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FIRST- AND SECOND-ORDER ANALYSIS OF AXIALLY LOADED CRYSTALS IN n-FOLD SYMMETRY

By K. S. HAVNER

Department of Civil Engineering, North Carolina State University, Raleigh, North Carolina 27695, *U.S.A.*

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CONTENTS

A comprehensive theoretical investigation of multiple slip in axially tensile-loaded f.c.c. crystals in n-fold symmetry positions ($n = 4, 6, 8$) is presented. The analysis is complete to second order in terms of series expansions of all variables in the prescribed small load increment. In the first part of the paper, general kinematic relations and slip-system inequalities are given, and several new results discovered that apply independently of hardening rule and degree of symmetry. Subsequent sections contain extensive first- and second-order analyses corresponding to four specific hardening theories, including Taylor's classical isotropic rule and the 'simple theory' of anisotropic latent hardening. For minimum work, unifying relations are found connecting a generic hardening parameter, its rate of change with load, and the first and second derivatives of axial stretch that hold for all four theories.

1. Introduction and scope of study

The initial (rigorous) analysis of the 'rate problem' for response of axially-loaded crystals in multiple-slip positions is found in Havner (1981). That work contains an exhaustive investigation of finite plastic straining of f.c.c. crystals (in tension) in sixfold axial symmetry according to both Taylor's classical isotropic hardening rule (Taylor & Elam 1923, 1925) and the 'simple theory' of finite distortional latent hardening introduced in Havner & Shalaby (1977). The latter hardening rule was the first (continuum) mechanics-based theory to account for the phenomenon of 'overshooting' in f.c.c. and b.c.c. crystals initially oriented for single slip, as established in the comprehensive series of papers: Havner & Shalaby (1977, 1978); Havner *et al.* (1979); Havner & Baker (1979); and Vause & Havner (1979) (also see the review article by Havner (1982*a*) for background to this theory).

The multiple-slip analysis in Havner (1981) was extended in Havner (1982*b*) to encompass compressive loading in sixfold symmetry and a two-parameter, empirical hardening rule from the metallurgical literature; and the rate problem in all double-symmetry positions was analysed for the three hardening rules. Subsequently, complete solutions for all cases of finite double slip according to the simple theory were obtained by Havner & Salpekar (1982, 1983); and Salpekar (1982) extended the tensile rate analysis in Havner (1981) to f.c.c. crystals in four and eightfold symmetry positions.

In the present work I have undertaken a substantial generalization and extension of the higher-symmetry analyses in Havner (1981, 1982*b*) and Salpekar (1982). My treatment here of tensile-loaded f.c.c. crystals, in four, six and eightfold symmetry, is in terms of series expansions of all variables, to second order, in the small yet finite load increment, taken as prescribed. Correspondingly, the first-order analysis both encompasses and extends all previous analyses of the rate problem in n-fold symmetry ($n = 4, 6, 8$), while the second-order analysis goes beyond the rate problem and so is totally new.

The balance of the paper is divided into three major sections, each containing three or more subsections. In § 2 is included a comprehensive presentation of the fundamental kinematics and critical slip-system inequalities, both first- and second-order, that must be applied in any analysis of axially-loaded crystals in n-fold symmetry, whatever hardening theory one may choose to adopt (or seek to discover from experiment). The possibilities for coincident rotation among material-, lattice-, and axis-co-rotational frames are carefully delineated and their consequences subsequently explored. Moreover, several simple relations are found that are independent of hardening rule and degree of symmetry (four, six or eightfold) and that later prove particularly useful in analysis of specific theories.

In §§ 3 and 4, four hardening theories are considered that are of value in the context of finite deformation of crystals. These are the previously mentioned Taylor hardening rule, 'simple theory', and two-parameter rule together with a recently proposed hardening theory introduced in Peirce *et al.* (1982). Particular emphasis is placed in these sections on a minimum work postulate for prescribed axial-load increment that corresponds to 'stiffest response' in n-fold symmetry and is the natural generalization of a postulate of minimum *rate* of plastic work introduced in Havner (1981).

From minimum work, a single unifying relation is established in § 3, connecting a generic hardening parameter h_0 and the rate of change of axial stretch with load, that applies to all four hardening theories and the three higher symmetry positions ($n = 4, 6, 8$). In addition, a complete first-order analysis of the hardening rule of Peirce *et al.* (1982) in sixfold symmetry is done (parallel to the rate analyses of the other three hardening theories in Havner (1981, 1982*b*) which are reviewed here). It is found that, for minimum work, this newest theory predicts axis stability, axisymmetric deformation, and isotropic hardening of both active and latent systems. The theory is alone among the four in these combined predictions.

In § 4, a second unifying relation is found connecting h_0, its rate of change with load, and the first and second derivatives of axial stretch that applies whenever the loading axis is stable in n-fold symmetry. Moreover, it is shown that in sixfold symmetry this relation is a direct consequence of minimum work for each of the four hardening theories. Thus, for 'stiffest response' of an f.c.c. crystal in sixfold symmetry (where such response is the norm), experimental information about the first and second derivatives of axial stretch is sufficient to determine the hardening modulus h_0 and its rate of change with load (at the onset of finite crystallographic slip) for all four hardening rules.

2. General analysis in n-fold symmetry

2.1. *Definitions and fundamental kinematic relations*

Let $\boldsymbol{\iota}$ denote a unit vector in the direction of prescribed tensile load per unit reference area (nominal stress) s, and λ denote the stretch of the gross crystalline material in that direction (with $\lambda\boldsymbol{\iota}$ an embedded vector). Then, Cauchy stress $\boldsymbol{\sigma}$ has the representation

$$\boldsymbol{\sigma} = \lambda s \boldsymbol{\iota} \otimes \boldsymbol{\iota}, \tag{2.1}$$

and the resolved shear stress on the kth crystallographic slip system is

$$\operatorname{tr}(N_k \boldsymbol{\sigma}) = m_k \lambda s, \quad N_k = \{(\boldsymbol{b} \otimes \boldsymbol{n})_k\}_{\mathrm{sym}}, \tag{2.2}$$

with

$$m_k = (\boldsymbol{b}_k \boldsymbol{\iota})(\boldsymbol{n}_k \boldsymbol{\iota}) = \boldsymbol{\iota} N_k \boldsymbol{\iota}, \tag{2.3}$$

where $\boldsymbol{b}_k$, $\boldsymbol{n}_k$ denote unit vectors in the slip and normal directions respectively of the kth slip system. Henceforth m_k will be called the 'Schmid factor' for that system. (Note: $\boldsymbol{ab}$ and $\boldsymbol{a}A\boldsymbol{b}$ are scalar products for vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and second-rank tensor A.)

Let $(\overset{\frown}{...})$, $\mathscr{D}/\mathscr{D}t(\ldots)$, and $(\ldots)^{\cdot}$ designate material derivatives of vector and tensor variables relative to observer frames, respectively rotating with the underlying atomic lattice, the gross crystalline material, or the loading axis. Also, let $(\ldots)^{\cdot}$ designate the frame-independent material derivative of a scalar invariant. Then, disregarding effects of infinitesimal lattice straining (typically of order 10^{-3} or less compared with unity) on slip-system directions $\boldsymbol{b}_k$, $\boldsymbol{n}_k$, one has the following alternative ways of expressing the material derivative of the invariant resolved shear stress on that system:

$$(m_k \lambda s)^{\cdot} = (\lambda s)^{\cdot} m_k + 2(\lambda s)\, \boldsymbol{\iota} N_k \hat{\boldsymbol{\iota}}, \tag{2.4}$$

$$(m_k \lambda s)^{\cdot} = (\lambda s)^{\cdot} m_k + 2(\lambda s)\, \boldsymbol{\iota} N_k \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t + (\lambda s)\, \boldsymbol{\iota}(\mathscr{D}N_k/\mathscr{D}t)\, \boldsymbol{\iota}, \tag{2.5}$$

$$(m_k \lambda s)^{\cdot} = (\lambda s)^{\cdot} m_k + (\lambda s)\, \boldsymbol{\iota}(N_k)^{\cdot}\, \boldsymbol{\iota}. \tag{2.6}$$

These expansions follow from (2.3) and the fact that N_k is constant only in a lattice-co-rotational frame while $\boldsymbol{\iota}$ is constant only in an axis-co-rotational frame.

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Let Ω and W designate material spin relative to lattice and axis-co-rotational frames respectively, and ω designate lattice spin relative to the latter frame. Then, choosing all frames momentarily to coincide, we have

$$W-\omega = \Omega = \sum_k \Omega_k \dot{\gamma}_k, \quad \Omega_k = [(\boldsymbol{b}\otimes\boldsymbol{n})_k]_{\text{skew}}, \tag{2.7}$$

a fundamental kinematic connection, with $\dot{\gamma}_k \geqslant 0$ the crystallographic slip rate in the kth system. As $-W$, $-\omega$ are the spins of the loading-axis frame relative to the material and lattice-co-rotational frames, and as $(\boldsymbol{\iota})^{\cdot} = \mathbf{0}$, there follow

$$\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = -W\boldsymbol{\iota} = D\boldsymbol{\iota} - (\dot{\lambda}/\lambda)\,\boldsymbol{\iota} = \sum_k \dot{\gamma}_k(N_k - m_k I)\boldsymbol{\iota}, \tag{2.8}$$

$$\dot{\boldsymbol{\iota}} = -\omega\boldsymbol{\iota} = (D+\Omega)\,\boldsymbol{\iota} - (\dot{\lambda}/\lambda)\,\boldsymbol{\iota} = \sum_k \dot{\gamma}_k[(\boldsymbol{b}\otimes\boldsymbol{n})_k - m_k I]\,\boldsymbol{\iota}, \tag{2.9}$$

where the terms on the extreme right in (2.8), (2.9) reflect a disregard of the contribution of infinitesimal lattice straining (at constant pressure) to the rate of deformation (Eulerian strain rate) D, whence

$$D = \sum_k N_k \dot{\gamma}_k, \quad (\dot{\lambda}/\lambda) = \boldsymbol{\iota}D\boldsymbol{\iota} = \sum_k m_k \dot{\gamma}_k. \tag{2.10}$$

Further, the rates of change of N_k in material and axis-co-rotational frames are given by

$$\mathscr{D}N_k/\mathscr{D}t = N_k\Omega - \Omega N_k = N_k \sum_j \Omega_j \dot{\gamma}_j - \sum_j \dot{\gamma}_j \Omega_j N_k, \tag{2.11}$$

$$(N_k)^{\cdot} = -N_k\omega + \omega N_k. \tag{2.12}$$

Henceforth we shall refer to the axis-co-rotational frame simply as the loading frame.

Consider a situation in which at least two of the defined reference frames remain coincident during multiple slip. From (2.7) there obviously are four possibilities: (i) $\omega = 0$, the lattice-co-rotational and loading frames rotate together while the material-co-rotational frame rotates separately; (ii) $W = 0$, the material-co-rotational and loading frames rotate together while the lattice-co-rotational frame rotates separately; (iii) $\Omega = 0$, the lattice and material-co-rotational frames rotate together while the loading frame rotates separately; (iv) $\omega = W = \Omega = 0$, all three frames rotate together (i.e. there is no rotation of either material or lattice relative to the loading frame). For the analysis of pure axial loading, we shall find it useful to modify these four cases by specifying only that: (i) $\dot{\boldsymbol{\iota}} = -\omega\boldsymbol{\iota} = \mathbf{0}$; (ii) $\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = -W\boldsymbol{\iota} = \mathbf{0}$; (iii) $\dot{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t$, whence $\Omega\boldsymbol{\iota} = \mathbf{0}$; (iv) $\dot{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = \mathbf{0}$, whence $\omega\boldsymbol{\iota} = W\boldsymbol{\iota} = \Omega\boldsymbol{\iota} = \mathbf{0}$. The corresponding equations in terms of slip rates are:

$$\text{(i)} \quad \dot{\boldsymbol{\iota}} = \mathbf{0}, \quad \sum_k \dot{\gamma}_k[(\boldsymbol{b}\otimes\boldsymbol{n})_k - m_k I]\,\boldsymbol{\iota} = \mathbf{0}; \tag{2.13}$$

$$\text{(ii)} \quad \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = \mathbf{0}, \quad \sum_k \dot{\gamma}_k[N_k - m_k I]\,\boldsymbol{\iota} = \mathbf{0}; \tag{2.14}$$

$$\text{(iii)} \quad \dot{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t, \quad \sum_k \dot{\gamma}_k \Omega_k \boldsymbol{\iota} = \mathbf{0}; \tag{2.15}$$

$$\text{(iv)} \quad \dot{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = \mathbf{0}; \text{ both (2.14) and (2.15) (whence (2.13)) are satisfied.} \tag{2.16}$$

The physical interpretation of (2.13)–(2.15) is of course that the respective axial vectors of spins ω, W or Ω are collinear with $\boldsymbol{\iota}$. In general, for one of these cases to occur, at least three slip systems must be active simultaneously. We shall consider this further in a later section.

Finally, we note the necessary and sufficient condition that the material and axis-co-rotational derivatives of N_k coincide. From (2.7), (2.11) and (2.12) this is

$$N_k W - W N_k = 0. \tag{2.17}$$

It is readily established that the combined conditions (2.14) and (2.17), corresponding to $\mathscr{D}\iota/\mathscr{D}t = (\iota)^{\cdot} = \mathbf{0}$ and $\mathscr{D}N_k/\mathscr{D}t = (N_k)^{\cdot}$, are satisfied only in the event that $W = 0$.

2.2. *First- and second-order inequalities in critical systems*

We denote the *critical strength* ('flow stress') in the kth crystallographic slip system by τ_k and consider its rate of change to be a linear function of the slip rates in all active systems (see Hill 1966; Hill & Havner 1982, §7):

$$\dot{\tau}_k = \sum_j H_{kj} \dot{\gamma}_j. \tag{2.18}$$

The H_{kj} will be called the physical slip-system hardening moduli. They may be both functions of the current stress state (for example dependent on the orientation of the tensile or compressive force relative to the lattice in axial loading) as well as functions of the slip-history; but they are assumed to be independent of which systems are momentarily active.† The critical strengths τ_k are considered to depend only on the slip history. Thus, the general hardening law (2.18) is consistent with the following scenario.

A crystal is unloaded from a plastically deformed state without further slipping. Then, a differently oriented specimen taken from the deformed 'parent' crystal is reloaded until measurable slip is initiated in one or more systems distinct from those (or that one) originally active. *The unknown critical strengths developed in these previously latent systems, as a consequence of the original deformation of the parent crystal, are taken to equal the respective resolved shear stresses on the systems at the onset of slip in the reloaded specimen.* (This is in fact the standard experimental procedure for determination of latent hardening in cubic crystals. See, for example, Jackson & Basinski 1967; Franciosi *et al.* (1980).)

In accordance with the above, a slip system in a crystal under load is defined as *critical* at a material point if its resolved shear stress (dependent only on current stress state) equals its critical strength (dependent only on slip history). In a critical system the rate of change of resolved shear stress, in quasi-static loading, may not exceed the rate of change of critical strength. An *active* system is of course one in which $\dot{\gamma}_k > 0$, and only a critical system can be active. Necessary (but not sufficient) conditions for a slip system to be active are therefore

$$\operatorname{tr}(N_k \boldsymbol{\sigma}) = \tau_k, \quad \operatorname{tr}(N_k \boldsymbol{\sigma})^{\cdot} = \dot{\tau}_k. \tag{2.19}$$

A system satisfying these necessary conditions (hence remaining critical) but in which $\dot{\gamma}_k = 0$ will be labelled *inactive-critical*. A critical system that does not satisfy the second necessary condition (i.e. in which $\operatorname{tr}(N_k \boldsymbol{\sigma})^{\cdot} < \dot{\tau}_k$) will be labelled *inactivated*.

† In Franciosi *et al.* (1980), equations encompassed by (2.18) are given in the form $\tau_k = \tau_0 + \Sigma_j H_{kj} \gamma_j$, requiring all physical hardening moduli to be constant. Then, experimental evidence of rapidly increasing (followed by decreasing) plastic anisotropy in single slip is offered as conclusive argument that the γ_j are not a sufficient set of kinematic variables for characterization of gross crystal hardening. Rather, various dislocation measures are introduced in order to express 'adequate' hardening laws. The problem, however, lies *not* with the adequacy of macroscopic slip rates as the independent kinematic variables but with the assumption that the H_{kj} are constant.

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Henceforth we shall be concerned only with the analysis of initially critical systems at $s = s_0$ for small but finite changes δs in the nominal stress. Define

$$f_k = \tau_k - m_k \lambda s \geqslant 0, \tag{2.20}$$

as the (non-negative) difference between critical strength and resolved shear stress in the kth slip system. Then, indicating differentiation with respect to s by $(\ldots)'$, we must have in each of the n initially critical systems

$$(f_k)_0 = 0, \quad (f'_k)_0 \geqslant 0, \quad f'_k \gamma'_k = 0, \quad \gamma'_k \geqslant 0, \tag{2.21}$$

and

$$\int_{s_0}^{s_0+\delta s} f'_k \, \mathrm{d}s \geqslant 0, \quad k = 1, \ldots, n, \tag{2.22}$$

with the equality in (2.22) of course satisfied for an active system.

Consider a unidirectional (i.e. $s \geqslant s_0$) Taylor series expansion of f'_k, in an initially critical system, about the reference stress s_0: $f'_k = (f'_k)_0 + (f''_k)_0 (s - s_0) + \ldots$. On substituting into (2.22) and integrating we find

$$(f'_k)_0 \delta s + \tfrac{1}{2}(f''_k)_0 \delta s^2 \geqslant 0, \quad k = 1, \ldots, n, \tag{2.23}$$

correct to second order in δs. For systems respectively active, inactive-critical, or inactivated during the small nominal stress change δs, there follow (from (2.21) and (2.23))

active: $(f'_k)_0 = 0, \quad (f''_k)_0 = 0;$ (2.24)

inactive-critical: $(f'_k)_0 = 0, \quad (f''_k)_0 \geqslant 0;$ (2.25)

inactivated: $(f'_k)_0 > 0$, sign of $(f''_k)_0$ undetermined. (2.26)

Thus, in all critical systems

$$(\tau'_k - m'_k \lambda s)_0 \geqslant (m_k (\lambda s)')_0, \tag{2.27}$$

and in each active or inactive-critical system

$$(\tau''_k - m''_k \lambda s - 2m'_k (\lambda s)')_0 \geqslant (m_k (\lambda s)'')_0. \tag{2.28}$$

Inequalities (2.27) and (2.28), henceforth called the *first- and second-order inequalities in critical systems*, will be the focus of our analysis herein. (It is important to emphasize that (2.28) necessarily holds in an initially critical system only if the *equality* holds in (2.27), that is only if the system remains critical during a small increment in load.)

From (2.3), (2.9) and (2.10) we have

$$m'_k = 2\boldsymbol{\iota} N_k \hat{\boldsymbol{\iota}} = \sum_j n_{kj} \gamma'_j - 2m_k (\lambda'/\lambda), \tag{2.29}$$

with

$$n_{kj} = 2\boldsymbol{\iota} N_k (\boldsymbol{b} \otimes \boldsymbol{n})_j \boldsymbol{\iota}, \quad \lambda'/\lambda = \sum_j m_j \gamma'_j. \tag{2.30}$$

Therefore the first-order inequalities (2.27) can be expressed in the form

$$(\tau'_k)_0 \geqslant (\lambda s)_0 \sum_j (n_{kj} \gamma'_j)_0 + (m_k)_0 (\lambda - \lambda' s)_0, \quad k = 1, \ldots, n, \tag{2.31}$$

which is of course completely general.

2.3. *F.c.c. crystals in four, six, or eightfold symmetry*

Consider a virgin or equally-hardened f.c.c. crystal with all $\tau_k = \tau_0$ (momentarily) and the tensile loading axis in a four, six or eightfold symmetry position at $s = s_0$. In each of the n critical systems $(m_k)_0 = m$, a constant dependent only on the axis position ($m = 1/\sqrt{6}$, $2/3\sqrt{6}$, or $1/\sqrt{6}$ in four, six or eightfold symmetry respectively). Moreover, in each of these multiple-slip positions the elements of any row of the corresponding matrix (n_{kj}) in (2.31) are permutations of the elements of any other row, as may be seen in the Appendix. Consequently,

$$\sum_k (n_{kj})_0 = M, \quad j = 1, \ldots, n, \tag{2.32}$$

with M also dependent only on the degree of symmetry. Specifically, $M = \frac{4}{3}$, $\frac{8}{9}$, or $\frac{8}{3}$ in four, six or eightfold symmetry, and we observe that

$$M = 2nm^2, \quad n = 4, 6, 8. \qquad (2.33)\dagger$$

Now let us sum the first-order inequalities (2.31) over the n critical systems in four, six or eightfold symmetry. On substituting the second equation in (2.30), (2.32) and (2.33), we discover the remarkably simple result

$$\sum_k (\tau'_k)_0 \geqslant nm(\lambda s)'_0, \quad n = 4, 6, 8, \tag{2.34}$$

which must hold for all f.c.c. crystals momentarily in a higher symmetry position, however they subsequently rotate and deform. That is, (2.34) presupposes neither a particular hardening law nor axis stability in the corresponding n-fold position. Comparing (2.27) with (2.34), we see that the essential content of the latter is

$$\sum_k (m'_k)_0 = 0, \quad \text{in four, six or eightfold symmetry}, \tag{2.35}$$

(with summation on all critical systems) which of course can be determined directly from (2.29), (2.30), (2.32), (2.33). Thus, *independent of how the Schmid factors m_k may change individually, whenever the loading axis rotates away from an n-fold symmetry position, the sum of their rates of change over all initially critical systems must be zero*. (This is a general result, previously unremarked, that I have not seen elsewhere in the literature.)

In terms of the slip-rates γ'_j and physical hardening moduli H_{kj}, (2.34) may be equivalently expressed

$$\sum_k \sum_j (H_{kj} \gamma'_j)_0 - nm^2(\lambda s)_0 \sum_j (\gamma'_j)_0 \geqslant nm\lambda_0, \quad n = 4, 6, 8, \tag{2.36}$$

with each summation taken over the n critical systems. Consider the set of 'effective' hardening moduli h_{kj}, related to the H_{kj} through (see, for example, Havner & Shalaby 1977, equation (22), or Hill & Havner 1982, equation (7.14))

$$H_{kj} = h_{kj} - \operatorname{tr}(N_k \boldsymbol{\alpha}_j), \quad \boldsymbol{\alpha}_j = 2\{\boldsymbol{\sigma}\Omega_j\}_{\text{sym}}. \tag{2.37}$$

For axial loading, from (2.1),

$$\operatorname{tr}(N_k \boldsymbol{\alpha}_j) = 2 \operatorname{tr}(N_k \boldsymbol{\sigma} \Omega_j) = (\lambda s)\, r_{kj}, \tag{2.38}$$

with

$$r_{kj} = -2\boldsymbol{\iota} N_k \Omega_j \boldsymbol{\iota}. \tag{2.39}$$

† In every double-symmetry orientation, namely along the three sides of standard stereographic triangle $a\bar{2}$ of figure 1, the 2×2 matrix (n_{kj}) is symmetric with equal diagonal terms (see Havner 1982*b*, §4). Thus, $\Sigma_k (n_{kj})_0$ is again a constant dependent only on orientation. However, (2.33) is not satisfied for $n = 2$.

In each of four, six or eightfold symmetry the kth row elements of the corresponding matrix (r_{kj}) are not only permutations of the elements of any other row, as in the case of matrix (n_{kj}), but also their sum is zero (see Appendix):

$$\sum_k (r_{kj})_0 = 0, \quad j = 1, \ldots, n. \tag{2.40}$$

Thus, the sums over critical systems of the effective and physical hardening moduli for each of the higher symmetry positions are equal:

$$\sum_k (H_{kj})_0 = \sum_k (h_{kj})_0, \quad n = 4, 6, 8. \tag{2.41}$$

Consequently, $\Sigma_k(H_{kj})_0$ in (2.36) may be replaced by $\Sigma_k(h_{kj})_0$ at will.

Lastly, we define

$$a_{kj} = H_{kj} - (\lambda s)\, n_{kj} = h_{kj} - (\lambda s)\, m_{kj}, \tag{2.42}$$

with

$$m_{kj} = n_{kj} + r_{kj} = 2\boldsymbol{\iota} N_k N_j \boldsymbol{\iota}, \tag{2.43}$$

and express the first-order inequalities (2.31) in the alternative form

$$\sum_j (a_{kj}\gamma'_j)_0 \geqslant (m_k)_0 (\lambda - \lambda' s)_0, \quad k = 1, \ldots, n, \tag{2.44}$$

with of course $(m_k)_0 = m$. Observe that (m_{kj}) is a symmetric matrix whereas (n_{kj}) is not. Thus, if matrix (a_{kj}) is symmetric so will be the moduli h_{kj}, while moduli H_{kj} will be unsymmetric. Conversely, both (a_{kj}) and h_{kj} are unsymmetric if the H_{kj} are symmetric.

3. First-order analyses of specific hardening rules

3.1. *Hardening theories to be considered*

In Havner & Salpekar (1983, § 2) four hardening rules are identified that are 'of demonstrated usefulness relevant to finite distortion of cubic crystals'. They are: (i) Taylor's classic theory of isotropic hardening (Taylor & Elam 1923, 1925); (ii) an empirically-based, two-parameter modification of Taylor's rule (see Nakada & Keh 1966; Jackson & Basinski 1967); (ii) the 'simple theory' of rotation-dependent† crystal anisotropy introduced by Havner & Shalaby (1977); and (iv) a modification and extension of the 'simple theory' proposed by Peirce *et al.* (1982), here called the 'P.A.N. rule'. The four theories, encompassed by the general hardening law (2.18), may be expressed as follows:

(i) Taylor's rule: $\dot{\tau}_k = H\sum_j \dot{\gamma}_j$ for all k, $H > 0$; (3.1)

(ii) two-parameter rule:
$$\left.\begin{aligned} \dot{\tau}_k &= H_1 \sum_l \dot{\gamma}_l + H_2 \sum_m \dot{\gamma}_m, \\ \boldsymbol{n}_l &= \boldsymbol{n}_k, \quad \boldsymbol{n}_m \neq \boldsymbol{n}_k, \quad H_2 > H_1 > 0; \end{aligned}\right\} \tag{3.2}$$

(iii) simple theory:
$$\left.\begin{aligned} \dot{\tau}_k &= h \sum_j \dot{\gamma}_j - 2\,\mathrm{tr}\,(N_k \boldsymbol{\sigma} \Omega) \\ &= \sum_j (h - \mathrm{tr}\, N_k \boldsymbol{\alpha}_j)\, \dot{\gamma}_j, \quad h > 0; \end{aligned}\right\} \tag{3.3}$$

(iv) P.A.N. rule:
$$\left.\begin{aligned} \dot{\tau}_k &= \hbar \sum_j \dot{\gamma}_j - \mathrm{tr}\,(N_k \boldsymbol{\sigma} \Omega) - \mathrm{tr}\,(\Omega_k \boldsymbol{\sigma} D) \\ &= \sum_j (\hbar - \tfrac{1}{2}\,\mathrm{tr}\, N_k \boldsymbol{\alpha}_j + \tfrac{1}{2}\,\mathrm{tr}\, \boldsymbol{\alpha}_k N_j)\, \dot{\gamma}_j, \quad \hbar > 0. \end{aligned}\right\} \tag{3.4}$$

† Here is meant *relative* rotation of material and lattice corresponding to the relative spin Ω.

(Peirce *et al.* (1982) also give a two-parameter modification of (3.4) in which $\hbar$ is replaced by $q\hbar+(1-q)\,\hbar\delta_{kj}$, with q an independent parameter and δ_{kj} the Kronecker delta. We shall consider only $q=1$, i.e. (3.4) here.)

It is instructive to give the 'effective' hardening moduli h_{kj} for each of the last two theories. From (2.37) with (3.3) and (3.4) one finds:

$$\text{simple theory: } h_{kj} = h \quad \text{for all} \quad k, j; \tag{3.5}$$

$$\text{P.A.N. rule: } h_{kj} = \hbar + \tfrac{1}{2}\,\mathrm{tr}\,(N_k \boldsymbol{\alpha}_j + N_j \boldsymbol{\alpha}_k). \tag{3.6}$$

The symmetry of the h_{kj} is evident in each of these theories, as is the motivation for the name 'simple theory' from (3.5). In contrast, the physical hardening moduli H_{kj} are symmetric in each of the other two theories (as the H_{kj} also are symmetric in the 'kinematic' hardening rules of Budiansky & Wu (1962) and Weng (1979)), whence the corresponding h_{kj} are unsymmetric. Symmetry of moduli h_{kj}, rather than H_{kj}, was explicitly proposed in the context of crystal mechanics by Havner & Shalaby (1977, §§ 3 and 4).

For axial loading, note from (2.38) that (3.6) can be expressed:

$$\text{P.A.N. rule: } h_{kj} = \hbar + \tfrac{1}{2}\lambda s(r_{kj} + r_{jk}). \tag{3.7}$$

We shall find this form convenient here.

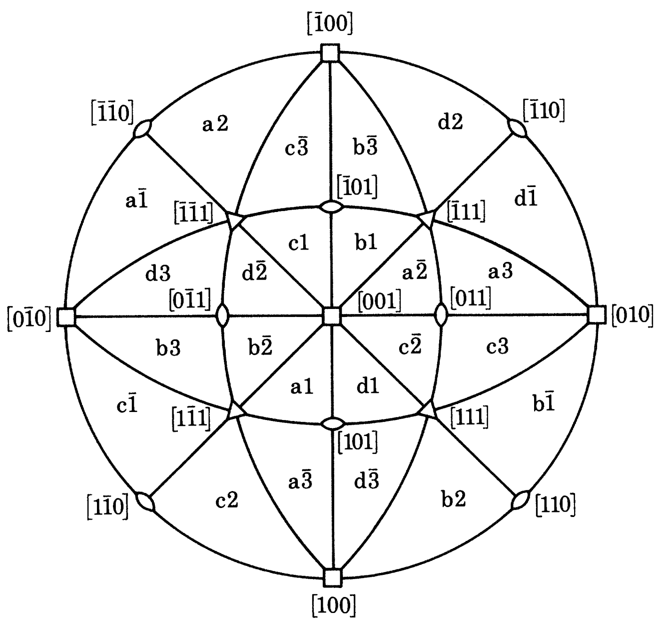

Figure 1. Standard [001] stereographic projection showing f.c.c. crystal slip systems.

3.2. *First-order analysis and a minimum work postulate*

In each of four, six and eightfold symmetry, using (2.40), (2.41), figure 1, table 1, and (3.1), (3.2), (3.5), or (3.7) as appropriate, we find:

(i) Taylor hardening: $\sum_k H_{kj} = nH;$ (3.8)

(ii) two-parameter rule: $\sum_k H_{kj} = 2H_1 + (n-2) H_2 = n\bar{H}$; (3.9)†

(iii) simple theory: $\sum_k H_{kj} = nh$; (3.10)

(iv) P.A.N. rule: $\sum_k H_{kj} = n\hbar$; (3.11)

each independent of j. For convenience in subsequent equations, let h_0 be a generic label for the various moduli H (Taylor modulus), $\bar{H}$ (defined by (3.9)), h, and $\hbar$ evaluated at s_0 in a particular symmetry position. Then, as

$$m \sum_j (\gamma_j')_0 = (\lambda'/\lambda)_0, \tag{3.12}$$

from the second equation of (2.10), there follows from the above

$$\sum_k \sum_j (H_{kj}\gamma_j')_0 = (n/m)\, h_0(\lambda'/\lambda)_0, \quad n = 4, 6, 8. \tag{3.13}$$

Whence, from (2.36), we have the following simple lower bound to the rate of change of axial stretch with respect to applied nominal stress, applicable to all four hardening rules in each of the three higher symmetry positions:

$$\lambda_0' \geqslant (m\lambda_0)^2/[h_0 - m^2(\lambda s)_0], \quad h_0 > m^2(\lambda s)_0. \tag{3.14}$$

Alternatively, if $\lambda_0' \equiv (d\lambda/ds)_0$ is available from experimental test, (3.14) gives a lower bound to the generic modulus h_0:

$$h_0 \geqslant m^2(\lambda s)_0 + (m\lambda_0)^2/\lambda_0'. \tag{3.15}$$

Table 1. Designation of slip systems in f.c.c. crystals

plane		(111)			$(\bar{1}\bar{1}1)$			$(\bar{1}11)$			$(1\bar{1}1)$	
direction	$[0\bar{1}1]$	$[10\bar{1}]$	$[\bar{1}10]$	$[011]$	$[\bar{1}0\bar{1}]$	$[1\bar{1}0]$	$[0\bar{1}1]$	$[\bar{1}0\bar{1}]$	$[110]$	$[011]$	$[10\bar{1}]$	$[\bar{1}\bar{1}0]$
system	a1	a2	a3	b1	b2	b3	c1	c2	c3	d1	d2	d3

For axially-loaded crystals in multiple-slip positions, different modes of finite-deformation response not only are kinematically possible, they indeed have been observed experimentally. (Note, however, that the precise specification of an n-fold symmetry position apparently is accurate only to within one or two degrees of orientation in an actual test.) These various responses correspond to different load–displacement (s–λ) curves, and the accepted experimental position seems to be that the highest number of active systems in a particular n-fold position, or at least the highest symmetry of deformation there, corresponds to the highest s–λ curve: that is, to the 'stiffest' response.

It is evident from figure 2 that the stiffest response is defined by the minimum increment in work δw, per unit reference volume, for a small increment δs in nominal stress (as this work is merely the area under the s–λ curve of a particular deformation response). From a Taylor series expansion it is readily found that

$$\delta w = \int_{s_0}^{s_0+\delta s} s\, d\lambda = (s\lambda')_0\, \delta s + \tfrac{1}{2}(\lambda' + s\lambda'')_0\, \delta s^2 + \dots. \tag{3.16}$$

† This follows from the fact that, for each critical slip system k in four, six or eightfold symmetry, one and only one other critical system l has a slip plane in common ($\boldsymbol{n}_l = \boldsymbol{n}_k$). Refer to figure 1 and table 1.

Consequently, to minimize δw correct to second order in δs and achieve the stiffest response from state $(s, \lambda)_0$,

$$\text{minimize } \lambda_0' \quad \text{and} \quad \lambda_0''. \tag{3.17}$$

This statement is of course independent of hardening rule, but upon comparing (3.17) with (3.14) we see that each of the considered theories provides the minimum λ_0', hence the stiffest response, if no critical system is *inactivated* (that is if every system is either active or inactive-critical as defined by (2.25)). Subsequently we shall find that this result is consistent with the (apparent) experimental position of highest symmetry deformation for each of the four hardening rules considered here.

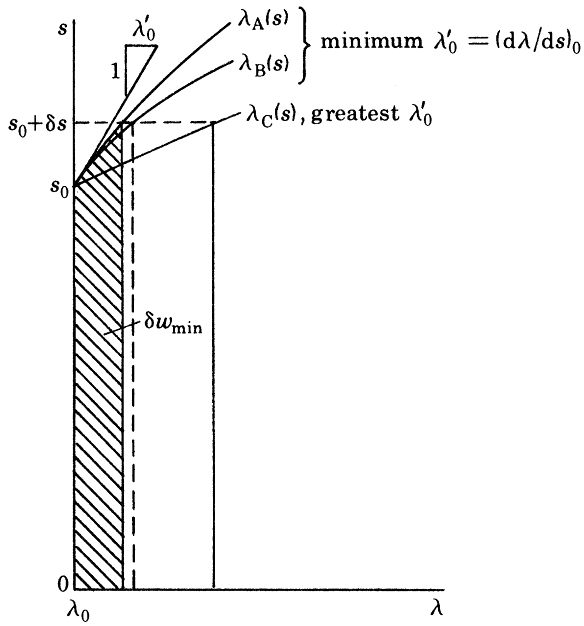

FIGURE 2. Possible deformation responses to nominal stress increment δs in an n-fold symmetry position: $\lambda_A(s)$, anticipated greatest number of active systems; $\lambda_C(s)$, anticipated least number of active systems (single or double slip).

A postulate of minimum *rate* of plastic work was introduced in Havner (1981) as a basis for the selection of axis stability and axisymmetric deformation from among the various solutions permitted by the rate-type constitutive inequalities, of either Taylor hardening or the simple theory, in sixfold symmetry. This connection was extended to the two-parameter rule in Havner (1982*b*, theorem 6.1), where is also included the analysis of rate-type inequalities in all double-symmetry positions for all three hardening theories. Rate-type inequalities and the minimization of plastic work rate for a given nominal stress rate (hence the highest $(ds/d\lambda)_0$) are, of course, fully equivalent to the first-order inequalities and first term in the series expansion of incremental work here. Hence, we shall call on these previous results for the first-order analyses of the above three hardening rules and extend the detailed analysis to the P.A.N. rule only in sixfold symmetry.

3.3. *First-order solutions in sixfold symmetry*

3.3.1. *Taylor hardening and the two-parameter rule*

For tensile loading in sixfold symmetry (namely $[\bar{1}11]$ in figure 1), Taylor hardening and the two-parameter rule may be treated together. (A separate analysis for Taylor hardening was first given in Havner (1981).) The corresponding first-order inequalities (Havner 1982*b*, equations (6.1)) follow by substituting (3.2) (with $\dot{\tau}_k$, $\dot{\gamma}_j$ replaced by τ'_k, γ'_j), (A 2), and $(m_k)_0 = m = 2/3\sqrt{6}$ into (2.31) for each of the six critical systems. For minimum work, hence the stiffest response, all *equalities* are satisfied (from (3.14) and (3.17)), and the system of six equations can be reduced to the following set of five (Havner 1982*b*, equations (6.5)):

$$(\gamma'_1+\gamma'_6)_0 = (\gamma'_2+\gamma'_4)_0 = (\gamma'_3+\gamma'_5)_0 = m\lambda_0/[3h_0-\tfrac{2}{9}(\lambda s)_0], \tag{3.18}$$

$$(a-1)\,(\gamma'_1-\gamma'_3)_0+a(\gamma'_2-\gamma'_4)_0+(\gamma'_5-\gamma'_6)_0 = 0, \tag{3.19}$$

$$a(\gamma'_1+\gamma'_2-\gamma'_5-\gamma'_6)_0 = 0, \tag{3.20}$$

in which

$$a = \tfrac{9}{2}(H_2-H_1)/(\lambda s)_0, \quad h_0 = \tfrac{1}{3}H_1+\tfrac{2}{3}H_2, \tag{3.21}$$

with the critical systems at $\boldsymbol{\iota}_0 = [\bar{1}11]$ (see figure 1) numbered 1–6 in the order a$\bar{2}$, a3, b1, b$\bar{3}$, d$\bar{1}$, d2. For $H_2 \neq H_1$, (3.18)–(3.20) are independent and one obtains (Havner 1982*b*, equations (6.6))

$$(\gamma'_1)_0 = (\gamma'_4)_0 = (\gamma'_5)_0 \quad \text{and} \quad (\gamma'_2)_0 = (\gamma'_3)_0 = (\gamma'_6)_0, \quad \gamma'_k \geqslant 0. \tag{3.22}$$

Equations (3.18), which hold for $H_2 = H_1 = H$ as well (that is for Taylor hardening), are precisely the conditions (2.13) for zero tensile-axis rotation relative to the lattice, namely $\dot{\boldsymbol{\iota}} = \mathbf{0}$, as shown in Havner (1981, equations (3.21)). The solution (3.22), which *necessarily* holds only for $H_2 \neq H_1$, corresponds to axisymmetric deformation relative to the sixfold axis (Havner 1981, § 3.4). Taylor hardening, then, requires axis stability for minimum λ'_0 but permits other deformation modes than axisymmetric, as first shown in Havner (1981). These results are summarized in the following two theorems:

THEOREM 3.1 (Havner 1981). *The tensile loading axis is stable in the sixfold symmetry position, corresponding to Taylor hardening, if and only if the rate of plastic work is a minimum.*

THEOREM 6.1 (Havner 1982*b*). *The tensile loading axis is stable and the deformation is axisymmetric in the sixfold symmetry position, corresponding to the two-parameter rule $H_2 > H_1$, if and only if the rate of plastic work is a minimum.*

(It may be noted in passing that theorem 6.1 also would hold for $H_2 < H_1$, or relative latent *softening*. Such a hardening rule has no basis in experiment however.)

3.3.2. *Simple theory of rotation dependent anisotropy*

For the simple theory, the required first-order inequalities in sixfold symmetry are identically equations (3.22) of Havner (1981); and the matrix from the left side of system (3.22) in that reference is the same as $(m_{kj})_0 = (n_{kj})_0+(r_{kj})_0$ from (A 2) and (A 5) here. Specifically, on substituting (3.5) and (3.12) into (2.42) and (2.44), one obtains

$$(h_0/m)\,(\lambda'/\lambda)_0 \geqslant (\lambda s)_0 \sum_j (m_{kj}\gamma'_j)_0+m(\lambda-\lambda' s)_0, \quad k = 1, \ldots, n, \tag{3.23}$$

with matrix $(m_{kj})_0$ singular of rank 3 for $n = 6$ as established in Havner (1981, § 3.3). As before, all equalities must hold for minimum work, hence at least three systems must be active. The corresponding general solution is given by equations (3.26) in Havner (1981). For the investigation here, it is convenient to have the reduced set of three equations in the alternative but algebraically equivalent form

$$\left.\begin{aligned} 3(\gamma_1'+\gamma_2')_0 &= \tfrac{2}{3}\sum_j(\gamma_j')_0+(\gamma_4'+\gamma_6')_0 > 0,\\ 3(\gamma_3'+\gamma_4')_0 &= \tfrac{2}{3}\sum_j(\gamma_j')_0+(\gamma_2'+\gamma_5')_0 > 0,\\ 3(\gamma_5'+\gamma_6')_0 &= \tfrac{2}{3}\sum_j(\gamma_j')_0+(\gamma_1'+\gamma_3')_0 > 0,\end{aligned}\right\} \tag{3.24}$$

with of course

$$\sum_j(\gamma_j')_0 = (1/m)\,(\lambda_0'/\lambda_0)_{\min} = \frac{m\lambda_0}{h_0-\frac{2}{27}(\lambda s)_0},\quad m = 2/3\surd 6, \tag{3.25}$$

from (3.12) and (3.14). It is evident from (3.24) that the simple theory requires there to be at least one non-zero slip rate from each pair (1, 2), (3, 4), and (5, 6), which means that there must be slip on each of the slip planes (111), $(\bar{1}\bar{1}1)$, and $(1\bar{1}\bar{1})$ at $\boldsymbol{\iota}_0 = [\bar{1}11]$ for minimum work. (This of course encompasses the axisymmetric deformation of (3.22).) Taylor hardening, however, requires only that (3.18) be satisfied; hence only two of the three critical planes need experience slip for minimum work (that is stiffest response).

Further manipulations of (3.24) lead to the following relations (Havner 1981, equations (3.28)):

$$\left.\begin{aligned} 7(\gamma_1'+\gamma_2')_0-2(\gamma_3'+\gamma_5')_0-5(\gamma_4'+\gamma_6')_0 &= 0,\\ 2(\gamma_1'+\gamma_6')_0+5(\gamma_2'+\gamma_5')_0-7(\gamma_3'+\gamma_4')_0 &= 0,\\ 5(\gamma_1'+\gamma_3')_0+2(\gamma_2'+\gamma_4')_0-7(\gamma_5'+\gamma_6')_0 &= 0,\end{aligned}\right\} \tag{3.26}$$

where the third equation, obviously dependent (being the difference between the first two), is given merely for completeness. It is implicit in Havner (1981, equations (3.27)), although not remarked there, that (3.26) are precisely the conditions (given here as (2.14), rotation case (ii)) for zero tensile axis rotation relative to a *material* co-rotational frame. That is,

$$(\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t)_0 = \mathbf{0},\quad \text{or}\quad (D\boldsymbol{\iota})_0 = (\dot{\lambda}/\lambda)_0\boldsymbol{\iota}_0, \tag{3.27}$$

according to the simple theory in sixfold symmetry. (Recall that the requirement for Taylor hardening is, in contrast, $\dot{\boldsymbol{\iota}}_0 = \mathbf{0}$.)

Finally, as shown in Havner (1981, § 3.4), if the condition of axis stability relative to the lattice is imposed on the simple theory, then the combination of (3.26) $(\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = \mathbf{0})$ with (3.18) $(\dot{\boldsymbol{\iota}}_0 = \mathbf{0})$ leads to the axisymmetric solution (3.22). That is, *for tensile axis stability in the sixfold symmetry position, the simple theory uniquely predicts axisymmetric deformation of the crystal* (Havner 1981, p. 344).

3.3.3. *P.A.N. rule*

To my knowledge the P.A.N. rule has not previously been investigated for the case of tensile loading of f.c.c. crystals in sixfold symmetry. Consequently, the first-order analysis for this theory is presented in somewhat more detail than was given for the other three hardening rules.

From (3.7), (2.42), (2.43), (3.12) and the symmetry of the m_{kj}, the first-order inequalities (2.44) become for the P.A.N. rule

$$(h_0/m)\,(\lambda'/\lambda)_0 \geqslant (\lambda s)_0\sum_j\{\tfrac{1}{2}(n_{kj}+n_{jk})\,\gamma_j'\}_0+m(\lambda-\lambda' s)_0,\quad k = 1,\dots,n, \tag{3.28}$$

where again the generic modulus h_0 has been used consistent with (3.14), which applies to all four theories. (As it stands, (3.28) governs solutions for the P.A.N. rule in each of four, six or eightfold symmetry.) From (A 2), the full equations in sixfold symmetry are (with $m = 2/3\sqrt{6}$):

$$\left.\begin{aligned}
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(2,1,5,3,3,2)\,\gamma_0' + m(\lambda-\lambda' s)_0,\\
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(1,2,3,2,5,3)\,\gamma_0' + m(\lambda-\lambda' s)_0,\\
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(5,3,2,1,2,3)\,\gamma_0' + m(\lambda-\lambda' s)_0,\\
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(3,2,1,2,3,5)\,\gamma_0' + m(\lambda-\lambda' s)_0,\\
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(3,5,2,3,2,1)\,\gamma_0' + m(\lambda-\lambda' s)_0,\\
(h_0/m)\,(\lambda'/\lambda)_0 &\geqslant \tfrac{1}{18}(\lambda s)_0\,(2,3,3,5,1,2)\,\gamma_0' + m(\lambda-\lambda' s)_0,
\end{aligned}\right\} \tag{3.29}$$

where γ_0' is the vector of slip rates in sequence 1–6.

The matrix on the right side of (3.29) is the *symmetric* part of the corresponding matrix for Taylor hardening, which is simply (n_{kj}). (Compare (3.29) with (3.13) of Havner 1981.) Remarkably, although (n_{kj}) is not even of rank 3, its symmetric part is of rank 5. Let B denote the 5×5 matrix consisting of the first five rows (including the factor $\frac{1}{18}$) of the full matrix, less the last column. Then

$$\begin{aligned}(\lambda s)_0\,(\gamma_1', \gamma_2', \gamma_3', \gamma_4', \gamma_5')_0^{\mathrm{T}} = \{(h_0/m + m(\lambda s)_0)\,(\lambda'/\lambda)_0 - m\lambda_0\}\,B^{-1}(1,1,1,1,1)^{\mathrm{T}}\\ -\tfrac{1}{18}(\lambda s)_0\,B^{-1}(2,3,3,5,1)^{\mathrm{T}}\,(\gamma_6')_0,\end{aligned} \tag{3.30}$$

with

$$B^{-1} = \frac{3}{4}\begin{bmatrix} 1 & -4 & 4 & 5 & -3\\ -4 & 4 & 2 & -8 & 6\\ 4 & 2 & 4 & -10 & 0\\ 5 & -8 & -10 & 13 & 3\\ -3 & 6 & 0 & 3 & -3\end{bmatrix}. \tag{3.31}$$

There follows $(\gamma_1')_0 = (\gamma_4')_0 = (\gamma_5')_0$ and $(\gamma_2')_0 = (\gamma_3')_0 = (\gamma_6')_0$ (with $\Sigma(\gamma_j')_0$ given by (3.25)), which is identically the axisymmetric solution of the two-parameter rule. Thus, the P.A.N. theory also corresponds to (2.16) (rotation case (iv)), namely

$$\dot{\boldsymbol{\imath}}_0 = (\mathscr{D}\boldsymbol{\imath}/\mathscr{D}t)_0 = \mathbf{0}. \tag{3.32}$$

Consider the effect of this solution on latent hardening. As (3.32) corresponds to $(\Omega\boldsymbol{\imath})_0 = \mathbf{0}$, there follows

$$(\boldsymbol{\sigma}\Omega)_0 = -(\lambda s)_0 \boldsymbol{\imath}_0 \otimes (\Omega\boldsymbol{\imath})_0 = 0. \tag{3.33}$$

(Equivalently, the axisymmetric solution (3.22) yields $\Sigma(\boldsymbol{\alpha}_j\gamma_j')_0 = 0$ as shown in Havner 1981.) Consequently, from (3.3) the simple theory immediately reduces to (Havner 1981, p. 345)

$$(\tau_k')_0 = h_0 \sum_j (\gamma_j')_0, \quad k = 1, \ldots, N, \tag{3.34}$$

or isotropic hardening; and the P.A.N. rule becomes, from (3.4),

$$(\tau_k')_0 = h_0 \sum_j (\gamma_j')_0 - \mathrm{tr}\,(\Omega_k \boldsymbol{\sigma} D). \tag{3.35}$$

Furthermore, as previously remarked, (3.32) is the axisymmetric solution (3.22) in sixfold symmetry. Therefore tensor D is a diagonal matrix when resolved on axis $\boldsymbol{\imath}_0 = [\bar{1}11]$ (of maximum principal strain rate) and any two orthogonal axes, as also is the matrix of stress $\boldsymbol{\sigma}$ for axial loading. Thus, $\boldsymbol{\sigma}D$ is a symmetric tensor, and its trace with any skew-symmetric tensor Ω_k is zero. The last term in (3.35) is therefore zero and we have

$$(\tau'_k)_0 = h_0 \sum_j (\gamma'_j)_0, \quad j = 1, \ldots, n;\ k = 1, \ldots, N, \tag{3.36}$$

for the P.A.N. rule as well (with $N = 24$, the total number of slip systems). We thus have established that *the P.A.N. rule* (as well as the simple theory) *predicts equal hardening of all systems, both active and latent, in axisymmetric deformation of f.c.c. crystals in sixfold symmetry*†.

3.3.4. *Summary of first-order solutions and kinematic possibilities*

Recall from § 2.1 the four possible cases of (partly) coincident rotation among lattice, material, and axis-co-rotational frames, defined in terms of loading-axis rotation: (i) $\mathring{\boldsymbol{\iota}} = -\omega\boldsymbol{\iota} = \mathbf{0}$; (ii) $\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = -W\boldsymbol{\iota} = \mathbf{0}$; (iii) $\mathring{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t$, whence $\Omega\boldsymbol{\iota} = \mathbf{0}$; (iv) $\mathring{\boldsymbol{\iota}} = \mathscr{D}\boldsymbol{\iota}/\mathscr{D}t = \mathbf{0}$, whence $\omega\boldsymbol{\iota} = W\boldsymbol{\iota} = \Omega\boldsymbol{\iota} = \mathbf{0}$. Also recall, in conjunction with case (ii), the added criterion $\mathscr{D}N_k/\mathscr{D}t = (N_k)^{\cdot}$, requiring $N_k W = WN_k$, from which $W = 0$. This condition is not a further restriction on case (ii), however. Whenever the loading axis is material-co-rotational ($W\boldsymbol{\iota} = \mathbf{0}$) one may arbitrarily choose the transverse axes of the 'loading frame' to be material-co-rotational as well. Thus, $W = 0$ and $W\boldsymbol{\iota} = \mathbf{0}$ are equivalent specifications of case (ii) for axial loading, and $\mathscr{D}N_k/\mathscr{D}t = (N_k)^{\cdot}$.

A parallel argument may be applied to case (i). If the loading axis is lattice-co-rotational ($\omega\boldsymbol{\iota} = \mathbf{0}$), we may choose the remaining axes of the loading frame so that they too are rotating with the lattice. Thus, $\omega = 0$ and $\omega\boldsymbol{\iota} = \mathbf{0}$ are equivalent specifications of case (i). Then, however, we should not have $\mathscr{D}N_k/\mathscr{D}t = (N_k)^{\cdot}$.

For case (iv) the combined analogy does not hold. If, for example, we arbitrarily choose the loading frame to be material-co-rotational (from $W\boldsymbol{\iota} = \mathbf{0}$), so that $\mathscr{D}N_k/\mathscr{D}t = (N_k)^{\cdot}$, we cannot simultaneously require (from $\omega\boldsymbol{\iota} = \mathbf{0}$) that the frame be lattice-co-rotational as well. The condition $\Omega\boldsymbol{\iota} = \mathbf{0}$ permits the material to have a pure spin about the loading axis relative to the underlying lattice. Specifically, in sixfold symmetry, the axisymmetric solution (3.22) corresponding to case (iv) may be written (Havner 1981, equations (3.33))

$$\left.\begin{aligned} \boldsymbol{\gamma}' &= \tfrac{1}{6}(1,1,1,1,1,1)\sum_j \gamma'_j + (-1,1,1,-1,-1,1)\,\gamma'_s, \\ -\tfrac{1}{6}\sum_j \gamma'_j &\leqslant \gamma'_s \leqslant \tfrac{1}{6}\sum_j \gamma'_j, \end{aligned}\right\} \tag{3.37}$$

in which the γ'_s-term corresponds to the relative spin Ω (of magnitude $\sqrt{2}\gamma'_s$) about $\boldsymbol{\iota}_0 = [\bar{1}11]$. Conversely, if we arbitrarily choose the loading frame to be lattice-co-rotational, whence $\omega = 0$, there follows $(N_k)^{\cdot} = 0$ while $\mathscr{D}N_k/\mathscr{D}t = N_k\Omega - \Omega N_k \neq 0$ (unless $\gamma'_s = 0$).

Consider now the results from minimum work in sixfold symmetry for the four hardening theories, grouped according to kinematics.

(*a*) Taylor hardening: $\mathring{\boldsymbol{\iota}}_0 = \mathbf{0}$, case (i), from which $\omega = 0$, whence $(N_k)^{\cdot} = 0$, but $(\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t)_0$ need not be zero; correspondingly, we may have $W \neq 0$ and $\mathscr{D}N_k/\mathscr{D}t \neq 0$.

(*b*) Simple theory: $(\mathscr{D}\boldsymbol{\iota}/\mathscr{D}t)_0 = 0$, case (ii), from which $W = 0$, whence $(N_k)^{\cdot} = \mathscr{D}N_k/\mathscr{D}t$, but $\mathring{\boldsymbol{\iota}}_0$ need not be zero; correspondingly, we may have $\omega \neq 0$ and $(N_k)^{\cdot} \neq 0$.

† I had not previously recognized the possibility of this result. Equation (3.36) and the italicized statement therefore correct an erroneous statement in Havner & Salpekar (1983, § 2) that the P.A.N. rule is 'incapable of predicting isotropic hardening in six or eightfold multiple slip'.

(*c*) Two-parameter rule and P.A.N. rule: $\hat{\iota}_0 = (\mathscr{D}\iota/\mathscr{D}t)_0 = \mathbf{0}$, case (iv), from which either (by choice) $\omega = 0$, whence $(N_k)^{\cdot} = 0$, but W need not be zero (correspondingly $\mathscr{D}N_k/\mathscr{D}t \neq 0$), or $W = 0$, whence $(N_k)^{\cdot} = \mathscr{D}N_k/\mathscr{D}t$, but ω need not be zero (correspondingly $(N_k)^{\cdot} \neq 0$).

Note in particular that for minimum work Taylor hardening does not require the loading axis to be material co-rotational whereas the other three theories do. Thus, to assume in advance of a theoretical analysis that $W = 0$ (hence $(N_k)^{\cdot} = \mathscr{D}N_k/\mathscr{D}t$), as do Franciosi & Zaoui (1982*a*, p. 1631, sentence following equation (6′)), is incorrect, for this condition is a *theory-specific* result.

It is instructive to pursue the issue of relative rotations in the case of *double-slip* from a sixfold symmetry position (a response 'less-stiff' than minimum work for each of the hardening rules considered here). In a recent experimental study of axially-loaded copper crystals, Franciosi & Zaoui (1982*b*) concluded that the (tensile) specimen tested in a $[\bar{1}11]$ orientation initially deformed on systems a$\bar{2}$, d$\bar{1}$ (figure 1), or 1 and 5 as numbered here, up to an axial strain (apparently logarithmic) of 5 %. (It should be noted, however, that their conclusion was based not only upon traces of slip lines on the faces of their triangular specimen and X-ray diffraction measurements, but also on their own conjectures about crystal hardening.) As mentioned in Havner (1981, p. 342), inequalities (3.23) of the simple theory permit equal double slip on systems a$\bar{2}$, d$\bar{1}$, with resultant axis rotation toward $[\bar{1}12]$. The two-parameter rule also permits equal double slip on these two systems (see Havner 1982*b*, equations (6.1)). However, neither Taylor hardening (as noted in Havner 1981, p. 339) nor the inequalities (3.29) of the P.A.N. rule permit double slip on a$\bar{2}$, d$\bar{1}$.

Consider the relative spin W of material and loading frame from the $[\bar{1}11]$ axis position. From (2.14), case (ii), the necessary conditions for $W\iota = \mathbf{0}$ in sixfold symmetry may be written (with the third equation dependent)

$$\left.\begin{aligned}(7,7,-2,-5,-2,-5)\,\gamma' &= 0,\\ (2,5,-7,-7,5,2)\,\gamma' &= 0,\\ (5,2,5,2,-7,-7)\,\gamma' &= 0,\end{aligned}\right\} \tag{3.38}$$

which are identically equations (3.26) introduced as the minimum-work solution for the simple theory. It is obvious that there is *no* combination of slip rates $\gamma'_k > 0$ on only two systems that can satisfy these equations. Consequently, in an initial sixfold symmetry position $W = 0$ *is kinematically impossible in double slip, independent of which systems are active.* Hardening theories are not at issue.

From (2.13), case (i), the necessary conditions for $\omega\iota = \mathbf{0}$ in sixfold symmetry are (Havner 1981, equations (3.21))

$$(\gamma'_1+\gamma'_6)_0 = (\gamma'_2+\gamma'_4)_0 = (\gamma'_3+\gamma'_5)_0. \tag{3.39}$$

Clearly, no double-slip combination can satisfy these conditions. For case (iii), $\Omega\iota = \mathbf{0}$, the necessary conditions in sixfold symmetry are, from (2.15),

$$\left.\begin{aligned}(-3,-3,2,1,2,1)\,\gamma' &= 0,\\ (-2,-1,3,3,-1,-2)\,\gamma' &= 0,\\ (-1,-2,-1,-2,3,3)\,\gamma' &= 0,\end{aligned}\right\} \tag{3.40}$$

with the third equation dependent. Again, no combination of only two active systems can satisfy these equations. Thus, for double slip (whatever the systems) from an initial axis position of sixfold symmetry, kinematics alone precludes each of cases (i) through (iv), and all three frames – material, lattice, and axis-co-rotational – rotate relative to each other.

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4. Second-order analyses of specific hardening rules

4.1. *General equations*

Henceforth, we shall assume that the systems which remain critical during a small load increment in a multiple-slip configuration have been identified, by minimum work rate or otherwise. (Recall the discussion that followed (2.28).) Let n now represent the total number of these active or inactive-critical systems, so that equations (2.25), which encompass (2.24), are satisfied for all $k = 1, \ldots, n$. Then the second-order inequalities (2.28) may be more conveniently expressed, from (2.29) and (2.31),

$$(\tau_k'')_0 \geqslant 2\lambda_0 \sum_j (n_{kj}\gamma_j')_0 + (\lambda s)_0 \sum_j (n_{kj}\gamma_j'')_0 + (\lambda s)_0 \sum_j (n_{kj}'\gamma_j')_0 - (m_k)_0(\lambda''s)_0 - 2(m_k)_0(\lambda'/\lambda)_0(\lambda - \lambda' s)_0, \quad k = 1, \ldots, n, \tag{4.1}$$

which are completely general. Further, from (2.18), (2.42) and (2.43) the left side of (4.1) has the equivalent representations, for all hardening rules,

$$\tau_k'' = \sum_j (H_{kj}\gamma_j'' + H_{kj}'\gamma_j'), \tag{4.2}$$

and

$$\tau_k'' = \sum_j (h_{kj}\gamma_j'' + h_{kj}'\gamma_j') - (\lambda s)\sum_j (r_{kj}\gamma_j'' + r_{kj}'\gamma_j'). \tag{4.3}$$

Consider once again a virgin f.c.c. crystal in a four, six or eightfold symmetry position at $s = s_0$. Adopting the postulate of minimum work, we seek to minimize both λ_0' and λ_0'' (3.17). For each of the four hardening rules investigated here, it was established in § 3.2 that λ_0' is minimized when the first-order equalities are satisfied in all critical systems (recall (3.14) and the discussion following (3.17)). Thus, every critical system is either active or inactive-critical and n is 4, 6 or 8 in the respective axis position. Consequently, for these hardening theories (and perhaps for others as well) one can utilize (2.32), (2.33), (2.35), (2.40) and (2.41) in summing the second-order inequalities (4.1) over the n critical systems, consistent with minimum work (stiffest response). We also shall use the following kinematic result, obtained by differentiating (2.30) and substituting (3.12):

$$m\sum_j (\gamma_j'')_0 = (\lambda'/\lambda)_0' - \sum_j (m_j'\gamma_j')_0, \tag{4.4}$$

with

$$(m_k')_0 = \sum_j (n_{kj}\gamma_j')_0 - 2m(\lambda'/\lambda)_0. \tag{4.5}$$

Upon summing inequalities (4.1) over the four, six or eight critical systems and substituting (4.2), (4.4), (2.32), (2.33) and (2.35), we obtain the following second-order counterpart of (2.36):

$$\sum_k \sum_j (H_{kj}\gamma_j'' + H_{kj}'\gamma_j')_0 \geqslant nm(2\lambda' + \lambda''s)_0 + (\lambda s)_0 \sum_k \sum_j (n_{kj}'\gamma_j')_0 - 2nm(\lambda s)_0 \sum_j (m_j'\gamma_j')_0, \quad n = 4, 6, 8. \tag{4.6}$$

Equivalently, from (4.3) with (2.40) and (2.41), in terms of the effective hardening moduli h_{kj} we have

$$\sum_k \sum_j (h_{kj}\gamma_j'' + h_{kj}'\gamma_j')_0 \geqslant nm(2\lambda' + \lambda''s)_0 + (\lambda s)_0 \sum_k \sum_j (m_{kj}'\gamma_j')_0 - 2nm(\lambda s)_0 \sum_j (m_j'\gamma_j')_0, \quad n = 4, 6, 8. \tag{4.7}$$

In each of the above the summations are taken over all n critical systems. Also, note that the left side of (4.6), but not (4.7), is equal to $\Sigma_k(\tau''_k)_0$. (Although (2.40) holds, it does not follow that $\Sigma_k(r'_{kj})_0 = 0$, whence $\Sigma_k(n'_{kj})_0 \neq \Sigma_k(m'_{kj})_0$ in general.)

In what follows we shall be particularly concerned with the calculation of the right side terms $\Sigma\,(m'_j\gamma'_j)_0$ and either $\Sigma\,\Sigma\,(n'_{kj}\gamma'_j)_0$ (from (4.6)) or $\Sigma\,\Sigma\,(m'_{kj}\gamma'_j)_0$ (from (4.7)). Consider the first of these. From (2.3) and the first equation in (2.10),

$$\sum_j (m'_j\gamma'_j)_0 = 2(\hat{\imath}D\imath)_0. \qquad (4.8)\dagger$$

Thus, upon substituting (2.7) through (2.9) and making use of $\imath\cdot\hat{\imath} = 0$, we obtain

$$\sum_j (m'_j\gamma'_j)_0 = -2(\hat{\imath}W\imath)_0. \qquad (4.9)$$

By following a similar procedure, also using (2.30), (2.35) and (2.43), one may express the double summations above as

$$\sum_k\sum_j (n'_{kj}\gamma'_j)_0 = 2\imath_0\sum_k N_k(\Gamma\hat{\imath})_0 + 2\imath_0\sum_k N_k\dot{\hat{\imath}}_0, \quad \Gamma = D + \Omega, \qquad (4.10)$$

$$\sum_k\sum_j (m'_{kj}\gamma'_j)_0 = 2\imath_0\sum_k N_k(D\hat{\imath})_0 - 2\hat{\imath}_0\sum_k N_k(W\imath)_0. \qquad (4.11)$$

Finally, it is re-emphasized that (4.6) and (4.7) are restricted only by the requirement that no critical system become inactivated (in the sense of (2.26)) in a four, six or eightfold symmetry position. For the four hardening rules considered here and the sixfold position, this can occur only in double slip (or single slip for two of the theories). The kinematics and theoretical results for *finite* changes are already available for double slip (save for the P.A.N. rule), and a series expansion, as here, is not needed (see Havner & Salpekar 1982, 1983).

4.2. *Solutions in n-fold symmetry with axis stability*

The specific case of initial axis stability (i.e. $\hat{\imath}_0 = \mathbf{0}$) is a possible solution of the first-order *equalities* in each of four, six and eightfold symmetry. This is evident from § 3 here for all four hardening rules in sixfold symmetry, and has been shown to hold for Taylor hardening and the simple theory in four and eightfold symmetry by Salpekar (1982). The result also can be extended to the other hardening rules in the latter symmetry positions. Thus, we briefly consider the consequences of axis stability in n-fold symmetry ($n = 4, 6, 8$).

Obviously, each of (4.9), (4.10), and (4.11) reduces to zero for $\hat{\imath}_0 = \mathbf{0}$. Then, from (3.1), (3.2), (3.5) and (3.7) in turn, together with $\Sigma_k(r'_{kj})_0 = 0$ from (2.43), (4.10), (4.11) and $\hat{\imath}_0 = \mathbf{0}$, inequalities (4.6) and (4.7) simplify to

$$nh_0\sum_j(\gamma''_j)_0 + nh'_0\sum_j(\gamma'_j)_0 \geqslant nm(2\lambda' + \lambda''s)_0. \qquad (4.12)$$

Here h_0 is the generic label, as before, for the various moduli H, $\bar{H} = 2H_1/n + (n-2)\,H_2/n$, h and $\hbar$ at $s = s_0$; and h'_0 is the generic label for their rates of change with respect to nominal stress. Thus, on substituting (3.12), (4.4), and (4.9) into (4.12), we obtain the following lower bound to λ''_0 in the event of axis stability in any of the three higher symmetry positions, applicable to all four hardening theories:

$$\lambda''_0 \geqslant [h_0(\lambda'/\lambda)_0 - h'_0 + 2m^2\lambda_0]\,\lambda'_0/(h_0 - m^2(\lambda s)_0), \qquad (4.13)$$

with

$$\lambda'_0 = (m\lambda_0)^2/(h_0 - m^2(\lambda s)_0) > 0. \qquad (4.14)$$

† Here and in subsequent equations (as appropriate) the time parameter t implicit in $\hat{\imath}$, D, and W is to be replaced by the variable s.

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Alternatively, and in parallel with (3.15), if both $\lambda_0'' = (\mathrm{d}^2\lambda/\mathrm{d}s^2)_0$ and $\lambda_0' = (\mathrm{d}\lambda/\mathrm{d}s)_0$ are available from experimental test, (4.13) gives a lower bound to the rate of change h_0' of the generic modulus:

$$h_0' \geqslant 2m^2\lambda_0 + h_0(\lambda'/\lambda)_0 - (m\lambda/\lambda')_0^2\lambda_0'', \tag{4.15}$$

with

$$h_0 = m^2(\lambda s)_0 + (m\lambda_0)^2/\lambda_0'. \tag{4.16}$$

If the axis remains in the n-fold position (that is, $\dot{\boldsymbol{\imath}} = \mathbf{0}$ throughout the loading increment) then (4.15) becomes an equality and yields the precise value of h_0' that corresponds to the experimentally determined behaviour. (This is not specific in the case of the two parameter rule, however, as (4.15) then only provides an n-fold mean for the rates of change of the individual parameters H_1, H_2 from (3.9).)

4.3. *The minimum-work solution in sixfold symmetry*

Recall from § 3.3.4 that, in sixfold symmetry, minimum work identically gives $\dot{\boldsymbol{\imath}}_0 = \mathbf{0}$ from the first-order inequalities for each of Taylor hardening, the two-parameter rule, and the P.A.N. rule. Consequently, (4.14) and the lower bound in (4.13) (with $m^2 = \frac{2}{27}$) form precisely the minimum work solution for λ_0' and λ_0'', in terms of the generic hardening modulus h_0 and its rate of change $h_0' = (\mathrm{d}h/\mathrm{d}s)_0$, for these three hardening rules. (Note that h_0' may be positive, negative, or zero.) For the simple theory, however, $\dot{\boldsymbol{\imath}}_0$ need not be zero for minimum work, as noted in § 3.3.4; hence the analysis in § 4.2 that led to (4.13) does not apply to this hardening rule. None the less, we shall establish in the following that the lower bound (4.13) is a consequence of minimum work for the simple theory as well.

Let us first consider the basic second-order inequalities themselves (rather than merely their sum) for each of the simple theory and Taylor hardening in sixfold symmetry. For the latter (as well as for the two-parameter and P.A.N. hardening rules) we necessarily have, from (2.2), (2.3), (2.7), (2.9), (2.10), (2.30) and $\dot{\boldsymbol{\imath}}_0 = \mathbf{0}$,

$$(m_k')_0 = 0, \quad (n_{kj}')_0 = 0, \quad \text{and} \quad \sum_j (n_{kj}\gamma_j')_0 = 2m(\lambda'/\lambda)_0. \tag{4.17}$$

Thus, on substituting (3.1), (3.12), (4.2) and (4.4) with (4.17) into (4.1), we find (for Taylor hardening only)

$$[H_0 + m^2(\lambda s)_0]\,(\lambda''/\lambda)_0 \geqslant m(\lambda s)_0 \sum_j (n_{kj}\gamma_j'')_0 + [H_0(\lambda'/\lambda)_0 - H_0' + 2m^2(\lambda + \lambda' s)_0]\,(\lambda'/\lambda)_0, \quad k = 1, \ldots, 6. \tag{4.18}$$

Summation of these inequalities with the aid of (2.32) and (4.4), which simplifies to

$$m \sum_j (\gamma_j'')_0 = (\lambda'/\lambda)_0', \tag{4.19}$$

provides the lower bound (4.13) for λ_0'' (with H_0 of course replaced by the generic modulus h_0). Moreover, in parallel with the results (3.18) from the first-order inequalities for Taylor hardening, minimum work gives (from (4.18), (4.19) and (4.13))

$$(\gamma_1'' + \gamma_6'')_0 = (\gamma_2'' + \gamma_4'')_0 = (\gamma_3'' + \gamma_5'')_0 = [m(2\lambda + \lambda' s)_0 - H_0'/m]\,(\lambda'/\lambda)_0/(3H_0 - \tfrac{2}{9}(\lambda s)_0). \tag{4.20}$$

(The individual second derivatives of the crystallographic slips, as their first derivatives, are not further determined by analysis.)

As $\dot{\imath}_0$ may be non-zero in the simple theory none of equations (4.17) apply. None the less, although the $(m'_k)_0$ are not necessarily zero, we still have

$$\sum_j (m'_j \gamma'_j)_0 = 0, \tag{4.21}$$

from (4.9) and $(\mathscr{D}\imath/\mathscr{D}t)_0 = -(W\imath)_0 = \mathbf{0}$, corresponding to minimum work in sixfold symmetry. Hence (4.19) still holds (from (4.4) and (4.21)). On substituting (3.5) and (4.3) with (2.43), (3.12) and (4.19) into (4.1), one obtains

$$\begin{aligned}[h_0 + m^2(\lambda s)_0](\lambda''/\lambda)_0 \geqslant m(\lambda s)_0 \sum_j (m_{kj}\gamma''_j)_0 + 2m\lambda_0(m'_k)_0 + m(\lambda s)_0 \sum_j (m'_{kj}\gamma'_j)_0 \\ + [h_0(\lambda'/\lambda)_0 - h'_0 + 2m^2(\lambda+\lambda' s)_0](\lambda'/\lambda)_0, \quad k = 1, \ldots, 6, \end{aligned} \tag{4.22}$$

for the simple theory, with

$$\sum_j (m'_{kj}\gamma'_j)_0 = 2\imath_0 N_k (D\dot{\imath})_0 + (\lambda'/\lambda)_0 (m'_k)_0, \tag{4.23}$$

from (2.43), the second equation of (3.27) and (2.29).

Consider now the summation of inequalities (4.22), with (4.19), (4.23) and (2.35). The result (after simplification) is

$$n[h_0 - m^2(\lambda s)_0](\lambda''/\lambda)_0 \geqslant n[h_0(\lambda'/\lambda)_0 - h'_0 + 2m^2\lambda_0](\lambda'/\lambda)_0 + 2m(\lambda s)_0 \imath_0 \sum_k N_k (D\dot{\imath})_0, \tag{4.24}$$

with, of course, $n = 6$, $m^2 = \frac{2}{27}$, and the equality necessarily satisfied for minimum λ''_0, hence minimum work. On comparing (4.24) with (4.13), we see that to establish applicability of the earlier lower bound to the simple theory in sixfold symmetry, there remains to prove that $\imath_0 \sum N_k (D\dot{\imath})_0 = 0$ for all solutions (3.24) of the first-order equalities. (As I found this result to be neither obvious nor straightforward to prove, a reasonable amount of detail is included here.)

We shall find it convenient to use the equivalence

$$2\imath_0 \sum_k N_k (D\dot{\imath})_0 = \sum_k \sum_j (m'_{kj}\gamma'_j)_0 \tag{4.25}$$

from (4.23) and (2.35) (or (4.11) and $(W\imath)_0 = \mathbf{0}$) and first evaluate

$$\sum_k (m'_{kj})_0 = 2\imath_0 \sum_k M_{kj} \dot{\imath}_0, \quad M_{kj} = N_k N_j + N_j N_k, \tag{4.26}$$

which follows from (2.43). The second-rank symmetric tensors M_{kj} in sixfold symmetry are given in the Appendix. Summing on k in (A 7), with $j = 1$ to 6 and $\imath_0 = (1/\surd 3)(-1, 1, 1)$, we find

$$\left.\begin{aligned} \hat{\imath}_0 \sum_k M_{k1} &= 1/(6\surd 3)(-3, 6, 7), & \imath_0 \sum_k M_{k2} &= 1/(6\surd 3)(-3, 7, 6), \\ \hat{\imath}_0 \sum_k M_{k3} &= 1/(6\surd 3)(-6, 3, 7), & \imath_0 \sum_k M_{k4} &= 1/(6\surd 3)(-7, 3, 6), \\ \hat{\imath}_0 \sum_k M_{k5} &= 1/(6\surd 3)(-6, 7, 3), & \imath_0 \sum_k M_{k6} &= 1/(6\surd 3)(-7, 6, 3). \end{aligned}\right\} \tag{4.27}$$

General kinematic equations for $\dot{\imath}$ in sixfold symmetry are given in Havner (1981, equations (3.20)). They are

$$\left.\begin{aligned} 3\surd 2(\hat{\imath}_1)_0 &= -(\gamma'_1 + \gamma'_2 + \gamma'_4 + \gamma'_6)_0 + \tfrac{2}{3}\sum_j (\gamma')_0, \\ 3\surd 2(\hat{\imath}_2)_0 &= (\gamma'_2 + \gamma'_3 + \gamma'_4 + \gamma'_5)_0 - \tfrac{2}{3}\sum_j (\gamma')_0, \\ 3\surd 2(\hat{\imath}_3)_0 &= (\gamma'_1 + \gamma'_3 + \gamma'_5 + \gamma'_6)_0 - \tfrac{2}{3}\sum_j (\gamma'_j)_0. \end{aligned}\right\} \tag{4.28}$$

Substituting solution (3.24) of the first-order equalities of the simple theory into (4.28), one obtains

$$\left.\begin{aligned}3\sqrt{2}(\hat{\iota}_1)_0 &= -\tfrac{4}{3}(\gamma_4'+\gamma_6')_0+\tfrac{4}{9}\sum_j(\gamma_j')_0,\\3\sqrt{2}(\hat{\iota}_2)_0 &= \tfrac{4}{3}(\gamma_2'+\gamma_5')_0-\tfrac{4}{9}\sum_j(\gamma_j')_0,\\3\sqrt{2}(\hat{\iota}_3)_0 &= \tfrac{4}{3}(\gamma_1'+\gamma_3')_0-\tfrac{4}{9}\sum_j(\gamma_j')_0.\end{aligned}\right\}\tag{4.29}$$

We now substitute (4.27) and (4.29) into (4.26). There follows, after simplification,

$$\left.\begin{aligned}\sum_k(m_{k1}')_0 &= m^3[-7(\gamma_4'+\gamma_6')_0+2(\gamma_2'+\gamma_5')_0+5(\gamma_1'+\gamma_3')_0],\\\sum_k(m_{k2}')_0 &= m^3[-7(\gamma_4'+\gamma_6')_0+5(\gamma_2'+\gamma_5')_0+2(\gamma_1'+\gamma_3')_0],\\\sum_k(m_{k3}')_0 &= m^3[2(\gamma_4'+\gamma_6')_0-7(\gamma_2'+\gamma_5')_0+5(\gamma_1'+\gamma_3')_0],\\\sum_k(m_{k4}')_0 &= m^3[5(\gamma_4'+\gamma_6')_0-7(\gamma_2'+\gamma_5')_0+2(\gamma_1'+\gamma_3')_0],\\\sum_k(m_{k5}')_0 &= m^3[2(\gamma_4'+\gamma_6')_0+5(\gamma_2'+\gamma_5')_0-7(\gamma_1'+\gamma_3')_0],\\\sum_k(m_{k6}')_0 &= m^3[5(\gamma_4'+\gamma_6')_0+2(\gamma_2'+\gamma_5')_0-7(\gamma_1'+\gamma_3')_0].\end{aligned}\right\}\tag{4.30}$$

It is readily confirmed that equations (4.30) are zero only for the axisymmetric solution with axis stability, given by (3.37)†. Correspondingly, a key step in the proof is substitution from (4.29) for each of $(\gamma_4'+\gamma_6')_0$, $(\gamma_2'+\gamma_5')_0$ and $(\gamma_1'+\gamma_3')_0$ above. The terms in $\sum(\gamma_j')_0$ cancel in every equation, and (4.30) may be expressed in the final simple form

$$\left.\begin{aligned}\sum_k(m_{k1}')_0 &= 1/(9\sqrt{3})\,(7\hat{\iota}_1+2\hat{\iota}_2+5\hat{\iota}_3)_0,\\\sum_k(m_{k2}')_0 &= 1/(9\sqrt{3})\,(7\hat{\iota}_1+5\hat{\iota}_2+2\hat{\iota}_3)_0,\\\sum_k(m_{k3}')_0 &= 1/(9\sqrt{3})\,(-2\hat{\iota}_1-7\hat{\iota}_2+5\hat{\iota}_3)_0,\\\sum_k(m_{k4}')_0 &= 1/(9\sqrt{3})\,(-5\hat{\iota}_1-7\hat{\iota}_2+2\hat{\iota}_3)_0,\\\sum_k(m_{k5}')_0 &= 1/(9\sqrt{3})\,(-2\hat{\iota}_1+5\hat{\iota}_2-7\hat{\iota}_3)_0,\\\sum_k(m_{k6}')_0 &= 1/(9\sqrt{3})\,(-5\hat{\iota}_1+2\hat{\iota}_2-7\hat{\iota}_3)_0.\end{aligned}\right\}\tag{4.31}$$

We now substitute (4.31) into (4.25), summing on j from 1 to 6 to obtain

$$\begin{aligned}\sum_k\sum_j(m_{kj}'\gamma_j')_0 = 1/(9\sqrt{3})\,[&\{7(\gamma_1'+\gamma_2')_0-2(\gamma_3'+\gamma_5')_0-5(\gamma_4'+\gamma_6')_0\}(\hat{\iota}_1)_0\\&+\{2(\gamma_1'+\gamma_6')_0+5(\gamma_2'+\gamma_5')_0-7(\gamma_3'+\gamma_4')_0\}(\hat{\iota}_2)_0\\&+\{5(\gamma_1'+\gamma_3')_0+2(\gamma_2'+\gamma_4')_0-7(\gamma_5'+\gamma_6')_0\}(\hat{\iota}_3)_0].\end{aligned}\tag{4.32}$$

But from (3.26) of the simple theory, we see that each of the algebraic multipliers of the components of $\hat{\boldsymbol{\iota}}_0$ is a *zero identity*! Thus, we have proven that

$$2\boldsymbol{\iota}_0\sum_k N_k(D\hat{\boldsymbol{\iota}})_0 = \sum_k\sum_j(m_{kj}'\gamma_j')_0 = 0\tag{4.33}$$

† The simple theory requires that $\boldsymbol{\iota}_0$ be a direction of principal strain rate for minimum work, from (3.27), but the theory does not require axis stability. The converse is true for Taylor hardening.

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for the simple theory in sixfold symmetry, corresponding to minimum work. (As the reader undoubtedly will have realized, we could have obtained expressions for the $\sum_k (m'_{kj})_0$ which are equally as simple as equations (4.31) by substituting (4.27) directly into (4.26) without using (4.29). The result would have been $\sum_k (m'_{k1})_0 = 1/(3\sqrt{3})\,(-3\hat{\iota}_1+6\hat{\iota}_2+7\hat{\iota}_3)_0$, etc. However, we should not then have found in (4.32) the readily recognizable identities (3.26). It is the double substitution of (4.29) from the simple theory that is the key to the proof.)

We now summarize the principal results in sixfold symmetry. None of the four hardening theories considered predicts an absolutely unique set of values, from minimum work ('stiffest response'), for the first or second derivatives of crystallographic slips†. Nevertheless, the minimum work postulate gives the following general connections between derivatives of the observable axis-stretch λ and the theoretical (generic) hardening modulus h_0 and its rate of change h'_0, applicable to all four theories:

$$\left.\begin{aligned} \lambda'_0 &= (m\lambda_0)^2/[h_0 - m^2(\lambda s)_0], \quad h_0 > m^2(\lambda s)_0, \\ \lambda''_0 &= [h_0(\lambda'/\lambda)_0 - h'_0 + 2m^2\lambda_0]\,\lambda'_0/[h_0 - m^2(\lambda s)_0]. \end{aligned}\right\} \tag{4.34}$$

(Recall that $(\lambda'/\lambda)_0$ is necessarily a principal strain rate for minimum work according to all the theories save Taylor hardening.) Furthermore, for each of Taylor hardening, the simple theory, and the P.A.N. rule, (4.34) is sufficient for determination of the respective h_0 and h'_0 from experimental values of λ'_0 and λ''_0, corresponding to triple or higher-order multiple slip in sixfold symmetry:

$$\left.\begin{aligned} h_0 &= m^2(\lambda s)_0 + (m\lambda_0)^2/\lambda'_0, \quad \lambda'_0 > 0, \\ h'_0 &= 3m^2\lambda_0 + m^2(\lambda' s)_0 - (m\lambda/\lambda')^2_0\,\lambda''_0. \end{aligned}\right\} \tag{4.35}$$

In addition to the foregoing results for sixfold symmetry, it was established in § 3.2 that the first of (4.34) (or (4.35)) applies to the four and eightfold symmetry positions as well. Whether the second of (4.34) (or (4.35)) also holds in these other positions remains to be determined.

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References

Budiansky, B. & Wu, T. T. 1962 Theoretical prediction of plastic strains of polycrystals. In *Proc. 4th U.S. Natn. Cong. Appl. Mech.*, pp. 1175–1185. New York: American Society of Mechanical Engineers.

Franciosi, P., Berveiller, M. & Zaoui, A. 1980 Latent hardening in copper and aluminium single crystals. *Acta metall.* 28, 273–283.

Franciosi, P. & Zaoui, A. 1982*a* Multislip in f.c.c. crystals, a theoretical approach compared with experimental data. *Acta metall.* 30, 1627–1637.

Franciosi, P. & Zaoui, A. 1982*b* Multislip tests on copper crystals: a junctions hardening effect. *Acta metall.* 30, 2141–2151.

Havner, K. S. 1981 A theoretical analysis of finitely deforming f.c.c. crystals in the sixfold symmetry position. *Proc. R. Soc. Lond.* A 378, 329–349.

Havner, K. S. 1982*a* The theory of finite plastic deformation of crystalline solids. In *Mechanics of solids, the Rodney Hill 60th anniversary volume* (ed. H. G. Hopkins & M. J. Sewell), pp. 265–302. Oxford: Pergamon Press.

Havner, K. S. 1982*b* Minimum plastic work selects the highest symmetry deformation in axially-loaded f.c.c. crystals. *Mech. Matl* 1, 97–111.

Havner, K. S. & Baker, G. S. 1979 Theoretical latent hardening in crystals – II. Bcc crystals in tension and compression. *J. Mech. Phys. Solids* 27, 285–314.

† For the two-parameter and P.A.N. rules, however, the results are unique to within a pure relative spin of material and lattice about the loading axis.

Havner, K. S., Baker, G. S. & Vause, R. F. 1979 Theoretical latent hardening in crystals – I. General equations for tension and compression with application to f.c.c. crystals in tension. *J. Mech. Phys. Solids* **27**, 33–50.

Havner, K. S. & Salpekar, S. A. 1982 Theoretical latent hardening of crystals in double slip – I. F.c.c. crystals with a common slip plane. *J. Mech. Phys. Solids* **30**, 379–398.

Havner, K. S. & Salpekar, S. A. 1983 Theoretical latent hardening of crystals in double slip – II. F.c.c. crystals slipping on distinct planes. *J. Mech. Phys. Solids* **31**, 231–250.

Havner, K. S. & Shalaby, A. H. 1977 A simple mathematical theory of finite distortional latent hardening in single crystals. *Proc. R. Soc. Lond.* A **358**, 47–70.

Havner, K. S. & Shalaby, A. H. 1978 Further investigation of a new hardening law in crystal plasticity. *J. appl. Mech.* **45**, 500–506.

Hill, R. 1966 Generalized constitutive relations for incremental deformation of metal crystals by multislip. *J. Mech. Phys. Solids* **14**, 95–102.

Hill, R. & Havner, K. S. 1982 Perspectives in the mechanics of elastoplastic crystals. *J. Mech. Phys. Solids* **30**, 5–22.

Jackson, P. J. & Basinski, Z. S. 1967 Latent hardening and the flow stress in copper single crystals. *Can. J. Phys.* **45**, 707–735.

Nakada, Y. & Keh, A. S. 1966 Latent hardening in iron single crystals. *Acta metall.* **14**, 961–973.

Peirce, D., Asaro, R. J. & Needleman, A. 1982 An analysis of nonuniform and localized deformation in ductile single crystals. *Acta metall.* **30**, 1087–1119.

Salpekar, S. A. 1982 A theoretical investigation of axially loaded f.c.c. crystals in multiple slip positions at finite strain. Ph.D. thesis, North Carolina State University.

Taylor, G. I. & Elam, C. F. 1923 The distortion of an aluminium crystal during a tensile test. *Proc. R. Soc. Lond.* A **102**, 643–667.

Taylor, G. I. & Elam, C. F. 1925 The plastic extension and fracture of aluminium crystals. *Proc. R. Soc. Lond.* A **108**, 28–51.

Vause, R. F. & Havner, K. S. 1979 Theoretical latent hardening in crystals – III. F.c.c. crystals in compression. *J. Mech. Phys. Solids* **27**, 393–414.

Weng, G. J. 1979 Kinematic hardening rule in single crystals. *Int. J. Solids Struct.* **15**, 861–870.

Appendix

Matrices (n_{kj}) for f.c.c. crystals in four, six and eightfold symmetry

In fourfold symmetry, with $\boldsymbol{\iota}_0 = [011]$ and the four critical systems (figure 1) taken in sequence a$\bar{2}$, a3, c$\bar{2}$, c3, the matrix of coefficients $n_{kj} = 2\boldsymbol{\iota}_0 N_k (\boldsymbol{b} \otimes \boldsymbol{n})_j \boldsymbol{\iota}_0$ is

$$(n_{kj}) = \frac{1}{3}\begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 2 & 0 & 1 \\ 1 & 0 & 2 & 1 \\ 0 & 1 & 1 & 2 \end{bmatrix}. \tag{A 1}$$

In sixfold symmetry, with $\boldsymbol{\iota}_0 = [\bar{1}11]$ and the six critical systems (figure 1) taken in sequence a$\bar{2}$, a3, b1, b$\bar{3}$, d$\bar{1}$, d2, matrix (n_{kj}) is

$$(n_{kj}) = \frac{1}{18}\begin{bmatrix} 2 & 1 & 5 & 1 & 5 & 2 \\ 1 & 2 & 5 & 2 & 5 & 1 \\ 5 & 1 & 2 & 1 & 2 & 5 \\ 5 & 2 & 1 & 2 & 1 & 5 \\ 1 & 5 & 2 & 5 & 2 & 1 \\ 2 & 5 & 1 & 5 & 1 & 2 \end{bmatrix}. \tag{A 2}$$

In eightfold symmetry, with $\boldsymbol{\iota}_0 = [001]$ and the eight critical systems (figure 1) taken in sequence a$\overline{2}$, c$\overline{2}$, b1, c1, d$\overline{2}$, b$\overline{2}$, a1, d1, matrix (n_{kj}) is

$$(n_{kj}) = \frac{1}{6}\begin{bmatrix} 2 & 2 & 3 & 1 & 2 & 2 & 1 & 3 \\ 2 & 2 & 3 & 1 & 2 & 2 & 1 & 3 \\ 3 & 1 & 2 & 2 & 3 & 1 & 2 & 2 \\ 3 & 1 & 2 & 2 & 3 & 1 & 2 & 2 \\ 2 & 2 & 1 & 3 & 2 & 2 & 3 & 1 \\ 2 & 2 & 1 & 3 & 2 & 2 & 3 & 1 \\ 1 & 3 & 2 & 2 & 1 & 3 & 2 & 2 \\ 1 & 3 & 2 & 2 & 1 & 3 & 2 & 2 \end{bmatrix}. \tag{A 3}$$

Observe that (n_{kj}) is symmetric only in fourfold symmetry.

Matrices (r_{kj}) for f.c.c. crystals in four, six and eightfold symmetry

In fourfold symmetry, in the same sequence as (A 1), the matrix of coefficients $r_{kj} = -2\boldsymbol{\iota}_0 N_k \Omega_j \boldsymbol{\iota}_0$ is

$$(r_{kj}) = \frac{1}{24}\begin{bmatrix} -5 & -1 & 1 & 5 \\ -1 & -5 & 5 & 1 \\ 1 & 5 & -5 & -1 \\ 5 & 1 & -1 & -5 \end{bmatrix}. \tag{A 4}$$

In sixfold symmetry, in the same sequence as (A 2), matrix (r_{kj}) is

$$(r_{kj}) = \frac{1}{36}\begin{bmatrix} 10 & 11 & -5 & -1 & -9 & -6 \\ 11 & 10 & -9 & -6 & -5 & -1 \\ -5 & -1 & 10 & 11 & -6 & -9 \\ -9 & -6 & 11 & 10 & -1 & -5 \\ -1 & -5 & -6 & -9 & 10 & 11 \\ -6 & -9 & -1 & -5 & 11 & 10 \end{bmatrix}. \tag{A 5}$$

In eightfold symmetry, in the same sequence as (A 3), matrix (r_{kj}) is

$$(r_{kj}) = \frac{1}{12}\begin{bmatrix} 1 & 1 & -2 & 2 & -1 & -1 & 2 & -2 \\ 1 & 1 & -2 & 2 & -1 & -1 & 2 & -2 \\ -2 & 2 & 1 & 1 & -2 & 2 & -1 & -1 \\ -2 & 2 & 1 & 1 & -2 & 2 & -1 & -1 \\ -1 & -1 & 2 & -2 & 1 & 1 & -2 & 2 \\ -1 & -1 & 2 & -2 & 1 & 1 & -2 & 2 \\ 2 & -2 & -1 & -1 & 2 & -2 & 1 & 1 \\ 2 & -2 & -1 & -1 & 2 & -2 & 1 & 1 \end{bmatrix}. \tag{A 6}$$

Matrix (r_{kj}), as (n_{kj}), is symmetric only in fourfold symmetry. However, $(m_{kj}) = (n_{kj}) + (r_{kj})$ is symmetric in all three higher symmetry positions.

Second-rank tensors M_{kj} for f.c.c. crystals in sixfold symmetry

The second-rank tensors $M_{kj} = N_k N_j + N_j N_k$ in sixfold symmetry, expressed as matrix arrays of their components on the f.c.c. lattice axes, are (in the same sequence as before):

$$
\left.
\begin{array}{ll}
M_{11} = \frac{1}{12}\begin{bmatrix} 5 & 2 & -1 \\ 2 & 2 & 2 \\ -1 & 2 & 5 \end{bmatrix}, &
M_{12} = M_{21} = \frac{1}{24}\begin{bmatrix} 8 & -1 & -1 \\ -1 & 2 & 5 \\ -1 & 5 & 2 \end{bmatrix}, \\
M_{13} = M_{31} = \frac{1}{24}\begin{bmatrix} 2 & 3 & -1 \\ 3 & 2 & 1 \\ -1 & 1 & 8 \end{bmatrix}, &
M_{14} = M_{41} = \frac{1}{24}\begin{bmatrix} -8 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & 2 \end{bmatrix}, \\
M_{15} = M_{51} = \frac{1}{24}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & -8 \end{bmatrix}, &
M_{16} = M_{61} = \frac{1}{24}\begin{bmatrix} -6 & 0 & -2 \\ 0 & 4 & 0 \\ -2 & 0 & -6 \end{bmatrix}, \\
M_{22} = \frac{1}{12}\begin{bmatrix} 5 & -1 & 2 \\ -1 & 5 & 2 \\ 2 & 2 & 2 \end{bmatrix}, &
M_{23} = M_{32} = \frac{1}{24}\begin{bmatrix} 2 & -1 & -1 \\ -1 & -8 & 1 \\ -1 & 1 & 2 \end{bmatrix}, \\
M_{24} = M_{42} = \frac{1}{24}\begin{bmatrix} -6 & -2 & 0 \\ -2 & -6 & 0 \\ 0 & 0 & 4 \end{bmatrix}, &
M_{25} = M_{52} = \frac{1}{24}\begin{bmatrix} 2 & -1 & 3 \\ -1 & 8 & 1 \\ 3 & 1 & 2 \end{bmatrix}, \\
M_{26} = M_{62} = \frac{1}{24}\begin{bmatrix} -8 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & 2 \end{bmatrix}, &
M_{33} = \frac{1}{12}\begin{bmatrix} 2 & 2 & -2 \\ 2 & 5 & 1 \\ -2 & 1 & 5 \end{bmatrix}, \\
M_{34} = M_{43} = \frac{1}{24}\begin{bmatrix} 2 & -1 & -5 \\ -1 & 8 & 1 \\ -5 & 1 & 2 \end{bmatrix}, &
M_{35} = M_{53} = \frac{1}{24}\begin{bmatrix} 4 & 0 & 0 \\ 0 & -6 & 2 \\ 0 & 2 & -6 \end{bmatrix}, \\
M_{36} = M_{63} = \frac{1}{24}\begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & 1 \\ -1 & 1 & -8 \end{bmatrix}, &
M_{44} = \frac{1}{12}\begin{bmatrix} 5 & -1 & -2 \\ -1 & 5 & -2 \\ -2 & -2 & 2 \end{bmatrix}, \\
M_{45} = M_{54} = \frac{1}{24}\begin{bmatrix} 2 & -1 & -1 \\ -1 & -8 & 1 \\ -1 & 1 & 2 \end{bmatrix}, &
M_{46} = M_{64} = \frac{1}{24}\begin{bmatrix} 8 & -1 & -1 \\ -1 & 2 & -3 \\ -1 & -3 & 2 \end{bmatrix}, \\
M_{55} = \frac{1}{12}\begin{bmatrix} 2 & -2 & 2 \\ -2 & 5 & 1 \\ 2 & 1 & 5 \end{bmatrix}, &
M_{56} = M_{65} = \frac{1}{24}\begin{bmatrix} 2 & -5 & -1 \\ -5 & 2 & 1 \\ -1 & 1 & 8 \end{bmatrix}, \\
M_{66} = \frac{1}{12}\begin{bmatrix} 5 & -2 & -1 \\ -2 & 2 & -2 \\ -1 & -2 & 5 \end{bmatrix}. &
\end{array}
\right\} \quad (A\,7)
$$