

Bifurcation into shear bands on the Bishop and Hill polyhedron. Part I: General analysis

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THE PRESENT PAPER is the first of a series of three papers devoted to the micro-mechanical conditions which render possible the appearance of shear bands in crystalline materials. The phenomenon is analysed as a bifurcation from an initially homogeneous mode of deformation. Following a previous work by Hill and Hutchinson, the criterion of bifurcation is seen as the compatibility between equilibrium, the particular form of the shear velocity field and the state of the material, expressed by its rate constitutive equation. The analysis is restricted to the case of rigid-plastic crystals with uniform strain hardening whose flow surface is the Bishop and Hill polyhedron. The paper discusses the form of the criterion according to the state of deviatoric stress on the yield surface, which determines the various geometries of the slip and the form of the rate law of behaviour. It shows that when only two or three independent slip systems are available, only coplanar and codirectional slip systems currently originate shear banding. With a higher number of slip systems, the conditions required for the bifurcation are different, as will be studied in the subsequent papers.

Key words: shear bands; rate constitutive law; Bishop and Hill polyhedron.

Notations

- t time,
- f arbitrary function of one variable,
- $C(t)$ current configuration,
- $\hat{C}(t)$ isoclinic configuration,
- a_i components of the vector a (in $C(t)$),
- A_{ij} components of the tensor \mathbf{A} (in $C(t)$),
- $\dot{a}, \dot{\mathbf{A}}$ derivative of the vector a (respectively: of the tensor \mathbf{A}) with respect to time,
- $\overset{\vee}{\mathbf{A}}^*$ derivative of the tensor \mathbf{A} with respect to time (components formed on axes which spin with the lattice),
- \bar{a} vector a transported in $\hat{C}(t)$,
- $\bar{\mathbf{A}}$ tensor \mathbf{A} transported in $\hat{C}(t)$,
- x_{ij} current position of a material point,

- V velocity field,
- η velocity field in a shear band,
- \mathbf{I} second order identity tensor,
- \mathbf{F} deformation gradient,
- \mathbf{P} plastic deformation gradient,
- \mathbf{R} rotation of the lattice,
- \mathbf{D} Eulerian strain rate,
- \mathbf{L} Eulerian velocity gradient,
- $\mathbf{\Omega}$ spin rate,
- $\mathbf{\Omega}^*$ crystallographic lattice spin rate,
- \mathbf{T} Cauchy stress,
- \mathbf{S} deviatoric Cauchy stress,
- \mathbf{X} deviatoric stress tensor on an edge of the Bishop and Hill polyhedron,
- \mathbf{S}_0 projection of the centre 0 on an edge of the Bishop and Hill polyhedron,
- \mathfrak{s} deviatoric stress tensor in a vectorial subspace comprising an edge, of the Bishop and Hill polyhedron,
- \mathbf{S}^v deviatoric stress at a vertex v ($v = 1 \dots 56$) of the Bishop and Hill polyhedron,
- \dot{W} rate of plastic work dissipated per unit volume,
- \mathbf{M} Schmid factor, after symmetrisation,
- \mathbf{M}' Schmid factor, before symmetrisation,
- p isostatic pressure,
- ν unit normal to a shear plane,
- τ_c critical resolved shear stress,
- h_a microscopic strain-hardening modulus,
- R ratio h_a/τ_c ,
- n unit normal to a crystallographic slip plane,
- g unit vector aligned with a crystallographic slip direction,
- $\dot{\gamma}$ glide rate on a crystallographic slip direction,
- \mathcal{E} vectorial space of the second order, three-dimensional symmetric tensors of trace 0,
- $\mathcal{E}\mathbf{v}$ vectorial subspace of \mathcal{E} comprising a flow cone,
- d dimension of a variety on the Bishop and Hill polyhedron,
- N number of active crystallographic slip systems on a variety of the Bishop and Hill polyhedron,
- μ_i components of the flow rate expressed as a combination of the crystallographic slip systems,
- (S) system of equations on which the bifurcation depends,
- λ^n parameters of the rate constitutive law of behaviour,
- y unknown proportional to the gradient of the rate of hydrostatic pressure,
- $C_{ij}, \alpha_{ij}, \beta_{ij}, \gamma_{ij}$ dimensionless quantities used to calculate the bifurcation criterion,
- CP coplanar crystallographic slip planes,
- CD codirectional crystallographic slip planes,
- ζ_{ij} parameter taking the values $-1, 0, 1$ in the system (S),
- Δ determinant,
- P_e homogeneous polynomial of degree e .

1. Introduction

SHEAR BANDS are zones of highly concentrated deformation between parallel planes. They are observed at large strains in various forming processes on all sorts of solids including polymers and geological materials. In metals, they form mainly at room temperature. They start as microscopic bands with a width of a few $1/10 \mu\text{m}$ within a grain; other microbands cluster parallel to the previous ones; then they may cross grain boundaries, generally without deflection, and form macrobands which extend over the scale of the whole sample. In spite of the variety of tested metals and deformation paths, they have striking common features in their dimensions, their patterns in the material, the way they propagate and saturate [1].

Numerous experimental investigations have been done on the factors which favour or hinder their development. They include metallurgical considerations like the substructure of dislocations [2, 3], the stacking fault energy [4] and a range of microstructural phenomena like the pinning of dislocations by solute atoms or, on the contrary, the breakdown of obstacle networks opposing the dislocation glide [5]. Mechanical factors have also been extensively reviewed. The fact that changes in the deformation path trigger off the shear bands has been documented [6]. Some investigators have pointed out that larger grains are more sensitive to shear banding than the smaller ones [7]; others have put in evidence the role of the crystallographic orientations [8].

The present series of papers is a contribution to the study of the micro-mechanical conditions which make possible the appearance of intragranular shear bands. It tries to determine the conditions under which the initially smooth evolving, homogeneous mode of deformation may change abruptly into a localised scheme, an intense shear between two limiting planes. The thermal effects, which play an important role in the bands that form when the metal is machined [9], are not taken into account here, and the constitutive law of the material is chosen as rate-insensitive, which is suitable, for example, for cold-rolling.

Localization phenomena can be studied by various methods. At the macroscopic level, successful analyses have been conducted by introducing initial non-uniformities. Such were the papers by MARCINIAK and KUCZYŃSKI [10] in which a variation of thickness in a sheet deepens into a groove, or various analyses using finite element methods [11, 12]. When no imperfections are created at the frontiers, an important tool is the study of uniqueness and stability performed by HILL [13]. In the case of rate-sensitive materials, localisation phenomena must be thought in terms of the development of an initially infinitesimal perturbation [14]. In the rate-insensitive case, on the contrary, they can be analysed in terms of a bifurcation, that is, an alternative to the homogeneous solution which fulfils the same boundary conditions. It must be stressed that in this approach,

the law of behaviour of the material is the same at the onset of shear banding in the matrix and in the affected zone.

Among the variants of the latter method, RICE's work [15] must be referred to because it gives, in the rigorous formalism of large deformations and rotations, the kinematic and equilibrium conditions for the bifurcation along a surface within the material. An application to the case of crystals has been done by PIERCE [16], although his results are restricted to the case of symmetric bi-slip. Here a slightly different approach is used, based on a 1975 work by HILL and HUTCHINSON [17]. These authors have proposed an analysis of the bifurcation in two dimensions of a continuous medium, deformed in tension along its axes of orthotropy. In spite of this restrictive presentation, their criterion can be adapted to various types of rate-insensitive, incompressible, incrementally linear materials, in particular ductile f.c.c. crystals which obey the Schmid law. Hence, rigid plasticity is assumed. The choice of the description of work hardening involved special difficulties. As shown by ASARO [18], latent hardening favours the localization, and there is no theoretical difficulty in adapting the present calculation to the case of heterogeneous strain hardening [19]. Anyhow, the testing of realistic representations of strain hardening is a complex task. Here, it was chosen to consider it as uniform, so that the flow surface of the material is the Bishop and Hill polyhedron. The deviatoric loading and the initially homogeneous flow may lay anywhere upon it, provided that the flow belongs to the adequate cone of the normals. The first paper gives the conditions of bifurcation all over the polyhedron; the second one is devoted to the vertices and the third to the edges of dimension one.

2. Fundamentals

2.1. Principles of the Hill and Hutchinson analysis

When the deformation is uniform in the material, the velocity field V_i , $i = 1 \dots 3$ is given by combining the fundamental principle of mechanics (in the present case, the equilibrium equations) and the constitutive law of the solid. The analysis of bifurcation by HILL and HUTCHINSON [17] states that heterogeneity becomes possible when, with the evolution of the mechanical properties of the solid, the compatibility with a third element, i.e. a particular form of the velocity field, can be achieved. It must be noticed from the start that for these calculations, the law of behaviour of the material has to be taken in the form of a rate constitutive equation, which involves the applied stress state (in the present paper the Cauchy stress \mathbf{T}), the stress rate (see below the choice of a derivative of \mathbf{T} with respect to time), the strain rate gradient $\mathbf{L} = \text{grad}(V)$ or, in various applications, the symmetrised strain rate tensor $\mathbf{D} = \frac{1}{2}(\text{grad}(V) + \text{grad}(V)^T)$,

and the strain itself, through its consequences on the strength of the material and its rate of work-hardening. When the latter is uniform, it can be represented by one parameter, the microscopic hardening modulus h_a . Since the material is incompressible, only the deviatoric part \mathbf{S} is responsible for the deformation; the hydrostatic pressure, denoted p , is such that $\mathbf{T} = -p\mathbf{I} + \mathbf{S}$.

Due to the fact that the shear band is bounded by planes of unit normal ν , as sketched in Fig. 1. the particular form of the velocity field is:

$$V_i = \eta_i f(\nu_k x_k), \quad i, k = 1\dots 3 \quad \text{with} \quad \eta_i \nu_i = 0, \quad i = 1\dots 3,$$

f depends only on the variable $\nu_k x_k$, and so is the hydrostatic pressure p . Bifurcation takes place if there is a non-trivial solution for the velocity field η in the shear band. The η_i are determined only within a scaling factor, and f is undetermined, except on the bounding planes of the shear band where $f = 0$, so that the continuity of the velocity field (but not the continuity of its gradient) is fulfilled.

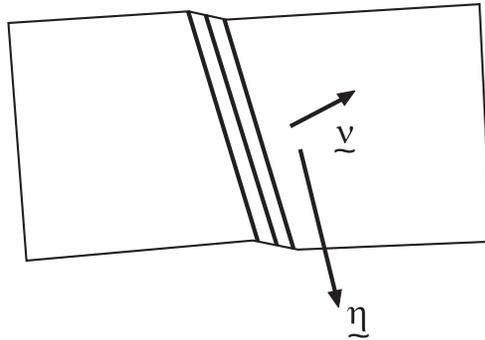


FIG. 1. Sketch of the shear band geometry.

2.2. The Bishop and Hill polyhedron

The yield surface of a purely plastic metal in which the slip systems are defined by $\{111\} \langle 110 \rangle$ or $\{110\} \langle 111 \rangle$ has been studied by BISHOP and HILL [20, 21]. The present section sums up the notations and some results of further works on the subject, particularly those classifying the edges: KOCKS *et al.*, [22], FORTUNIER *et al.* [23].

Let \bar{n}^s and \bar{g}^s be the unit normal to the slip plane and the unit vector aligned with the slip direction of a crystallographic system of index s , noted, for example, in the isoclinic configuration (see below). The symmetrised Schmid factors are defined by $\bar{\mathbf{M}}^s = \frac{1}{2} (\bar{g}^s \otimes \bar{n}^s + \bar{n}^s \otimes \bar{g}^s)$, the unsymmetrised Schmid factors by

$\bar{\mathbf{M}}'^s = \bar{g}^s \otimes \bar{n}^s$. Since a shear line can work in two opposite directions, a total of 24 slip systems are considered, numbered so that $\bar{n}^{s+12} = \bar{n}^s$, $\bar{g}^{s+12} = -\bar{g}^s$, $\bar{\mathbf{M}}'^{s+12} = -\bar{\mathbf{M}}'^s$. The critical resolved shear stress common to all the systems is denoted τ_c . Thus, all the glide rates $\dot{\gamma}^s$ $s = 1 \dots 24$ on the crystallographic slip systems are taken as positive or zero.

The Bishop and Hill polyhedron is a convex hypersurface, symmetric with respect to the origin 0. The deviatoric stress states which correspond to it can be described as a subset \mathcal{E}_V of the five-dimensional vectorial space \mathcal{E} of the second order, three-dimensional symmetric tensors of trace zero. So are the Schmid factors and the flow strain rates. Like a polyhedron in the Euclidian space, which exhibits facets, edges and vertices, the polyhedron is composed of subsets of dimension $d = 0$ to 4: a total of 698 ones, recapitulated in Table 1. These subsets are sometimes called varieties [23]. The varieties $d = 4$ are the hyperplanes (facets) corresponding to the activity of only one crystallographic slip system; there are $12 \times 2 = 24$ of them. The $28 \times 2 = 56$ vertices are the varieties $d = 0$; each one corresponds to only one state of deviatoric stress which is denoted S^v $v = 1 \dots 56$. $\mathbf{S}^{\nu+28} = -\mathbf{S}^\nu$. The case of the varieties $d = 1$ to 3 (edges) is more complex; some of their characteristics have been summarised in Table 1. Altogether, there are 26 crystallographically distinct types [22].

Let N be the number of slip systems active on a given variety of dimension d . The corresponding Schmid factors $\bar{\mathbf{M}}'^s$ $s = 1 \dots N$ form a subspace of \mathcal{E} , the dimension of which is $(5-d)$; of course, $N \geq 5-d$. It is important to note at this stage that, whatever is the stress on the Bishop and Hill polyhedron, the velocity field η must belong to the cone of the normals to the corresponding facet, edge or vertex. Hence, only a limited number of systems can be activated, depending on the stress state of the crystal; when the bifurcation occurs, the glide rates change, causing a discontinuity in the velocity gradient, but the Schmid law stands and no extra system is activated. This is in accordance with the postulate of bifurcation, which states that pre-localization conditions prevail at the onset of the phenomenon. Besides, it will be seen in the applications of this theory that characteristic cases of shear banding correspond to the stoppage of the glide on certain crystallographic slip systems, while others continue at an increased rate.

A classical description of the uniform strain hardening is that the rate of resolved shear stress $\dot{\tau}_c$ on all the slip systems is given by $\dot{\tau}_c = h_a \sum_{k=1}^N \dot{\gamma}^k$ where h_a is the above-mentioned microscopic strain hardening modulus, and $\dot{\gamma}^k$ the glide rates on the N active slip systems of the variety on which the deformation takes place; $N = 1, 2, 3, 4, 5, 6$ or 8, see Table 1.

Table 1. The facets, edges and vertices on the Bishop and Hill polyhedron.

Dimension (d)	Number and nature	Number crystallographic classes	Variety	Number of active slip systems (N)
0	56 vertices	5	4A	8
			4B	6
			4C	8
			4D	6
			4E	8
1	216 edges ($d = 1$)	8	3A	4
			3B	6
			3C	4
			3D	4
			3E	4
			3F	4
			3G	4
			3H	5
2	270 edges ($d = 2$)	7	2A	3
			2B	4
			2C	4
			2D	3
			2E	3
			2F	3
			2G	3
3	132 edges ($d = 3$)	5	1A	2
			1B	
			1C	
			1D	
			1E	
4	24 facets	1	0A	1

2.3. The mechanical framework

Much work has been done to define with rigour the various representations which describe the elasto-viscoplastic deformation of a solid [24]. Although the case of rigid plasticity is much simpler, it is worth referring to the isoclinic configuration, introduced by LEE [25] and discussed by MANDEL [26] and other authors, since it is the framework of all theoretical work on plasticity today.

Let $C(t)$ be the current configuration, to which belongs the Cauchy tensor \mathbf{T} , and $C(0)$ – the initial configuration. The deformation gradient tensor \mathbf{F} is the product of the plastic deformation gradient \mathbf{P} and of the rotation of the lattice \mathbf{R} , so that $\mathbf{F} = \mathbf{R} \cdot \mathbf{P}$. \mathbf{P} results from the contribution of various crystallographic slip systems. The isoclinic configuration $\hat{C}(t)$ corresponds to a fictitious state of the material in which the glide has taken place on the active systems, but no rotation has affected the crystal lattice, which remains the same as in the reference configuration $C(0)$. When transported from $C(t)$ to $\hat{C}(t)$, the vectors and tensors (for example a and \mathbf{A}) are written \bar{a} and $\bar{\mathbf{A}}$. In $\hat{C}(t)$, the crystallographic slip systems do not rotate, hence the above-mentioned notations \bar{g}^s , \bar{n}^s and $\bar{\mathbf{M}}^s$ to introduce the Schmid factors. When expressed in the current configuration $C(t)$, \bar{g}^s becomes g^s such as $g^s = \mathbf{R} \cdot \bar{g}^s$ and \bar{n}^s becomes n^s such as $n^s = \mathbf{R} \cdot \bar{n}^s$, so that $\mathbf{M}^s = \mathbf{R} \cdot \bar{\mathbf{M}}^s \cdot \mathbf{R}^T$ and $\dot{\bar{\mathbf{M}}}^s = 0$ whereas $\dot{\mathbf{M}}^s \neq 0$. All the usual tensors of stress and kinematics have been defined in the isoclinic configuration, but for the present work it is only necessary to consider:

- the isoclinic strain rate $\bar{\mathbf{D}} = \frac{1}{2}(\dot{\mathbf{P}} \cdot \mathbf{P}^{-1} + \mathbf{P}^{-T} \cdot \dot{\mathbf{P}}^T)$, which is the correspondent in $\hat{C}(t)$ of the Eulerian tensor \mathbf{D} , which belongs to $C(t)$:

$$(2.1) \quad \bar{\mathbf{D}} = \mathbf{R}^T \cdot \mathbf{D} \cdot \mathbf{R}$$

- the isoclinic stress $\bar{\mathbf{T}}$ and its deviatoric part $\bar{\mathbf{S}}$ which are such that:

$$(2.2) \quad \begin{aligned} \bar{\mathbf{T}} &= \mathbf{R}^T \cdot \mathbf{T} \cdot \mathbf{R}, \\ \bar{\mathbf{S}} &= \mathbf{R}^T \cdot \mathbf{S} \cdot \mathbf{R}. \end{aligned}$$

The tensors $\bar{\mathbf{T}}$ and $\bar{\mathbf{D}}$ are conjugated, as shown by calculating the rate of plastic work dissipated by unit volume \dot{W} :

$$(2.3) \quad \dot{W} = \mathbf{T} : \mathbf{D} = \mathbf{S} : \mathbf{D} = \bar{\mathbf{T}} : \bar{\mathbf{D}} = \bar{\mathbf{S}} : \bar{\mathbf{D}}.$$

The isoclinic configuration allows to write the Schmid law straightforwardly:

$$(2.4) \quad \tau_c = \bar{\mathbf{M}}^{s_k} : \bar{\mathbf{T}} = \bar{\mathbf{M}}^{s_k} : \bar{\mathbf{S}} \quad \text{for } k = 1 \dots N.$$

(When elasticity is considered, which is not the case here, it offers the advantage to give an expression of the law independent the deformation of the crystal lattice). But the main interest of $\hat{C}(t)$ is that it provides a reference frame invariant throughout the deformation, so that the derivatives $\dot{\bar{\mathbf{T}}}$ and $\dot{\bar{\mathbf{S}}}$ are objective tensors. On the contrary in $C(t)$, the objective stress rate tensor must be defined as a derivative in some frame which accompanies the material in its rotation. In the

present case the axes which spin with the crystal lattice are chosen to derivate the components of \mathbf{T} . This particular derivative is noted $\overset{\vee}{\mathbf{T}}^*$, and is different from the usual Jaumann derivative [18]. The lattice rotates with respect to the initial or isoclinic frame with a rotation rate $\mathbf{\Omega}^* = \dot{\mathbf{R}} \cdot \mathbf{R}^{\mathbf{R}}$ so that:

$$(2.5) \quad \begin{aligned} \overset{\vee}{\mathbf{T}}^* &= \dot{\mathbf{T}} + \mathbf{T} \cdot \mathbf{\Omega}^* - \mathbf{\Omega}^* \cdot \mathbf{T}, \\ \overset{\vee}{\mathbf{S}}^* &= \dot{\mathbf{S}} + \mathbf{S} \cdot \mathbf{\Omega}^* - \mathbf{\Omega}^* \cdot \mathbf{S}. \end{aligned}$$

The Schmid law can be derived straightforwardly in $\hat{C}(t)$ as $\dot{\tau}_c = \overline{\mathbf{M}}^{s_k} \cdot \overset{\vee}{\mathbf{S}}$ for $k = 1 \dots N$ and some algebra involving Eqs. (2.4) and (2.5) shows that:

$$(2.6) \quad \begin{aligned} \dot{\tau}_c = \overline{\mathbf{M}}^{s_k} : \overset{\vee}{\mathbf{S}} &= (\mathbf{R}^T \cdot \mathbf{M}^{s_k} \cdot \mathbf{R}) : (\dot{\mathbf{R}}^T \cdot \mathbf{S} \cdot \mathbf{R} + \mathbf{R}^T \cdot \dot{\mathbf{S}} \cdot \mathbf{R} + \mathbf{R}^T \cdot \mathbf{S} \cdot \dot{\mathbf{R}}) \\ &= \mathbf{M}^{s_k} : (\dot{\mathbf{S}} + \mathbf{S} \cdot \mathbf{\Omega}^* - \mathbf{\Omega}^* \cdot \mathbf{S}), \end{aligned}$$

hence the consistency condition, expressing that the stress remains on the flow surface when deformation goes on, becomes:

$$(2.7) \quad \mathbf{M}^{s_k} : \overset{\vee}{\mathbf{S}}^* = \dot{\tau}_c \quad \text{for } k = 1 \dots N.$$

It can be noted that Eqs. (2.4) and (2.7) can also be written with the unsymmetrised Schmid tensors \mathbf{M}^{s_k} (or $\overline{\mathbf{M}}^{s_k}$ in the isoclinic configuration), since the involved stress tensors are symmetric.

2.4. The equilibrium equations

Since a rate constitutive law is used, the usual equilibrium equations must be derived with respect to time, and adapted to the case of a bifurcating crystal.

Bifurcation along a plane considers only the gradients perpendicular to this plane, hence the description of the velocity field as $V_i = \eta_i f(\nu_k x_k)$. The same applies to the hydrostatic pressure which is taken as a function $p(\nu_k x_k)$. In the pre-localization state, the deformation of the crystal is considered as uniform, without gradients in the strain rate or the applied stress (stress and strain, nevertheless, vary with time). Hence $\partial \dot{\gamma}^s / \partial x_k = 0$ and $\partial \mathbf{T}_{ij} / \partial x_k = 0$.

These assumptions are fully justified because the shear bands are very thin (1/10 μm wide), thus no gradient of applied stress in their width would be significant. When shear banding occurs, it extends along the whole plane throughout the crystal, at least as long as the lattice, hence the n^s and g^s retain rigorously their orientation. This actually happens in real crystals in which the shear bands

are seldom stopped in their straight development, except by grain boundaries or outer surfaces.

If there are no body forces (e.g. weight) and no accelerations, as usual in metal forming problems, the equilibrium equations can be written in $C(t)$ as $\partial \mathbf{T}_{ij} / \partial x_j = 0$ for $i = 1 \dots 3$. They are derived with respect to time by considering the total derivative of $\mathbf{T}(t, x_k)$ $k = 1 \dots 3$:

$$(2.8) \quad \dot{\mathbf{T}}_{ij} = \frac{d\mathbf{T}_{ij}}{dt} = \frac{\partial \mathbf{T}_{ij}}{\partial t} + \frac{\partial \mathbf{T}_{ij}}{\partial x_k} V_k \quad \text{for } i, j, k = 1 \dots 3.$$

Hence:

$$(2.9) \quad \frac{\partial \dot{\mathbf{T}}_{ij}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\partial \mathbf{T}_{ij}}{\partial t} \right) + \frac{\partial}{\partial x_j} \left(\frac{\partial \mathbf{T}_{ij}}{\partial x_k} \right) V_k + \frac{\partial \mathbf{T}_{ij}}{\partial x_k} \frac{\partial V_k}{\partial x_j} \quad \text{for } i, j, k = 1 \dots 3.$$

Inverting the partial derivatives and taking $\partial \mathbf{T}_{ij} / \partial x_j$ as zero yields:

$$(2.10) \quad \frac{\partial \dot{\mathbf{T}}_{ij}}{\partial x_j} - \frac{\partial \mathbf{T}_{ij}}{\partial x_k} \frac{\partial V_k}{\partial x_j} = 0 \quad \text{for } i, j, k = 1 \dots 3.$$

By introducing the derivative $\overset{\vee}{\mathbf{T}}^*$ and taking advantage of the fact that $\mathbf{\Omega}^*$ is a skew tensor, it is possible to write the equilibrium equations under the form:

$$(2.11) \quad \frac{\partial \overset{\vee}{\mathbf{T}}_{ij}^*}{\partial x_j} + \mathbf{T}_{ik} \frac{\partial \mathbf{\Omega}_{jk}^*}{\partial x_j} + \mathbf{T}_{jk} \frac{\partial \mathbf{\Omega}_{ik}^*}{\partial x_j} + \frac{\partial \mathbf{T}_{ik}}{\partial x_j} \cdot \mathbf{\Omega}_{jk}^* - \frac{\partial \mathbf{T}_{ij}}{\partial x_k} \frac{\partial V_k}{\partial x_j} = 0 \quad \text{for } i = 1 \dots 3.$$

As seen above, $\partial \mathbf{T}_{ij} / \partial x_k = 0$ in the present analysis. One important consequence of the local uniformity of the glide rates concerns the relation between the rigid body rotation rate $\mathbf{\Omega} = \frac{1}{2}(\text{grad}(V) - \text{grad}(V)^T)$ and the lattice rotation rate $\mathbf{\Omega}^*$. Their difference is the plastic spin due to the activity of the slip systems $\mathbf{\Omega} = \mathbf{\Omega}^* + \frac{1}{2} \sum_{k=1}^N \dot{\gamma}_k (g^{sk} \otimes n^{sk} - n^{sk} \otimes g^{sk})$. With the above-mentioned hypotheses:

$$(2.12) \quad \text{grad } \mathbf{\Omega} = \text{grad } \mathbf{\Omega}^*.$$

But $\text{div}(\overset{\vee}{\mathbf{T}}^*) = -\text{grad}(\dot{p}) + \text{div}(\overset{\vee}{\mathbf{S}}^*)$. Since the $\partial \mathbf{\Omega}_{ij} / \partial x_k$ are skew tensors, it is easy to find that:

$$(2.13) \quad \mathbf{T}_{ik} \frac{\partial \mathbf{\Omega}_{jk}}{\partial x_j} + \mathbf{T}_{jk} \frac{\partial \mathbf{\Omega}_{ik}}{\partial x_j} = \mathbf{S}_{ik} \frac{\partial \mathbf{\Omega}_{jk}}{\partial x_j} + \mathbf{S}_{jk} \frac{\partial \mathbf{\Omega}_{ik}}{\partial x_j}.$$

This allows to specialise the equilibrium equations as:

$$(2.14) \quad \frac{\partial \mathbf{S}_{ij}^*}{\partial x_j} + \mathbf{S}_{ik} \frac{\partial \Omega_{jk}}{\partial x_j} + \mathbf{S}_{jk} \frac{\partial \Omega_{ik}}{\partial x_j} - \frac{\partial \dot{p}}{\partial x_i} = 0 \quad \text{for } i = 1 \dots 3$$

which are used in this form infra.

3. The criterion of bifurcation

3.1. The differential constitutive equation

The most important task to implement Hill and Hutchinson's analysis in the case of a crystalline solid is to find the expressions of the rate constitutive law which, due to the incompressibility of the material, can be taken in the form $\mathbf{S}^* = F_{h_a}(\mathbf{S}, \mathbf{L})$. As pointed out in [17], this law can be piecewise linear, and on the Bishop and Hill polyhedron its expression is different on each variety. It is obtained by combining:

- i) the flow rule, written in $C(t)$ as $\mathbf{L} = \sum_{k=1}^N \dot{\gamma}^k \mathbf{M}^{s_k} \dot{\gamma}^k \geq 0$,
- ii) the hardening rule, already written as $\dot{\tau}_c = h_a \sum_{k=1}^N \dot{\gamma}^k$,
- iii) the consistency condition $\dot{\tau}_c = \mathbf{M}^{s_k} : \mathbf{S}^* = \mathbf{M}^{s_k} : \mathbf{S}^*$.

These relations allow to calculate the rate of plastic work dissipated per unit volume as:

$$(3.1) \quad \dot{W} = \mathbf{S} : \mathbf{L} = \mathbf{S} : \sum_{k=1}^N \dot{\gamma}^k \mathbf{M}^{s_k} = \tau_c \frac{\dot{\tau}_c}{h_a}$$

so that the differential constitutive law verifies the set of relations:

$$(3.2) \quad \forall k \ k = 1 \dots N \quad \mathbf{M}^{s_k} : \mathbf{S}^* = \frac{h_a}{\tau_c} \mathbf{S} : \mathbf{L}.$$

This can be written as a set of N linear equations of five of the variables S_{ij} ($S_{ii} = 0$). The rank of this system cannot be greater than five since the \mathbf{M}^{s_k} belong to the vectorial space \mathcal{E} . An arbitrary facet, edge or vertex on the Bishop and Hill polyhedron is part of the set of the tensors ς such as:

$$(3.3) \quad \mathbf{M}^{s_k} : \varsigma = \tau_c$$

for $k = 1 \dots N$ (slip systems active on the variety). The ς do not know the restriction imposed on the deviatoric states \mathbf{S} because the Bishop and Hill polyhedron

is convex and finite. As noted supra, the flow cone is orthogonal to the subset of deviatoric stress states. Hence, for a given flow rate \mathbf{D} , for any \mathbf{S} of the activated variety or for any element $\boldsymbol{\varsigma}$ of the subset defined by Eq. (2.4), it is possible to write:

$$(3.4) \quad \forall \boldsymbol{\varsigma} \mathbf{S} : \mathbf{D} = \boldsymbol{\varsigma} : \mathbf{D} = \mathbf{S}_0 : \mathbf{D} = \mathbf{S} : \mathbf{L} = \boldsymbol{\varsigma} : \mathbf{L} = \mathbf{S}_0 : \mathbf{L}$$

where \mathbf{S}_0 is the projection of the centre 0 on the variety. Equation (2.5) gives multiple expressions of the rate of plastic work, which is unique on a variety when \mathbf{D} is known. Substituting \mathbf{L} to \mathbf{D} does not change this result. The solution of Eq. (2.3) is:

$$(3.5) \quad \mathbf{S}^* = \frac{h_a}{\tau_c^2} (\boldsymbol{\varsigma} \otimes \boldsymbol{\varsigma}) : \mathbf{L}$$

as can be checked by writing:

$$\begin{aligned} \forall k = 1 \dots N, \\ M_{ij}^{sk} \overset{\vee}{S}_{ij}^* = M_{ij}^{sk} \left(\frac{h_a}{\tau_c^2} \varsigma_{ij} \varsigma_{mn} L_{mn} \right) = \frac{h_a}{\tau_c^2} \left(M_{ij}^{sk} \varsigma_{ij} \right) \varsigma_{mn} L_{mn} = \frac{h_a}{\tau_c} S_{mn} L_{mn}. \end{aligned}$$

In the calculations infra, it is used in the form:

$$(3.6) \quad \overset{\vee}{S}_{ij}^* = \frac{h_a}{\tau_c^2} \varsigma_{ij} S_{0mn} D_{mn}.$$

Some important features of this result are:

- i. At the vertices \mathbf{S}^v $v = 1 \dots 56$, the solution is unique since $\boldsymbol{\varsigma} = \mathbf{S} = \mathbf{S}_0 = \mathbf{S}^v$.
- ii. This is not true on the edges of the polyhedron, on which the expression of the rate constitutive law includes a tensor $\boldsymbol{\varsigma}$ whose value cannot be determined by mechanics of the crystal itself, but results from other considerations, the bifurcation requirements for instance. The same happens with the state of deviatoric stress which, in incompressible solids, can be determined by considerations of equilibrium, while the complete stress tensor is known only by adding the boundary conditions.

3.2. Existence of a criterion of bifurcation

The considerations above show that bifurcation occurs when there are non trivial solutions η_i to the system (S) of equations composed of:

- i. Three equilibrium equations:

$$(3.7) \quad \operatorname{div} \left(\frac{h_a}{\tau_c^2} (\boldsymbol{\varsigma} \otimes \mathbf{S}_0) : \mathbf{D} + \boldsymbol{\Omega} \cdot \mathbf{S} - \mathbf{S} \cdot \boldsymbol{\Omega} \right) - \operatorname{grad}(\dot{p}) = 0$$

in which the tensorial expressions can be calculated using $\frac{\partial f}{\partial x_j} = \nu_j f'$ and

$\frac{\partial \dot{p}}{\partial x_i} = \nu_i \dot{p}'$, since hydrostatic pressure is taken as a function of $\nu_k \eta_k$ only; then $\frac{\partial \mathbf{D}_{mn}}{\partial x_j} = \frac{1}{2} \nu_j (\nu_m \eta_n + \nu_n \eta_m) f''$ and $\frac{\partial \mathbf{\Omega}_{im}}{\partial x_j} = \frac{1}{2} \nu_j (\nu_m \eta_i - \nu_i \eta_m) f''$, and similarly $\frac{\partial \mathbf{\Omega}_{jm}}{\partial x_j}$.

ii. The condition of orthogonality $\eta \cdot \nu = 0$.

iii. Five equations due to the fact that the bifurcation flow, $\mathbf{D}_{ij} = \frac{1}{2} (\nu_i \eta_j + \nu_j \eta_i) f'$, which has five independent components, belongs to the cone of the normals to the considered variety. This condition requires different treatments whether the number N of active slip systems is equal to or greater than $(5 - d)$: see Table 1.

- if $N = (5 - d)$, \mathbf{D} can be decomposed in a unique way on the Schmid factors which define the cone, so that the five equations express that:

$$\exists \mu'_k \quad k = 1 \dots N \quad \text{with} \quad \mathbf{D} = \sum_{k=1}^N \mu'_k \mathbf{M}^{s_k}.$$

It must be verified later that the μ'_k are all of the same sign, so that \mathbf{D} actually belongs to the flow cone and not simply to the vectorial subspace \mathcal{E}_V of dimension $(5 - d)$ which contains it. In this case the μ'_k are the glide rates $\dot{\gamma}^k$ on the slip systems;

- if $K > (5 - d)$, it is necessary to choose a base among the \mathbf{M}^{s_k} , that is $(5 - d)$ of them which generate the subspace \mathcal{E}_V . The five equations of the system express that \mathbf{D} belongs to \mathcal{E}_V :

$$\exists \mu''_m \quad m = 1 \dots (5 - d) \quad \text{with} \quad \mathbf{D} = \sum_{m=1}^{5-d} \mu''_m \mathbf{M}^{s_m}$$

and the μ''_m $m = 1 \dots (5 - d)$ do not give directly the glide rates, since several combinations of $\dot{\gamma}^k$ can produce the same strain rate \mathbf{D} .

The system (S) has nine equations \dot{p}' and f'' only intervene through their ratio in the three equilibrium equations. For a given state of deviatoric stress \mathbf{S} , for a given ν (all the planes of the Euclidian space will be successively tested for bifurcation), (S) is linear with respect to the η_i , $i = 1 \dots 3$ the ratio \dot{p}'/f'' and the coefficients μ'_m or μ''_m , $m = 1 \dots (5 - d)$. The criterion of bifurcation, which is the condition for the existence of non zero solutions, is calculated below.

3.3. Principle of calculation of the criterion

In order to solve the system (S) , the first task is to determine the tensors ς which represent the part of the differential constitutive law which is still un-

determined at this point of the analysis. For this, a base \mathbf{X}^n , $n = 1 \dots d$ is taken on the variety of the Bishop and Hill polyhedron, so that it is possible to write $\boldsymbol{\varsigma} = \mathbf{S}_0 + \sum_{n=1}^d \lambda^n \mathbf{X}^n$, the λ^n being quantities which can take any real value and on which depends the existence of non zero solutions. The \mathbf{X}^n are orthogonal to the \mathbf{M}^{s_k} of the cone of the normals, and $\forall n \mathbf{X}^n : \mathbf{D} = 0$. Hence, the equilibrium equations take the form:

$$(3.8) \quad \left[\frac{h_a}{\tau_c^2} (\mathbf{S}_{0ik} + \sum_{n=1}^d \lambda^n \mathbf{X}_{ik}^n) \mathbf{S}_{0jl} \nu_k \nu_l + \frac{1}{2} (\mathbf{S}_{ik} \nu_j \nu_k - \mathbf{S}_{jk} \nu_i \nu_k - \mathbf{S}_{ij} + \delta_{ij} \mathbf{S}_{kl} \nu_k \nu_l) \right] \eta_j - \nu_i \frac{\dot{p}'}{f''} = 0$$

for $i = 1 \dots 3$. Results are easier to present with the help of:

- the variable $y = \dot{p}' / (f'' \tau_c)$,
- the dimensionless quantities α_{ij} , β_{ij}^n and γ_{ij} , defined by:

$$\alpha_{ij} = \frac{1}{\tau_c^2} \mathbf{S}_{0ik} \mathbf{S}_{0jl} \nu_k \nu_l, \quad \beta_{ij}^n = \frac{1}{\tau_c^2} \mathbf{X}_{ik}^n \mathbf{S}_{0jl} \nu_k \nu_l,$$

$$\gamma_{ij} = \frac{1}{\tau_c} (\mathbf{S}_{ik} \nu_j \nu_k - \mathbf{S}_{jk} \nu_i \nu_k - \mathbf{S}_{ij} + \delta_{ij} \mathbf{S}_{kl} \nu_k \nu_l),$$

- the ratio $R = h_a / \tau_c$,

which, taken together, allow to define $C_{ij} = R (\alpha_{ij} + \sum_{n=1}^d \lambda^n \beta_{ij}^n) + \gamma_{ij}$.

In the same way, it can be noted that the components of the \mathbf{M}^{s_k} in the axes of the crystal are $0, \pm \frac{1}{\sqrt{6}}, \pm \frac{1}{2\sqrt{6}}$. So, by introducing the coefficients $\mu_m = -\frac{\mu'_m}{\sqrt{6} f'}$ or $\mu_m = -\frac{\mu''_m}{\sqrt{6} f'}$, it is possible to write that \mathbf{D} belongs to \mathcal{E}_V with the help of coefficients ζ_{ij} which take the values 0, 1 or -1, and are characteristic of the variety. Hence the system (S) takes the form:

$$(3.9) \quad \begin{aligned} C_{11}\eta_1 + C_{12}\eta_2 + C_{13}\eta_3 + \nu_1 y &= 0, \\ C_{21}\eta_1 + C_{22}\eta_2 + C_{23}\eta_3 + \nu_2 y &= 0, \\ C_{31}\eta_1 + C_{32}\eta_2 + C_{33}\eta_3 + \nu_3 y &= 0, \end{aligned}$$

$$\begin{aligned}
& \nu_1\eta_1 + \nu_2\eta_2 + \nu_3\eta_3 = 0, \\
& \nu_1\eta_1 + \zeta_{11}\mu_1 + \dots + \zeta_{1(5-d)}\mu_{(5-d)} = 0, \\
& \nu_2\eta_2 + \zeta_{21}\mu_1 + \dots + \zeta_{2(5-d)}\mu_{(5-d)} = 0, \\
(3.9) \quad & \nu_2\eta_1 + \nu_1\eta_2 + \zeta_{31}\mu_1 + \dots + \zeta_{3(5-d)}\mu_{(5-d)} = 0, \\
[\text{cont.}] \quad & \nu_3\eta_1 + \nu_1\eta_3 + \zeta_{41}\mu_1 + \dots + \zeta_{4(5-d)}\mu_{(5-d)} = 0, \\
& \nu_3\eta_2 + \nu_2\eta_3 + \zeta_{51}\mu_1 + \dots + \zeta_{5(5-d)}\mu_{(5-d)} = 0.
\end{aligned}$$

Hence, (S) is a linear, homogeneous system of nine equations with $(9 - d)$ unknowns η_i , μ_j and y , whose coefficients depend on the quantities R and λ^n , $n = 1\dots d$, plus the ν_k , which are taken as the data. Another way of looking at it is to consider (S) as a system of nine equations, linear and homogeneous with respect to the $(8 - d)$ unknowns η_i and μ_j , nonlinear with respect to the $(d + 1)$ unknowns R and λ^n . The value of y can be fixed arbitrarily since the velocities η_i and the related quantities μ_j need only to be known within a scalar factor. With this approach, it appears that for a given shear plane ν , (S) might provide the orientation of the shear, the ratio R of strain hardening, and fix the quantities λ^n .

The approach of (S) as a homogeneous linear system with $(9 - d)$ unknowns has been favoured in the algorithm of resolution, all the planes in the Euclidian space being successively tested for bifurcation. Whether the latter is actually possible is discussed infra. When the parameter R can be calculated, its values form a continuous set limited by R_{\max} and R_{\min} . The physical sense of the calculation is the following: at the beginning of the deformation, h_a is high and so is the ratio $R = h_a/\tau_c$; but as the deformation goes on, h_a drops and τ_c rises steadily, so that R diminishes. So the bifurcation becomes possible on certain planes R_{\max} corresponding to the most favoured ones.

3.4. Cases in which the criterion can actually be calculated

Bifurcation is impossible on the facets of the polyhedron, since only one direction of flow is possible because of the Schmid law. Only deviations from this law allow to consider bifurcation when a single slip is active [27].

The more numerous are the active slip systems on a variety, the easier is the bifurcation. At the vertices (6 or 8 available slip systems, no λ^n , only one possible state of deviatoric stress), the solution of the system (S) is simple because Eqs. (3.9)₁ to (3.9)₄ contain the four unknowns η_i and y , and can be solved separately. This case is studied in the second paper of the series.

On the edges $d = 1$ (4, 5 or 6 available slip systems), the system (S) can be solved as a linear, homogeneous system of nine equations and eight unknowns, which has non-trivial solutions if all its nine determinants of order eight are zero. In practice, the nullity of two of them is sufficient so that R and λ can be determined, as seen in the third paper of the series.

Examining (S) in the case $d = 2$ (3 or 4 available slip systems) shows that Eqs. (3.9)₄ to (3.9)₉ form a linear, homogeneous system of six unknowns η_i and μ_i which has non-trivial solutions only if the determinant $\Delta = 0$:

$$(3.10) \quad \Delta = \begin{vmatrix} \nu_1 & \nu_2 & \nu_3 & 0 & 0 & 0 \\ \nu_1 & 0 & 0 & \zeta_{11} & \zeta_{12} & \zeta_{13} \\ 0 & \nu_2 & 0 & \zeta_{21} & \zeta_{22} & \zeta_{23} \\ \nu_2 & \nu_1 & 0 & \zeta_{31} & \zeta_{32} & \zeta_{33} \\ \nu_3 & 0 & \nu_1 & \zeta_{41} & \zeta_{42} & \zeta_{43} \\ 0 & \nu_3 & \nu_2 & \zeta_{51} & \zeta_{52} & \zeta_{53} \end{vmatrix}$$

($\zeta_{ij} = 1, -1$ or 0 according to the case). Hence only the planes such that their normal components ν_k abide a certain polynomial relation are suitable for bifurcation. This is distinctive from the case $d = 0$ and $d = 1$, for which the ν form continuous cones in the Euclidean space.

The complete study of the shear flows on all the edges of the Bishop and Hill polyhedron is in progress in [28] and the results for $d = 2$ are summarized in Table 2. For the suitable ν , Eqs. (3.9)₄ to (3.9)₉ yield the values of η . Conversely, with the suitable ν_i and η_i , Eqs. (3.9)₁ to (3.9)₃ give three relations linear in R , $R\lambda^1$, $R\lambda^2$ and y . This leaves R undetermined. Hence, for $d = 2$, the present theory does not provide a threshold of bifurcation. Basically, three types of situations happen:

- Only two coplanar (CP) systems are active (one or two $\mu_i = 0$, according to the edge). Their combination according to any new glide rates gives a shear flow different from the initial one. This is consistent with the fact that this mode of shear banding needs no condition on strain hardening, hence no threshold for R .
- The same, but with codirectional (CD) systems.
- A particular combination of the μ_i (hence of the $\dot{\gamma}^k$) is necessary. It takes the form of a homogeneous polynomial of degree $n = 1, 2$ or 3 in μ_i , according to the case. These polynomials are uniformly referred to as P_e in Table 2, e being their degree (1, 2 or 3) although they are all different. These conditions involve such a specific geometry for the flow that it is doubted whether they correspond to actual shear banding. On the contrary, there

is plenty of evidence that coplanar or codirectional slip systems combine to originate shear bands: see JAOUL [29].

Table 2. Bifurcation on the edges $d = 2$.

Class	Slip System	Conditions of bifurcation
2A	CP + CP+X	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0$
		b- $P_2(\mu_1, \mu_2, \mu_3)$
2B	CP + CP + CD + CD	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0, \quad \mu_4 = 0$
		b- $\forall \mu_1 = 0, \quad \forall \mu_2 = 0 \quad \mu_3 \geq 0, \quad \mu_4 \geq 0$
2C	CP + CP + X + X	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0, \quad \mu_4 = 0$
		b- $P_2(\mu_1, \mu_2, \mu_3)$
2D	(CD/CP) + CD + CP	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0$
		b- $\forall \mu_1 \geq 0, \quad \forall \mu_2 = \mu_3 \geq 0$
		c- $P_1(\mu_1, \mu_2, \mu_3)$
2E	CD + CD + X	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0$
		b- $P_1(\mu_1, \mu_2, \mu_3)$
2F	CP + CP + X	a- $\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0 \quad \mu_3 = 0$
		b- $P_2(\mu_1, \mu_2, \mu_3)$
2G	X + X + X	a- $P_3(\mu_1, \mu_2, \mu_3)$

Three or four slip systems available. X means that the system is neither (CP) nor (CD).

Table 3. Bifurcation on the edges $d = 3$.

Class	Slip Systems	Conditions of bifurcation
1A	CP + CP	$\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0$
1B	CD + CD	$\forall \mu_1 \geq 0, \quad \forall \mu_2 \geq 0$
1C	X + X	Impossible
1D	X + X	Impossible
1E	X + X	$P_1(\mu_1, \mu_2)$

Two slip systems available. Same conventions as in Table 2.

The same occurs in the case $d = 3$ (two available slip systems) but here the conditions on ν are more rigorous, since all the determinants of order 5 formed by Eqs. (3.9)₄ to (3.9)₉ must be zero. Table 3 recapitulates the possible cases, which are, with one exception, combinations of (CD) and (CP) systems. Five unknowns $R, R\lambda^1, R\lambda^2, R\lambda^3$ and y are found in the equilibrium equations, so that there is no condition on work hardening. Such results differ from those of PIERCE [16]

who found that only a low value of strain hardening leads to bifurcation in the case of two slip systems. This discrepancy could come from the fact that Pierce considers elasto-plasticity, instead of the rigid-plastic model used here.

4. Partial conclusion

In this paper, several elements necessary for the study of the localisation into shear bands of the rigid plastic f.c.c. crystals with uniform strain hardening have been presented, in the wake of Hill and Hutchinson's work. The differential constitutive relations, classical at the vertices [15], have been formulated for all the varieties of the Bishop and Hill polyhedron. The equilibrium requirements, the kinematic compatibility and the normality rule impose conditions which form a system (S) of nine equations. Additional inequalities ensure that the flow rate is compatible with the deviatoric state of stress. The appearance of the band corresponds to a redistribution of the glide rates on the available slip systems. The occurrence of such events has been repeatedly pointed out in metallurgical studies, both the obstruction of certain systems (due, for example, to a lamellar substructure of dislocations) and, with the opposite effect, the ease of the dislocation glide in privileged directions after some critical work hardening [30].

The form of the system (S) changes according to the state of the applied deviatoric stress, which determines the dimension d of the activated variety on the Bishop and Hill polyhedron. The bifurcation criterion is the compatibility condition which ensures that the velocity field in the shear band is not identically zero. When $d = 2$ or 3 (edges with few available slip systems), only specific geometries allow shear banding and the rigid-plastic analysis provides no threshold for bifurcation. The conditions of the latter are quite different in the case of the edges $d = 1$ or at the vertices $d = 0$, which will be studied in the subsequent papers.

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