, which is not in accord with experimental evidence[6].

[6] We have also simulated the uniaxial tension test by using the symmetrization rule proposed more recently in [14] with $\beta = 1/2$. Initially the material behaviour is similar to that shown in Fig. 3, and next activation of the slip-system $c\bar{2}$ is predicted, which is also not satisfactory.

To summarize, the proposed selective symmetrization rule removes the drawbacks observed in the present modelling of uniaxial tension of a single crystal at finite plastic deformation that are induced by geometric terms in the P.A.N. [4] and H.S. [13] rules of full symmetrization of the slip-system interaction matrix (g_{KL}).

The above example is, of course, insufficient to draw a conclusion that the proposed selective symmetrization does not contradict experimental observations in general. We have deliberately avoided here any quantitative comparison with existing rich experimental data for uniaxial tension tests of different metals, as this would be a matter of curve fitting. It is fully possible that for a number of tests from a big collection discussed so far, cf. [6], satisfactory predictions are obtained by other approaches. Nevertheless, the above example is sufficient to conclude that the selective symmetrization, restricted to the set of currently active slip-systems, allows us to avoid certain undesired features introduced into the model by symmetrization of the entire matrix (g_{KL}). In particular, the proposed symmetrization eliminates (by definition) artificial latent hardening or softening of inactive slip-systems that is introduced by terms proportional to stress in the full symmetrization rules.

6. Conclusion

We have re-examined the symmetry issue of the slip-system interaction matrix in the theory of crystal plasticity at finite deformation. It has been shown that partial symmetrization of the representative matrix can be supported by physically plausible reasoning, although it requires certain specific assumptions given in Section 3. The key point is that this finding refers only to the submatrix of interaction between the *active* slip-systems in the representative space-time element of a crystal, and not to the entire interaction matrix for all slip-systems.

In accord with this observation, a new selective symmetrization rule has been proposed that is restricted to active slip-systems only. The latent hardening of inactive slip-systems, specified by any physical hardening law, remains unaffected.

In comparison to the earlier proposals of unrestricted symmetrization of the interaction matrix, no extra stress-dependent hardening or softening of *inactive* slip-systems is introduced here. The illustrative simulation of uniaxial tension test has revealed that this is advantageous as it avoids undesired effects met when applying the full symmetrization. Further work on examining other consequences of the present proposal is in progress.

Acknowledgement

This work has been partially supported by the Ministry of Science and Higher Education in Poland through Grant No. N N501 071935.

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Received December 13, 2010; revised version April 4, 2011.