Int. J. Solids Structures Vol. 29, No. 6, pp. 745–765, 1992
Printed in Great Britain.

0020-7683/92 $5.00 + .00

ON DISCRETIZED PLASTICITY PROBLEMS WITH BIFURCATIONS

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(*Received 6 July 1990; in revised form January 1991*)

Abstract—A spatially discretized non-linear rate problem for a time-independent plastic solid is examined with particular reference to bifurcation. Constitutive non-linearity in a general form encompassing the yield-surface vertex effect is considered under the restriction that the tangent stiffness matrix for the whole system is symmetric. Theorems concerning existence, uniqueness and stability of solutions are presented. As an outcome of the theoretical analysis, a computational method is proposed for crossing bifurcation points with automatic rejection of an unstable post-bifurcation branch. An illustrative example of plane strain tension is calculated by using the finite element method.

1. INTRODUCTION

In this paper, spatially discretized non-linear rate problems are discussed which accompany numerical step-by-step analysis of large quasi-static deformations of time-independent inelastic solids. In particular, attention is focused on the possibility that the continuation of the deformation is not unique, i.e. there is a bifurcation of a deformation path. A familiar method of numerical initiation of a secondary post-bifurcation path follows from Hill's bifurcation theory [cf. Hill (1959, 1961)]. The instant of primary bifurcation is to be found as a point on the fundamental deformation path at which the tangent stiffness matrix ceases to be positive definite and becomes singular. The respective eigenvector is computed and added to the fundamental solution in velocities with a multiplier such that the resulting strain rates do not fall outside the constitutive domain of applicability of the stiffness moduli corresponding to the fundamental solution. The actual value of the multiplier results from a higher-order condition of continuing equilibrium which usually reduces to the requirement that at one or more material elements the strain rate must lie *on* the boundary of the domain of fundamental moduli; for more details see e.g. Needleman (1972), Hutchinson (1973) and Needleman and Tvergaard (1982). However, that approach is not very convenient in practical computations since it requires implementation of numerical techniques other than those used along a regular path without bifurcations; there may also be difficulties raised by an ill-conditioned tangent stiffness matrix in a vicinity of the bifurcation point. A more fundamental difficulty is met if the secondary branch emanates at the primary bifurcation point "tangentially" to the fundamental path so that the above approach cannot be directly applied; this is a rule when the constitutive rate equations are thoroughly non-linear (Klushnikov, 1980; Needleman and Tvergaard, 1982; Triantafyllidis, 1983) but is also possible in classical elastic–plastic solids (Petryk and Thermann, 1985). Moreover, the above approach fails when the bifurcation is induced by a discontinuous drop of the incremental stiffness of the material so that the tangent stiffness matrix along the fundamental path becomes indefinite without being singular.

A common method used to pass over those difficulties is to analyze numerically a system with imperfections such that the unperturbed post-bifurcation path is approximated by a perturbed path which does not exhibit bifurcations. Results obtained for an imperfect system are often regarded as being closer to reality. Nevertheless, such an analysis is not always satisfactory since the results can strongly depend on the form and magnitude of the assumed initial imperfection.

In the present paper the bifurcation problem in a general setting [cf. Hill (1961)] is revisited under the additional assumption that an initial-boundary value problem posed originally for a plastically deformed continuum has been *spatially* discretized. The resulting *discretized non-linear rate problems*† are treated in their own merit: no attempt is made to study convergence of discretized solutions to the exact solution for the continuum. Incremental non-linearity of the material in a general form encompassing the yield-surface vertex effect is taken into account. Classical plasticity problems, such as column buckling, for instance, are also covered by the analysis and may serve as illustrations. The generality of considerations is motivated by the known inadequacy of classical elastoplastic models (as J_2-flow theory) in certain bifurcation calculations which are sensitive to details of the incremental constitutive law; for a review, see e.g. Christoffersen and Hutchinson (1979). The basic restriction here is that the global tangent stiffness matrix (which at a given deformation stage is non-linearly dependent on the current "direction" of further deformation) must be symmetric. In Section 3 the statements concerning existence, uniqueness and stability of discretized solutions are presented which are not contained in Hill's general theory for a continuum [cf. Hill (1978)] nor in an alternative theory developed by Nguyen (1990).

As an outcome of the theoretical analysis, a computational method is proposed which is applicable to large strain plasticity problems for non-linear constitutive rate equations. The method leads to a unified treatment of a class of problems where bifurcations are present and problems where the continuation of deformation is unique: there is no need to introduce any imperfections or perturbations to the analyzed system nor to apply another numerical technique when a bifurcation is met. The essence of the method lies in solving a non-linear first-order rate problem by minimizing the value of a velocity functional. This might be regarded as an extension to finite deformations of the known approach to a class of plasticity problems where geometric changes are disregarded which is based on the classical minimum principle for velocities [cf. Koiter (1960)]. However, there is a fundamental distinction, namely, the minimum principle is no longer unconditionally valid when geometric non-linearity is taken into account (Hill, 1959). Only the stationarity principle for velocities is guaranteed in the latter case (op. cit.) and therefore the minimization procedure which excludes certain solutions requires another theoretical justification. This is offered by the energy criterion of *instability* of a quasi-static deformation *process* [cf. Petryk (1982, 1985, 1991)]. In Section 3 it is shown that a deformation path along which the actual velocity field does not correspond to an absolute minimum of the functional should be regarded as unstable, although each of the equilibrium states separately may still be stable. As a rule, that instability concerns the fundamental post-bifurcation path. The minimization procedure enables calculation of another solution in velocities and automatic switching to a secondary branch emanating immediately beyond the primary bifurcation point. It is emphasized that a *non-linear* bifurcation problem is solved in this way rather than the usual linear eigenvalue problem. The procedure has the advantage that it is also applicable when the bifurcation is induced by a discontinuous change of material parameters since singularity of the tangent stiffness matrix at the critical point is not required. Moreover, it can be applied irrespectively whether the primary bifurcation takes place through non-uniqueness in velocities or in a higher-order rate of displacements. Certain limitations will be discussed later; for instance, the method is *not* suited for crossing bifurcation points in purely elastic solids.

There are well known numerical deficiencies of the explicit Euler time integration scheme, therefore the question arises how to implement in practice the above solution method which theoretically applies to rate problems. Our suggestion is to take advantage of the fact that in usual circumstances the regular second-order rate problem is linear

† We were unable to find in the literature any comprehensive study of bifurcations in a general problem of that type, especially for a non-singular tangent stiffness matrix. It will be shown in Section 3 that the assumption of a finite-dimensional system allows conclusions to be drawn that are unavailable at present for the continuum problem of similar generality.

[cf. Klushnikov (1980); Triantafyllidis (1983); Petryk and Thermann (1985)], with the respective matrix being exactly the tangent stiffness matrix associated with the first-order solution. In the second-order algorithm discussed in Section 4 the linear problem for quasi-static accelerations is solved at each time step, and the solution is used for updating purposes in order to improve the time integration accuracy and hence total effectiveness of the method.

A finite element program has been developed for numerical simulation of large plastic deformation processes by using the method proposed here. It is not our present aim to examine numerical features of the algorithm; the numerical results shown below are thought of merely as illustrations of potentialities of the method. As a testing example, the localization of deformation in a rectangular specimen subject to plane strain tension is analyzed for a solid obeying J_2-corner theory of plasticity (Christoffersen and Hutchinson, 1979). In comparison with the analysis by Tvergaard *et al.* (1981), no initial imperfection is assumed so that the necking starts at a bifurcation point. To illustrate the possibility of calculating bifurcations caused by a discontinuous change of the tangent modulus, a piecewise linear stress–strain curve is also used in addition to the usual power hardening law.

Notation

The standard symbolic notation is used throughout the paper. Spatial vectors or tensors are denoted by boldface letters, and their Cartesian components are denoted by lower case Latin subscripts for which the summation convention is adopted. A dot between two tensor symbols denotes contraction over two pairs of the subscripts in the sense that $a_{ij}b_{ij} = \mathbf{a} \cdot \mathbf{b}$, $A_{ijkl}b_{kl} = (\mathbf{A} \cdot \mathbf{b})_{ij}$, $a_{ij}A_{ijkl}b_{kl} = \mathbf{a} \cdot \mathbf{A} \cdot \mathbf{b}$, while the product $a_i b_j$ is denoted by $\mathbf{ab}$. Components of vectors or matrices obtained via a discretization procedure are denoted by Greek subscripts.

Since only time-independent materials and isothermal quasi-static deformations are considered, the role of a natural time is played by a time-like parameter t, called time for simplicity. A dot superimposed over a symbol denotes the material time derivative, understood in the *right-hand* sense. To simplify the notation, the same symbol is frequently used for a function and its value.

2. CONSTITUTIVE RATE EQUATIONS AND A DISCRETIZED RATE PROBLEM

Constitutive rate equations

Constitutive rate equations for a time-independent material, no matter what their original (objective) form, can generally be written as [cf. Hill (1959)]

$$\dot{\mathbf{S}} = \dot{\mathbf{S}}(\dot{\mathbf{F}}, \mathscr{H}), \tag{1}$$

where $\mathbf{S}$ is the first Piola-Kirchhoff stress tensor (the transpose of the nominal stress tensor), $\mathbf{F}$ is the deformation gradient, and $\mathscr{H}$ symbolizes the influence of the deformation history from a given initial state up to the considered instant, including the current stress and deformation; in the following the symbolic argument $\mathscr{H}$ will for simplicity be omitted. The function $\dot{\mathbf{S}}(\dot{\mathbf{F}})$ (at the actual state of the material element) is assumed to be continuous and piecewise smooth but need not be invertible, also when expressed in other variables, so that the analysis also applies to so-called softening materials. For the material to be time-independent $\dot{\mathbf{S}}(\dot{\mathbf{F}})$ must be positively homogeneous of degree one but otherwise it can be arbitrarily non-linear. By the Euler theorem, at a point of differentiability of $\dot{\mathbf{S}}(\dot{\mathbf{F}})$ the constitutive equation (1) can be written in the form

$$\dot{\mathbf{S}} = \mathbf{C}(\dot{\mathbf{F}}) \cdot \dot{\mathbf{F}}, \quad \mathbf{C}(\dot{\mathbf{F}}) = \frac{\partial \dot{\mathbf{S}}(\dot{\mathbf{F}})}{\partial \dot{\mathbf{F}}}. \tag{2}$$

The dependence of instantaneous "stiffness" moduli $\mathbf{C}$ on $\dot{\mathbf{F}}$ is homogeneous of degree zero and may be discontinuous and non-linear, not necessarily piecewise constant as in the classical elastoplastic models.

The equation $(2)_1$ can serve as a starting point to define the relationship (1), but then the continuity of $\dot{\mathbf{S}}(\dot{\mathbf{F}})$ requires appropriate restrictions to be imposed on possible discontinuities of $\mathbf{C}(\dot{\mathbf{F}})$. Moreover, if the equality $(2)_2$ (which will be needed later) is to be maintained then the condition

$$\partial C_{ijkl}/\partial \dot{F}_{mn} = \partial C_{ijmn}/\partial \dot{F}_{kl} \tag{3}$$

must be satisfied wherever $\mathbf{C}(\dot{\mathbf{F}})$ is differentiable. Conversely, $(2)_1$ with (3) imply $(2)_2$, by the required homogeneity of $\mathbf{C}(\dot{\mathbf{F}})$.

We shall assume, following Hill (1959), that the constitutive equation (1) admits a potential, viz.

$$\dot{\mathbf{S}} = \frac{\partial U}{\partial \dot{\mathbf{F}}}, \quad U(\dot{\mathbf{F}}) = \tfrac{1}{2}\dot{\mathbf{S}}(\dot{\mathbf{F}})\cdot\dot{\mathbf{F}}. \tag{4}$$

This is equivalent to imposing the symmetry restriction on the moduli $(2)_2$, viz.

$$C_{ijkl} = C_{klij}; \tag{5}$$

necessity for (4) is obvious since $\mathbf{C} = \partial^2 U/\partial\dot{\mathbf{F}}\,\partial\dot{\mathbf{F}}$, and sufficiency for (4) follows from (2).

For elastic materials, (5) is a consequence of existence of a strain energy potential. It is well known [cf. Hill (1958, 1978)] that the property (5) also holds for the classical elastoplastic model which obeys the normality flow rule relative to a smooth yield surface (for work-conjugate variables). If the phenomenological law (1) is intended to describe more accurately the *incremental* behaviour of metal polycrystals in the plastic range then the effect of the formation of a vertex on the yield surface at the current loading point should be taken into account [cf. Hill (1967); Hutchinson (1970)]. At a yield-surface vertex, (5) is no longer a consequence of the normality flow rule alone but represents an additional assumption.

Still another restriction on the constitutive model will be considered which is based on micromechanical considerations. Contrary to (5), it is not necessary for applicability of the proposed method but provides justification for assuming that there is no bifurcation along a smooth deformation path so long as the tangent stiffness matrix is positive definite. Suppose that the material at a micro-level is elastic-plastic and obeys the normality and piecewise-linearity postulates, which are commonly regarded as acceptable for time-independent models of metal single crystals [cf. Hill and Rice (1972)]. Suppose also that an analog of the symmetry condition (5) is valid at the micro-level. Then the normality flow rule and existence of a velocity-gradient potential (4) at the macro-level can be inferred (Hill, 1972; Petryk, 1989). Further, consider a smooth segment of a deformation path along which the rates of macroscopic stress and strain and the respective tangent moduli vary smoothly in time, and denote by superscript "0" the corresponding quantities. Then one can argue that the rates $\dot{\mathbf{S}}^0$ and $\dot{\mathbf{F}}^0$ at the macro-level do not correspond to abrupt unloading at the micro-level, with the following consequence for the macroscopic constitutive law (Petryk, 1989)

$$\dot{\mathbf{S}}^0\cdot\dot{\mathbf{F}} - \dot{\mathbf{S}}\cdot\dot{\mathbf{F}}^0 \geqslant 0 \quad \text{for every } \dot{\mathbf{F}}, \tag{6}$$

where $(\dot{\mathbf{S}}, \dot{\mathbf{F}})$ is an arbitrary pair of *virtual* stress and deformation rates, related by (4). The significance of (6) for a study of bifurcation problems stems from the fact that if (6) is satisfied then a sufficient condition for uniqueness of a solution in velocities to a class of boundary value problems can be formulated in terms of the tangent moduli $\mathbf{C}^0 = \mathbf{C}(\dot{\mathbf{F}}^0)$ alone, no matter what is the actual non-linear constitutive law (4) (op. cit.).

Relationships needed to express the above formulae in terms of other measures of stress and strain and their rates can be found in Hill (1978). For instance, let the corotational (Zaremba-Jaumann) flux of the Kirchhoff stress be denoted by $\overset{\nabla}{\tau}$, the Eulerian strain rate by **D**, and the respective moduli by $\partial\overset{\nabla}{\tau}(\mathbf{D})/\partial\mathbf{D} = \mathbf{L}(\mathbf{D})$, so that (2) is equivalent to $\overset{\nabla}{\tau} = \mathbf{L}(\mathbf{D})\cdot\mathbf{D}$. Denote by $\boldsymbol{\sigma}$ the current Cauchy stress and by δ_{ij} the Kronecker symbol. Then the relationship between **L** and **C** reads

$$\det(\mathbf{F}^{-1})F_{ip}F_{kq}C_{jplq} = L_{ijkl} - \tfrac{1}{2}(\sigma_{jk}\delta_{il} - \sigma_{ik}\delta_{jl} + \sigma_{il}\delta_{jk} + \sigma_{jl}\delta_{ik}). \tag{7}$$

(5) is equivalent to $L_{ijkl} = L_{klij}$, while (6) is equivalent to

$$\overset{\nabla}{\tau}{}^{0}\cdot\mathbf{D} - \overset{\nabla}{\tau}\cdot\mathbf{D}^{0} \geqslant 0 \quad \text{for every } \mathbf{D}, \tag{8}$$

with the same meaning of the superscript 0 as before.

Later we shall also need constitutive equations for the *second-order* rates of stress. Since the second-order problem plays only an auxiliary role here in the computational algorithm, we introduce certain simplifying assumptions. We shall assume that within a single time step the deformation history influence is represented by a *smooth* dependence of $\dot{\mathbf{S}}$ on a finite number of material parameters H^K varying in a prescribed way with the deformation (it is inessential here whether they are scalars, vectors or tensors) which are substituted in place of the symbolic argument $\mathscr{H}$ in (1). For simplicity of the notation, the current stress and deformation are also regarded as elements of the set $\{H^K\}$. Formal differentiation of (1) with respect to time then yields

$$\ddot{\mathbf{S}} = \mathbf{C}(\dot{\mathbf{F}})\cdot\ddot{\mathbf{F}} + \frac{\partial\dot{\mathbf{S}}}{\partial H^K}\dot{H}^K, \tag{9}$$

with the summation over all K. We can assume that $\dot{H}^K = \dot{H}^K(\dot{\mathbf{F}}, H^L)$ so that the last term in (9) can be found from a first-order solution. It follows that if the moduli $\mathbf{C}(\dot{\mathbf{F}})$ are defined for the actual $\dot{\mathbf{F}}$ then the relationship between $\ddot{\mathbf{S}}$ and $\ddot{\mathbf{F}}$ is *linear* (although inhomogeneous). This observation (Klushnikov, 1980) is essential for efficiency of the second-order algorithm described in Section 4; we note that the existence of a potential (4), and hence the symmetry property (5) are not needed for the validity of (9).

Formulation of discretized rate problem

A convenient starting point to formulate a discretized rate problem in Lagrangian description is the rate form of the virtual work principle†

$$\int_V \dot{\mathbf{S}}\cdot(\nabla\mathbf{w})\,\mathrm{d}V = \int_V \dot{\mathbf{b}}\mathbf{w}\,\mathrm{d}V + \int_S \dot{\mathbf{T}}\mathbf{w}\,\mathrm{d}S, \tag{10}$$

where V and S are respectively the body volume and surface in the reference configuration, **b** and **T** are nominal body forces and nominal surface tractions per unit reference volume and area, respectively, the symbol ∇ denotes a gradient evaluated in the reference configuration, and $\mathbf{w} = \delta\mathbf{v}$ is any kinematically admissible variation of velocities **v**. The reference configuration is assumed to be fixed; in the case of updated Lagrangian formulation all considerations remain valid within each separate time step. We shall consider a *discretized* rate problem in which velocity fields are restricted to having the form

$$\mathbf{v}(\boldsymbol{\xi}) = \boldsymbol{\varphi}_\alpha(\boldsymbol{\xi})v_\alpha \tag{11}$$

where $\boldsymbol{\xi}$ is a position vector of a material point in the reference configuration, $\boldsymbol{\varphi}_\alpha$,

† It is assumed that all strong discontinuities in **S**, **b** or **T** are *material* surfaces or lines, at least within some time interval starting from the considered instant.

$\alpha = 1, \ldots, N$, are linearly independent, continuous and piecewise sufficiently smooth "shape functions" given on $\bar{V}$ and v_α are numbers whose meaning depends on the adopted method of discretization. In a finite element formulation, v_α correspond to velocity components at nodal points but that restriction is not necessary here. The summation convention over the range from 1 to N is adopted for repeated Greek indices; a different range of summation shall be indicated explicitly. Since φ_α are fixed functions of material coordinates, the decomposition (11) is equally valid for displacements $\mathbf{u}(\xi) = \varphi_\alpha(\xi)u_\alpha$, velocity variations $\mathbf{w}(\xi) = \varphi_\alpha(\xi)w_\alpha$, etc. A column vector with components v_α, $\alpha = 1, \ldots, N$, will be denoted by $\tilde{\mathbf{v}}$ and identified with a velocity field, with analogous convention for $\tilde{\mathbf{u}}$, $\tilde{\mathbf{w}}$, etc.

Values of v_α can be constrained by boundary data for velocities; the attention is confined here to equality constraints such that rigid translations or rotations of the whole body are excluded. We assume that the form and numeration of the functions φ_α have been chosen such that in a kinematically admissible velocity field $\tilde{\mathbf{v}}$ the components v_α remain unconstrained for $\alpha \leqslant M$ and take prescribed values $\bar{v}_\alpha$ for $\alpha = M+1, \ldots, N$. Consequently, kinematically admissible velocity variations $\tilde{\mathbf{w}}$ are subject to the restriction $w_\alpha = 0$ for $\alpha > M$. It will be convenient to formally define the respective sets:

$$\begin{aligned} \mathscr{V} &= \{\tilde{\mathbf{v}} : v_\alpha = \bar{v}_\alpha \quad \text{for} \quad \alpha = M+1, \ldots, N\} \\ \mathscr{W} &= \{\tilde{\mathbf{w}} : w_\alpha = 0 \quad \text{for} \quad \alpha = M+1, \ldots, N\} \end{aligned} \tag{12}$$

and to reserve the symbol $\tilde{\mathbf{w}}$ for an element of $\mathscr{W}$ only. Note that any function on $\mathscr{V}$ can be equivalently regarded as a certain other function on the linear space $\mathscr{W}$.

For the sake of simplicity we shall assume that the external loading, in the form of *nominal* body forces and *nominal* surface tractions, is independent of the body configuration; a possible extension to a class of configuration-dependent *conservative* loading will be briefly discussed below. Hence, $\dot{\mathbf{b}}$ and $\dot{\mathbf{T}}$ in (10) are regarded as given, with the usual restriction that only those components of $\dot{\mathbf{T}}$ are prescribed which are complementary to prescribed velocity components. Components of a prescribed vector of discretized loading rate are obtained in the standard way as

$$\dot{P}_\alpha = \int_V \dot{\mathbf{b}}\varphi_\alpha \, \mathrm{d}V + \int_S \dot{\mathbf{T}}\varphi_\alpha \, \mathrm{d}S, \quad \alpha = 1, \ldots, M. \tag{13}$$

The first-order problem of continuing equilibrium, defined by (10), reduces after discretization to the system of non-linear algebraic equations

$$\dot{Q}_\alpha(\tilde{\mathbf{v}}) = \dot{P}_\alpha, \quad \alpha = 1, \ldots, M, \quad \tilde{\mathbf{v}} \in \mathscr{V}, \tag{14}$$

where

$$\dot{Q}_\alpha(\tilde{\mathbf{v}}) = \int_V \dot{\mathbf{S}}(\nabla\mathbf{v}) \cdot (\nabla\varphi_\alpha) \, \mathrm{d}V, \quad \alpha = 1, \ldots, N \tag{15}$$

are the rates of "internal forces". The rates are non-linearly dependent on $\tilde{\mathbf{v}}$; the dependence is homogeneous of degree one, on account of homogeneity of (1).

The system (14) can generally be rewritten in terms of a tangent stiffness matrix which is dependent on the velocity field due to the non-linearity of the constitutive rate equation (1). However, it should be mentioned that a tangent stiffness matrix is not defined for $\tilde{\mathbf{v}} = \tilde{\mathbf{0}}$, or more generally when $\nabla\mathbf{v}$ corresponds to a non-differentiability point of $\dot{\mathbf{S}}(\dot{\mathbf{F}})$ in a body domain of finite volume. To avoid repetitions, those particular circumstances will be tacitly excluded below from considerations in all cases when the notion of a tangent stiffness matrix is used. Under that reservation, the augmented $(N \times N)$ tangent stiffness matrix, on account of $(2)_2$, is given by

$$K_{\alpha\beta}(\tilde{\mathbf{v}}) \equiv \frac{\partial \dot{Q}_\alpha(\tilde{\mathbf{v}})}{\partial v_\beta} = \int_V (\nabla\varphi_\alpha)\cdot\mathbf{C}(\nabla\mathbf{v})\cdot(\nabla\varphi_\beta)\,\mathrm{d}V. \tag{16}$$

By $(2)_1$, the system of equations in (14) takes the form

$$K_{\alpha\beta}(\tilde{\mathbf{v}})v_\beta = \dot{P}_\alpha, \quad \alpha = 1,\dots,M. \tag{17}$$

In a more explicit but less concise form, (17) can be written as

$$\sum_{\beta=1}^{M} \hat{K}_{\alpha\beta}(\tilde{\mathbf{v}})v_\beta = \dot{P}_\alpha - \sum_{\beta=M+1}^{N} K_{\alpha\beta}(\tilde{\mathbf{v}})\bar{v}_\beta, \quad \alpha = 1,\dots,M, \tag{18}$$

where $[\hat{K}]$ is the tangent stiffness matrix, being the first $M\times M$ minor of $[K]$.

We have assumed that the constitutive rate equation (1) admits a potential, so that (14) or (17) can be given a variational formulation, viz.

$$\delta J(\tilde{\mathbf{v}};\tilde{\mathbf{w}}) \equiv \frac{\partial J(\tilde{\mathbf{v}})}{\partial v_\alpha}w_\alpha = 0 \quad \text{for every } \tilde{\mathbf{w}}\in\mathscr{W}, \tag{19}$$

where

$$J(\tilde{\mathbf{v}}) \equiv \tfrac{1}{2}\dot{Q}_\alpha(\tilde{\mathbf{v}})v_\alpha - \sum_{\alpha=1}^{M}\dot{P}_\alpha v_\alpha = \int_V U(\nabla\mathbf{v})\,\mathrm{d}V - \sum_{\alpha=1}^{M}\dot{P}_\alpha v_\alpha. \tag{20}$$

This is a discretized form of Hill's (1959) variational theorem for a continuum. J and its partial derivatives $\partial J/\partial v_\alpha$ are everywhere continuous functions of $\tilde{\mathbf{v}}$, by the assumed continuity of the constitutive relationship (1). The variational equality (19) is equivalent to vanishing of $\partial J/\partial v_\alpha$ for $\alpha = 1,\dots,M$, and hence to (14). The augmented tangent stiffness matrix can be determined from

$$K_{\alpha\beta}(\tilde{\mathbf{v}}) = \frac{\partial^2 J(\tilde{\mathbf{v}})}{\partial v_\alpha\,\partial v_\beta} \tag{21}$$

and is obviously symmetric.

It is possible to extend the considerations to cases where the incremental loading consists not only of the prescribed part but also of a deformation-sensitive *conservative* part,† viz.

$$\dot{P}_\alpha = \dot{\bar{P}}_\alpha - \sum_{\beta=1}^{M} k_{\alpha\beta}v_\beta, \quad k_{\alpha\beta} = k_{\beta\alpha}, \quad \alpha = 1,\dots,M, \tag{22}$$

where the quantities $k_{\alpha\beta}$ may depend on the deformation state but are independent of $\tilde{\mathbf{v}}$. For instance, elastic supports or the loading by prescribed fluid pressure can lead to expressions of type (22). In such cases the tangent stiffness matrix has to be modified by replacing $\hat{K}_{\alpha\beta}$ by the sum $\hat{K}_{\alpha\beta}+k_{\alpha\beta}$, with respective modification of the function (20). For simplicity, we take $P_\alpha = \bar{P}_\alpha(\lambda)$, $\alpha = 1,\dots,M$, as given functions of a scalar loading parameter λ which in turn varies in a prescribed way in time, $\lambda = \lambda(t)$.‡ Consistently, the geometric constraints are taken in the form $u_\alpha = \bar{u}_\alpha(\lambda)$, $\alpha = M+1,\dots,N$, where $\bar{u}_\alpha(\lambda)$ are given functions, with $\bar{v}_\alpha = (\mathrm{d}\bar{u}_\alpha/\mathrm{d}\lambda)\dot{\lambda}$.

† In the sense that the *total* work done by that part of loading is path-independent to second-order terms; cf. Hill (1962).

‡ Note that λ need not be a multiplier but is simply a time-like parameter; it will be convenient later to treat the loading parameter λ and the "time" t as being distinct.

Second-order rate problem

The second-order rate equations of continuing equilibrium are obtained by differentiating (14) with respect to time and can be written as

$$\ddot{Q}_\alpha(\tilde{\mathbf{v}}, \tilde{\dot{\mathbf{v}}}) = \ddot{P}_\alpha, \quad \alpha = 1, \ldots, M, \tag{23}$$

with the kinematic restriction $\dot{v}_\alpha = \dot{\bar{v}}_\alpha$ for $\alpha = M+1, \ldots, N$, imposed on admissible "acceleration" fields. We shall assume that spatial discontinuities in $\dot{\mathbf{S}}$ are not moving relative to the material.† Under this restriction, on taking the time derivative of (15) and substituting (9) and (16), we transform (23) to

$$K_{\alpha\beta}(\tilde{\mathbf{v}})\dot{v}_\beta = \ddot{P}_\alpha - R_\alpha(\tilde{\mathbf{v}}), \quad \alpha = 1, \ldots, M, \tag{24}$$

where the quantities

$$R_\alpha(\tilde{\mathbf{v}}) = \int_V (\nabla\varphi_\alpha) \cdot \frac{\partial \dot{\mathbf{S}}}{\partial H^K} \dot{H}^K \, \mathrm{d}V \tag{25}$$

are independent of accelerations $\tilde{\dot{\mathbf{v}}}$ and can be calculated once the first-order solution has been found; the arguments of the integrand functions in (25) have been omitted for simplicity. If the augmented tangent stiffness matrix $[K](\tilde{\mathbf{v}})$ is well defined then (24) constitutes a *linear* system of equations for the unknowns $\dot{v}_\alpha$.

3. BIFURCATION AND INSTABILITY

Energy interpretation of continuing equilibrium

The deformation work in the body during a process of deformation in a time interval $(0, t)$ is expressed as

$$W = \int_0^t Q_\alpha v_\alpha \, \mathrm{d}\tau, \quad Q_\alpha|_\tau = \bar{Q}_\alpha + \int_0^\tau \dot{Q}_\alpha(\tilde{\mathbf{v}}) \, \mathrm{d}t, \tag{26}$$

where $\bar{Q}_\alpha$ and Q_α are related to the stresses at an initial state at $t = 0$ and at the current state, respectively, by the formula analogous to (15) but with the rate symbol omitted. Along any kinematically admissible deformation path, the energy functional is defined as (Petryk, 1982, 1985)

$$E = W + \Omega, \tag{27}$$

where $\Omega = \Omega(\tilde{\mathbf{u}}, \lambda)$ is the potential energy of the loading device which in the considered case can be expressed as

$$\Omega = -\sum_{\alpha=1}^{M} P_\alpha u_\alpha, \quad P_\alpha = -\frac{\partial \Omega}{\partial u_\alpha}. \tag{28}$$

In general, E is a functional of the deformation history due to path-dependence of W. Let a deformation path be followed in a quasi-static manner, in general under the action of additional perturbing forces varying continuously in time. An increment of the value of E along such a path can be interpreted as the amount of energy which has to be supplied from external sources to the mechanical *system* consisting of the body and the loading device according to the energy balance. It is emphasized that an increment of the value of

† This is in accord with the simplifying assumptions concerning dependence of $\dot{\mathbf{S}}$ on H^K within a single time step. However, the possibility of step-wise propagation of a discontinuity of $\dot{\mathbf{S}}$ is not excluded.

$(-\Omega)$ is generally *not* equal to the work done by the loads P_α unless the loads are constant in time.

The first (right-hand) time derivative of E reads

$$\dot{E} = \dot{E}(\tilde{\mathbf{v}}) = Q_\alpha v_\alpha - \sum_{\alpha=1}^{M} (P_\alpha v_\alpha + \dot{P}_\alpha u_\alpha). \tag{29}$$

The values of $\dot{P}_\alpha$ for $\alpha \leqslant M$, and of v_α for $\alpha > M$, are prescribed. It follows that the internal forces are in equilibrium with the external forces, that is $Q_\alpha = P_\alpha$ for $\alpha = 1, \ldots, M$, if and only if $\dot{E}$ is independent of $\mathbf{v} \in \mathscr{V}$. Hence, the equilibrium condition can be written as

$$\dot{E}(\tilde{\mathbf{v}}) = \text{const.} \quad \text{in } \mathscr{V}. \tag{30}$$

The second time derivative of E, when calculated at an equilibrium state, reads

$$\ddot{E} = \ddot{E}(\tilde{\mathbf{v}}) = \dot{Q}_\alpha v_\alpha - 2\sum_{\alpha=1}^{M} \dot{P}_\alpha v_\alpha + \sum_{\alpha=M+1}^{N} Q_\alpha \dot{v}_\alpha - \sum_{\alpha=1}^{M} \ddot{P}_\alpha u_\alpha. \tag{31}$$

Let $\tilde{\mathbf{v}}^{(1)}$ and $\tilde{\mathbf{v}}^{(2)}$ be any pair of admissible velocity fields at the equilibrium state. Since the last two terms in (31) have prescribed values, by comparison with (20) we obtain the identity [cf. Petryk (1982, 1985)]

$$\tfrac{1}{2}\ddot{E}(\tilde{\mathbf{v}}^{(2)}) - \tfrac{1}{2}\ddot{E}(\tilde{\mathbf{v}}^{(1)}) = J(\tilde{\mathbf{v}}^{(2)}) - J(\tilde{\mathbf{v}}^{(1)}). \tag{32}$$

Hence, the first-order rate equations of continuing equilibrium (14) can be equivalently written down as

$$\delta\ddot{E}(\tilde{\mathbf{v}}; \tilde{\mathbf{w}}) = 0 \quad \text{for every } \tilde{\mathbf{w}} \in \mathscr{W}. \tag{33}$$

This means that any solution in velocities corresponds to a stationary value, with respect to variations in the set $\mathscr{V}$ of admissible velocity fields, of the increment of the energy functional E calculated with accuracy to second order terms.

Stability of equilibrium

Consider now an equilibrium state under constant loading, $\lambda(t) = \text{const.}$, so that $\dot{P}_\alpha = 0$ for $\alpha = 1, \ldots, M$, $\dot{v}_\alpha = 0$ for $\alpha = M+1, \ldots, N$, and $\mathscr{V} = \mathscr{W}$. The energy criterion of stability of equilibrium, formulated in the literature with various degrees of exactness, is obtained by comparison of the deformation work done along arbitrary (non-equilibrium) paths starting from the equilibrium state with the respective work done by external loads. Since the external loads are assumed constant, the work difference coincides now with the increment of the energy functional (27). The increment of E has to be calculated with accuracy at least to second-order terms since $\dot{E} \equiv 0$ at an equilibrium state. An equilibrium state is said to be directionally stable if

$$\ddot{E}(\tilde{\mathbf{w}}) > 0 \quad \text{at } \lambda = \text{const.} \quad \text{for every } \tilde{\mathbf{w}} \neq \tilde{\mathbf{0}}. \tag{34}$$

For the considered problem this is equivalent to

$$\dot{Q}_\alpha(\tilde{\mathbf{w}}) w_\alpha > 0 \quad \text{for every } \tilde{\mathbf{w}} \neq \tilde{\mathbf{0}}. \tag{35}$$

This inequality is a discretized version of Hill's (1958, 1959) condition of stability; cf. also Drucker (1964). By the physical interpretation of an increment of E, (34) excludes a spontaneous departure from equilibrium along a direct path by imposing an energy barrier in all directions (but does not guarantee stability in a rigorous sense for arbitrarily circuitous paths without additional assumptions). If

$$\dot{Q}_\alpha(\tilde{\mathbf{w}})w_\alpha < 0 \quad \text{for some } \tilde{\mathbf{w}} \tag{36}$$

then such a departure is energetically possible; moreover, with the help of (4) the equilibrium state can also be shown to be unstable in a dynamic sense (Petryk, 1991). Therefore, we may accept that (36) is excluded along any equilibrium path which has a physical meaning: other paths may be regarded as unobservable solutions under the assumed loading conditions.

Existence of first-order solution

Since the system of eqns (14) is non-linear, it is not evident under which circumstances it has a solution. However, the system admits the variational formulation (19) while the leading term in the potential function (20) is a homogeneous function of degree two of the unknowns v_α; this aids the proof of [cf. Petryk (1991)] the existence of a solution under an assumption which has a clear physical interpretation.

Theorem 1. *The system of eqns* (14) *at a directionally stable equilibrium state has a solution which assigns to J its absolute minimum value in* $\mathcal{V}^{+}$.

The proof of Theorem 1 is given in the Appendix.

As long as equilibrium is directionally stable, Theorem 1 provides a basis for the computational method in which the stationarity condition for J, equivalent to (14), is replaced by the stronger condition for a minimum of J in $\mathcal{V}^{+}$. In that range, both conditions are equivalent to each other if the solution to (14) is unique; the case of non-uniqueness is discussed below. On the other hand, if (36) is satisfied so that the equilibrium is unstable then one can easily show [cf. Petryk (1985)] that J is unbounded from below. The minimization procedure then fails, although a solution to (14) may exist and may even be unique. As indicated above, such solutions are not expected to have a physical meaning.

Bifurcation and uniqueness

If a solution $\tilde{\mathbf{v}}$ to (14) at a directionally stable equilibrium state does not correspond to an absolute minimum of J in $\mathcal{V}^{+}$ then $\tilde{\mathbf{v}}$ cannot coincide with the solution guaranteed by Theorem 1 and is thus not unique. Suppose that a solution $\tilde{\mathbf{v}}$ does correspond to the absolute minimum but the minimum is also reached for some other field $\tilde{\mathbf{v}}^*$ from $\mathcal{V}^{+}$. Since J is everywhere differentiable, each minimum point is also a stationary point, so that $\tilde{\mathbf{v}}^*$ is also a solution to (14) and $\tilde{\mathbf{v}}$ is again not unique. Hence, we have proved the following statement.†

Theorem 2. *For uniqueness of a solution* $\tilde{\mathbf{v}}$ *to* (14) *at a directionally stable equilibrium state it is necessary that* $\tilde{\mathbf{v}}$ *assigns to J a strict and absolute minimum value in* $\mathcal{V}^{+}$, *viz.*

$$J(\tilde{\mathbf{v}}) < J(\tilde{\mathbf{v}}^*) \quad \text{for every } \tilde{\mathbf{v}}^* \neq \tilde{\mathbf{v}}, \quad \tilde{\mathbf{v}}^* \in \mathcal{V}^{+}. \tag{37}$$

Since positive semi-definiteness of the second variation is necessary for a minimum, from (21) we obtain that for uniqueness of a solution $\tilde{\mathbf{v}}$ to (14) at a directionally stable equilibrium state it is necessary that the respective tangent stiffness matrix $[\hat{K}]$ is at least positive semi-definite,‡ that is

$$K_{\alpha\beta}(\tilde{\mathbf{v}})w_\alpha w_\beta \geqslant 0 \quad \text{for every } \tilde{\mathbf{w}}. \tag{38}$$

We thus arrive at the following conclusion [cf. Petryk (1991)].

† This is a stronger result than proving (37) from the strict convexity of J which is merely *sufficient* for uniqueness and for (34) [cf. Hill (1959, 1978)]. Although Theorem 2 is merely a corollary of Theorem 1, it is distinguished as a separate theorem since it provides a fairly general condition *necessary* for uniqueness, with far reaching implications.

‡ If the incremental constitutive law (2.1) is piecewise linear then equality in (38) for some non-zero $\tilde{\mathbf{w}}$ usually implies non-uniqueness of the solution $\tilde{\mathbf{v}}$; this is related to a typical primary bifurcation point. If the relationship is thoroughly non-linear then the implication is generally not true, however, it should be noted that if $[\hat{K}]$ is singular then the solution to the *second-order* problem (24) is non-unique.

Corollary 1. *The solution in velocities is non-unique at every point on a solution path along which* (35) *holds but* (38) *does not; this means that the bifurcation points are then not isolated but form a continuous non-uniqueness range.*

This may be regarded as a generalization of the known observation (Shanley, 1947) that the incremental response of a model of a straight plastic column under increasing compressive loading is non-unique for the load between the tangent modulus load and reduced modulus load; note that (38) holds up to the former load while (35) up to the latter. On the other hand, the column response at a buckled state along a secondary post-bifurcation path can still be unique.

It is well known that for uniqueness of a solution to (19), and thus also to (14), it is sufficient (but not necessary) that J is strictly convex. Hill (1959, 1978) has formulated a property of constitutive equations for the material, called the relative convexity property, which allows the establishment of the strict convexity of J, and hence uniqueness, from positive definiteness of the stiffness matrix for an incrementally linear comparison material. Recently, it has been shown (Petryk, 1989) that for a certain class of materials uniqueness can be inferred from positive definiteness of the tangent stiffness matrix without the need for convexity of J. In the present notation, the uniqueness criterion takes the following form.

Theorem 3. *If there exists a solution* $\mathbf{\tilde{v}}^0$ *to* (14) *such that*

(i) *the respective tangent stiffness matrix* $[\hat{K}^0]$ *is positive definite, and*

(ii) *the stress and deformation rates* $\dot{\mathbf{S}}^0$ *and* $\dot{\mathbf{F}}^0$ *corresponding to* $\mathbf{\tilde{v}}^0$ *satisfy the constitutive inequality* (6),

then the solution $\mathbf{\tilde{v}}^0$ *is unique.*

The proof runs on exactly the same lines as in the non-discretized case discussed by Petryk (1989) and therefore need not be repeated here.

The constitutive restriction (6) is generally weaker than the relative convexity property and, moreover, can be derived from micromechanical considerations. Under the restrictions imposed on the material behaviour at the micro-level as indicated in Section 2, the constitutive inequality (6) is appropriate for time-independent models of plastically deformed polycrystals, provided that $\mathbf{\tilde{v}}^0$ corresponds to a smooth continuation of the deformation path. Theorem 3 thus provides justification for the common assumption that positive definiteness of the tangent stiffness matrix excludes bifurcation; we note that the second-order problem (24) then also has a unique solution. The conditions (i) and (ii) of Theorem 3 can be satisfied not only before the first bifurcation point on the fundamental path but also along a secondary post-bifurcation path, of course, with the exception of the bifurcation point itself. From Theorems 2 and 3 we also obtain the following conclusion.

Corollary 2. *If* (35) *and* (6) *hold along a deformation path then positive definiteness of the tangent stiffness matrix* $[\hat{K}^0]$ *is necessary and sufficient for uniqueness of the first- and second-order solutions.*

Instability of a deformation path

Although a quasi-static deformation path is a one-parameter family of equilibrium states, path-sensitivity of plastic materials results in the necessity of treating a plastic deformation path as a unity rather than as a collection of independent points. Therefore, there is no reason to identify the notion of stability of a plastic deformation path with stability of equilibrium states reached along that path. Below we briefly recall the concept of instability of a quasi-static deformation process (or path, in the present terminology) in the energy sense, introduced by Petryk (1982, 1985) for the class of materials and loading conditions encompassing those considered here.

The following criterion of path instability is adopted: Along a stable deformation path the actual deformation increment must minimize the value of the increment of the energy functional E, calculated with accuracy to second-order terms, within the class of all kinematically admissible deformation increments. This may be regarded as a specification of the intuitive engineering hypothesis that a real deformation mode in metals exhibits a tendency to minimize the energy consumption; justification of the criterion is discussed below. Since, as shown above, the value of $\dot{E}$ at an equilibrium state is independent of the actual deformation mode, the instability criterion can be expressed in terms of $\ddot{E}$ only. If

$$\ddot{E}(\tilde{\mathbf{v}}^*) < \ddot{E}(\tilde{\mathbf{v}}) \quad \text{for some } \tilde{\mathbf{v}}^* \in \mathscr{V} \tag{39}$$

then a continuation of the deformation process with the velocity field $\tilde{\mathbf{v}}$ is unstable in the energy sense. For λ = const. and $\tilde{\mathbf{v}} = \tilde{\mathbf{0}}$, (39) reduces to (36). For $\lambda \neq$ const., (39) is implied by (36) [cf. Petryk (1985)], but the converse is false in general.

From the identity (32) by negation of (39) we find that for stability of a deformation path in the energy sense it is necessary that at each point on the path the respective velocity field $\tilde{\mathbf{v}}$ assigns to J an absolute minimum value in $\mathscr{V}$, viz.

$$J(\tilde{\mathbf{v}}^*) \geqslant J(\tilde{\mathbf{v}}) \quad \text{for every } \tilde{\mathbf{v}}^* \in \mathscr{V}. \tag{40}$$

It can be shown [cf. Petryk (1991)] that (40) is satisfied by the fundamental solution $\tilde{\mathbf{v}} = \tilde{\mathbf{v}}^0$ in the uniqueness range defined by the conditions (i) and (ii) of Theorem 3. In turn, (38) is necessary for (40) and is thus necessary for stability of the process. Hence, a continuation of deformation with velocities $\tilde{\mathbf{v}}$ is unstable in the energy sense when

$$K_{\alpha\beta}(\tilde{\mathbf{v}})w_\alpha w_\beta < 0 \quad \text{for some } \tilde{\mathbf{w}} \tag{41}$$

which usually takes place along the fundamental path immediately beyond the primary bifurcation point.

To determine the nature of the instability of a deformation path predicted by the energy criterion, two typical cases have to be distinguished. If (39) is satisfied along a segment of a quasi-static deformation path simultaneously with (36) then, as mentioned above, the equilibrium states are unstable and a spontaneous dynamic departure from any such state at constant loading should be expected. If (39) is satisfied along a segment of the path simultaneously with (35) then instability has a different character, namely, a quasi-static deviation from the path at varying loading should be expected at any instant. For, from Theorem 2 and (32) it follows that at *every* point along the segment there is a bifurcation in velocities such that the secondary continuation corresponds to a minimum of $\ddot{E}$ and is thus energetically preferable. It is also reasonable to conclude that such segments of theoretical deformation paths, and not only segments along which equilibrium is unstable, do not have a physical meaning.

Critical stage of deformation

Suppose that the tangent stiffness matrix $[\hat{K}]$ evaluated for the actual velocity field along a fundamental deformation path is positive definite up to a certain critical point and becomes indefinite beyond that point. We focus attention on the question, essential for the proposed computational method, under which circumstances the directional stability of equilibrium is preserved on the fundamental deformation path just beyond that point. Suppose that the fundamental solution $\tilde{\mathbf{v}}$ and the tangent moduli vary smoothly along the path so that $[\hat{K}](\tilde{\mathbf{v}})$ is just positive semi-definite at the critical point, with one or more eigenmodes, i.e. eigenvectors corresponding to the zero eigenvalue. The instability condition (36) can be written down in the form

$$K_{\alpha\beta}(\tilde{\mathbf{w}})w_\alpha w_\beta < 0 \quad \text{for some } \tilde{\mathbf{w}} \tag{42}$$

and compared with (41). If $\tilde{\mathbf{w}}^*$ is an eigenmode at the critical point then in general we have (41) for $\tilde{\mathbf{w}} = \tilde{\mathbf{w}}^*$ just beyond that point. This implies instability of equilibrium immediately beyond the critical point if $\tilde{\mathbf{w}}^*$ happens to correspond everywhere in the body to the constitutive regime of the fundamental moduli (i.e. $\mathbf{C}(\nabla\mathbf{w}^*) = \mathbf{C}(\nabla\mathbf{v})$ everywhere) so that the stiffness matrices in (41) and (42) coincide. (This is always so in incrementally linear materials, in particular in elastic solids.) As mentioned above when discussing the existence of the solution, J then becomes unbounded from below and the minimization procedure fails. However, available results suggest that this case is rather an exception in elastic–plastic solids so long as a limit point (at which $\tilde{\mathbf{v}}$ itself is an eigenmode) is not reached, especially when the presence of a yield-surface corner diminishes the constitutive domain of fundamental moduli.

Consider thus a typical critical point at which the gradient $\nabla\mathbf{w}^*$ of any eigenmode is in some spatial domain directed outside the constitutive regime of the fundamental moduli, that is, $\dot{\mathbf{S}}(\nabla\mathbf{w}^*) \neq \mathbf{C}(\dot{\mathbf{F}}^0)\cdot(\nabla\mathbf{w}^*)$ in some domain; from now on we identify $\tilde{\mathbf{v}}$ with $\tilde{\mathbf{v}}^0$ and assume that the condition (ii) of Theorem 3 is satisfied. From (6) it can be concluded (Petryk, 1989) that

$$\dot{\mathbf{S}}(\dot{\mathbf{F}})\cdot\dot{\mathbf{F}} \geqslant \dot{\mathbf{F}}\cdot\mathbf{C}(\dot{\mathbf{F}}^0)\cdot\dot{\mathbf{F}} \quad \text{for every } \dot{\mathbf{F}}, \tag{43}$$

with equality only if $\dot{\mathbf{S}}(\dot{\mathbf{F}}) = \mathbf{C}(\dot{\mathbf{F}}^0)\cdot\dot{\mathbf{F}}$. On integrating (43) over the body volume and substituting (15) and (16), we find that at the critical point

$$\dot{Q}_\alpha(\tilde{\mathbf{w}})w_\alpha \geqslant K_{\alpha\beta}(\tilde{\mathbf{v}}^0)w_\alpha w_\beta \geqslant 0 \quad \text{for every } \tilde{\mathbf{w}} \neq \tilde{\mathbf{0}}, \tag{44}$$

with the left-hand equality only if $\nabla\mathbf{w}$ corresponds everywhere to the fundamental constitutive regime, and with the right-hand equality only if $\tilde{\mathbf{w}} = \tilde{\mathbf{w}}^*$. Let $|\tilde{\mathbf{w}}|$ denote a norm in $\mathscr{W}$, and

$$\mu = \min_{|\tilde{\mathbf{w}}|=1} \dot{Q}_\alpha(\tilde{\mathbf{w}})w_\alpha. \tag{45}$$

Since one equality in (44) excludes the other by the assumption concerning $\nabla\tilde{\mathbf{w}}^*$, it follows that $\mu > 0$ at the critical point. If the constitutive relationship along the fundamental path, assumed smooth, does not change discontinuously then μ must remain positive along some subsequent segment of that path. By homogeneity of $\dot{Q}_\alpha(\tilde{\mathbf{w}})$, this implies directional stability of equilibrium along the fundamental path in some interval beyond the critical point. The conclusion remains valid for a secondary post-bifurcation path provided the material stiffness in any direction does not decrease discontinuously at the bifurcation point.

Conclusions

For incrementally non-linear time-independent materials, deformation paths can exist along which the actual tangent stiffness matrix is indefinite but each equilibrium state is still directionally stable. Nevertheless, such a path itself should be regarded as unstable since at each point the solution in velocities is not unique, so that infinitely many secondary paths can emanate from the path; moreover, the secondary continuations of deformation are energetically preferable. This kind of instability is avoided only when along the path, except possibly at isolated points, $J(\tilde{\mathbf{v}})$ attains its absolute minimum in $\mathscr{V}$ at the actual velocity solution. Existence of a solution to (14) which minimizes $J(\tilde{\mathbf{v}})$ is ensured as long as the equilibrium state is directionally stable. Such a solution has the energy interpretation as a minimizer of the second-order increment of the energy functional E.

On this theoretical basis we propose below a computational algorithm which selects a solution by minimizing the value of $J(\tilde{\mathbf{v}})$ in $\mathscr{V}$. Since (41) excludes $\tilde{\mathbf{v}}$ as a minimum point of J, in that algorithm the primary solution path is left automatically as soon as the tangent stiffness ceases to be positive definite and becomes indefinite. The secondary solution in velocities is also determined automatically† provided the directional stability of equilibrium is preserved. Other qualities of the proposed method have been listed in the Introduction and are illustrated below in a numerical example.

† We recall that the actual rate problem is *non-linear*, so that a minimum point of J defines both the direction and magnitude of the bifurcation mode.

4. COMPUTATIONAL ALGORITHM

The basic step in the proposed computational procedure is to find a solution to the rate problem (14) by minimizing in $\mathscr{V}$ the value of the velocity functional J defined by (20). This can be done by using one of the known methods for unconstrained optimization [see e.g. Fletcher (1980)]. As a natural starting point in a minimization procedure one can take the velocity field from the previous time step. In our finite element calculations we have used Newton's method combined with the negative curvature line search when the tangent stiffness matrix is not positive definite (cf. the discussion below). However, this choice should be regarded only as preliminary since other numerical techniques may prove more efficient for the type of non-linearity of J; this question requires further study. It should be pointed out that in the non-uniqueness range it may happen that a minimization routine terminates at the saddle point, corresponding to the fundamental deformation mode, rather than at a required minimum point corresponding to a secondary mode. It is therefore reasonable to compute and factorize the tangent stiffness matrix $[\hat{K}]$ corresponding to the final velocity vector obtained after minimization, even if this is not necessary for other purposes, in order to check whether the matrix is positive definite. If it is not then our suggestion is to perform a line search in a negative curvature direction which can easily be calculated (Fiacco and McCormick, 1968) and then to return to a general minimization routine. Unfortunately, it is difficult to ensure that the minimum found is a global one. If during minimization the value of J exhibits a tendency to decrease unboundedly then this means that the current (approximate) equilibrium is unstable. Further continuation of calculations without changing the algorithm is not possible. According to the theoretical analysis from the preceding section, this is generally *not* expected in the vicinity of a typical primary bifurcation point in an incrementally non-linear solid.

It is well known that the straightforward time integration of first-order rate solutions according to the explicit Euler scheme is generally unsatisfactory unless very small time steps are used. To improve accuracy of time integration, we propose to use the following second-order algorithm.† At each time step not only the first- but also the second-order rate problem is solved and then used in an updating procedure similar to a dynamic-response analysis. An advantage of doing this stems from the fact that once a first-order rate solution has been found, the linear second-order rate problem (24) with quasi-static accelerations as unknowns can be solved by using the actual (already factorized as suggested above) tangent stiffness matrix. There are different possibilities to compute the values of R_α needed for this purpose. It is essential that contributions to (25) from individual integration points can be computed separately. The values of integrand function in (25) at an integration point can be found analytically if the material model is not too complicated; a mixed technique can also be used in which the values of certain $\dot{H}^K$ defined implicitly in the model are determined numerically by a finite difference approximation. In principle, it is always possible to find the value of the needed product numerically, simply as a quotient.

$$\frac{\partial \dot{S}}{\partial H^K}\dot{H}^K \approx \frac{\dot{S}(\dot{F}, H^K+\Delta H^K)-\dot{S}(\dot{F}, H^K)}{\Delta t} \tag{46}$$

where ΔH^K are increments of H^K due to the deformation increment $\dot{F}\Delta t$, and Δt is a small time increment which can be chosen independently of the time step discussed below; such increments ΔH^K must in principle be determinable in any time integration algorithm. In practice, calculation of R_α may require lengthy although rather straightforward transformations to be carefully implemented since the primary variables in the constitutive rate equations are usually different from $\dot{S}$, $\dot{F}$.

It is emphasized that the first- and second-order problems can be solved *before* specifying the current time step used for updating. Advantage of this can be taken in establishing an adaptive step-size control based on an estimate of the error introduced by neglecting

† We note that the second-order algorithm does not require symmetry of the tangent stiffness matrix, and could be used independently of the method adopted for solving the first-order rate problem.

higher-order terms. Moreover, an extrapolated value of the determinant or lowest eigenvalue of $[\hat{K}]$ can be used to select the time step such that the calculated point of branch switching lies within required tolerance from (but always somewhat beyond) a primary bifurcation point.

Summary of the algorithm

Step 1. Initialize.

Step 2. Calculate $\dot{\tilde{\mathbf{v}}}$ by minimizing $J(\dot{\tilde{\mathbf{v}}})$ in $\mathcal{V}'$. If $J(\dot{\tilde{\mathbf{v}}})$ decreases unboundedly then stop. If $|\text{grad}\, J(\dot{\tilde{\mathbf{v}}})|$ is sufficiently small then compute $[\hat{K}]$ corresponding to $\dot{\tilde{\mathbf{v}}}$ and factorize.

Step 3. Check whether $[\hat{K}]$ is positive definite. If not then perform the negative curvature line search and go to Step 2.

Step 4. Compute R_α and find $\ddot{\tilde{\mathbf{v}}}$ from the linear system of eqn (24).

Step 5. Determine the time step and update using the first- and second-order solutions. Go to Step 2 if further computations are needed, otherwise stop.

5. NUMERICAL EXAMPLE

Constitutive equations

A finite strain version of the J_2 corner theory of plasticity proposed by Christoffersen and Hutchinson (1979) is employed. At a conical vertex which is thought to be formed on the yield surface at the current loading point, the constitutive rate equations are taken in the form

$$\mathbf{D} = \frac{\partial \bar{W}(\check{\boldsymbol{\tau}})}{\partial \check{\boldsymbol{\tau}}} = \mathbf{M}(\check{\boldsymbol{\tau}})\cdot\check{\boldsymbol{\tau}}, \quad \mathbf{M}(\check{\boldsymbol{\tau}}) = \frac{\partial^2 \bar{W}(\check{\boldsymbol{\tau}})}{\partial \check{\boldsymbol{\tau}}\,\partial \check{\boldsymbol{\tau}}},$$

$$\bar{W}(\check{\boldsymbol{\tau}}) = \tfrac{1}{2}\check{\boldsymbol{\tau}}\cdot\mathbf{M}^e\cdot\check{\boldsymbol{\tau}} + \tfrac{1}{2}f(\Theta)\check{\boldsymbol{\tau}}\cdot\mathbf{M}^p\cdot\check{\boldsymbol{\tau}}, \quad \cos\Theta = \frac{\mathbf{s}\cdot\mathbf{M}^p\cdot\check{\mathbf{s}}}{(\mathbf{s}\cdot\mathbf{M}^p\cdot\mathbf{s})^{1/2}(\check{\mathbf{s}}\cdot\mathbf{M}^p\cdot\check{\mathbf{s}})^{1/2}}, \tag{47}$$

where $\mathbf{M}^e$ and $\mathbf{M}^p$ are symmetric positive-definite tensors of the linear elastic compliances† and the plastic total loading compliances, respectively, such that $\mathbf{M}^e+\mathbf{M}^p$ is the tensor of compliances of the hyperelastic version of J_2 deformation theory, $\mathbf{s}$ is the Kirchhoff stress deviator, and $f(\Theta)$ is a smooth transition function equal to unity in the total loading range $0 \leqslant \Theta < \Theta_0$, equal to zero in the total unloading range $\Theta_c < \Theta \leqslant \pi$ and decreasing monotonically in the transition regime $\Theta_0 \leqslant \Theta \leqslant \Theta_c$ such that the potential $\bar{W}(\check{\boldsymbol{\tau}})$ is continuously differentiable and strictly convex. The reader is referred to the paper cited above for more details concerning the theory and to the paper by Tvergaard *et al.* (1981) for the specifications which have also been used in the present computations. By inverting the relationship $(47)_1$ the stiffnesss moduli $\mathbf{L}$ are obtained, and then the moduli $\mathbf{C}$ and the value of U can be found from (7).

Once the elastic constants, uniaxial Kirchhoff stress/logarithmic strain curve and the (stress-dependent) transition function have been specified, the potential $\bar{W}$ becomes a function of $\check{\boldsymbol{\tau}}$ and of the current Cauchy stress $\boldsymbol{\sigma}$ only. The compliances at finite strain can be conveniently determined by using the "principal axes technique" [cf. Hill (1970, 1978)]. Similarly, it is convenient to begin computations of the last term (equal to $\dot{\mathbf{C}}\cdot\dot{\mathbf{F}}$) in the second-order constitutive equation (9) by assuming first the rotating triad $\mathbf{a}_r$ of the principal directions of $\boldsymbol{\sigma}$ as a reference basis. For this purpose, once the first-order solution has been found and the principal Cauchy stress rates $\dot{\sigma}_r$ are known, the quantities

† In our calculations, a slightly different $\mathbf{M}^e$ was actually determined for a hyperelastic solid, but the difference can have no appreciable effect on the present results.

$$\dot{D}_{ij}|_{\overset{\nabla}{\tau}=\text{const.}} = \frac{\partial}{\partial\sigma_r}\left(\frac{\partial W}{\partial\overset{\nabla}{\tau}_{ij}}\right)\dot{\sigma}_r \approx \frac{D_{ij}(\overset{\nabla}{\tau},\sigma_r+\dot{\sigma}_r\delta t)-D_{ij}(\overset{\nabla}{\tau},\sigma_r)}{\delta t} \tag{48}$$

can be determined† and substituted into the equation

$$\dot{L}_{ijkl}D_{kl}+L_{ijkl}\dot{D}_{kl} \equiv (\overset{\nabla}{\tau})^{\cdot}_{ij} = 0, \tag{49}$$

in order to compute components of $\dot{\mathbf{L}}\cdot\mathbf{D}$ on the triad $\mathbf{a}_r$. It is emphasized that the product, contrary to $\dot{\mathbf{L}}$ itself, is independent of the second-order rates (cf. the comments on eqn (9)); in particular, $\dot{\mathbf{L}}\cdot\mathbf{D} = (\overset{\nabla}{\tau})^{\cdot}|_{\mathbf{D}=\text{const.}}$. The components of $\dot{\mathbf{L}}\cdot\mathbf{D}$ on a fixed reference basis can then be expressed in terms of the current spin ω of the triad $\mathbf{a}_r$ which can readily be found from the equation

$$\omega_{rs}-\bar{w}_{rs} = \overset{\nabla}{\sigma}_{rs}/(\sigma_s-\sigma_r) \quad \text{(no sum)}, \quad r\neq s, \quad \sigma_r\neq\sigma_s, \tag{50}$$

where $\bar{\mathbf{w}}$ is the material spin and the components refer to a fixed triad which coincides momentarily with $\mathbf{a}_r$. Transformation to variables $(\dot{\mathbf{S}}, \dot{\mathbf{F}})$ can be deduced from the bridging equation (7) and its time derivative. The resulting formulae are rather lengthy but are obtained in a straightforward manner and hence need not be given here in detail.

Finite element discretization

A homogeneous rectangular specimen subjected to plane strain tension is considered. Standard boundary conditions (given normal velocities and zero shear tractions at the ends and zero tractions on lateral boundaries) are adopted; the additional restriction to deformations symmetric about the mid-planes allows numerical analysis of only one quadrant of the specimen. The quadrant is assumed to consist of 48 × 16 quadrilaterals, each made up of four constant-strain triangular elements. The updated Lagrangian description is used, and at each time step the triangles are formed by the two diagonals of the deformed quadrilateral so that the elements are well suited to accommodate nearly isochoric deformations (Nagtegaal *et al.*, 1974). The diagonals have been appropriately oriented to accommodate expected shear band formation (Tvergaard *et al.*, 1981). Calculations have been performed by using the algorithm described in Section 4 which has been implemented into the finite element code developed by K. Thermann.

Results

(i) *Smooth hardening law*. The calculations are intended to complement the numerical study of flow localization under plane strain tension by Tvergaard *et al.* (1981), where initial geometric inhomogeneities have been assumed, with an analysis of deformation of the initially perfect specimen. Material parameters are taken to be the same, e.g. the power hardening law with an exponent 0.1 is assumed, the initial aspect ratio l_0/h_0 (length/thickness) is also taken as 3, and a similar non-uniform grid is employed with the initial angle between the diagonals and the tensile axis in the necking region equal to 54.4°.

Contrary to the case with imperfections, the deformation is here initially uniform and necking starts at a bifurcation point. This takes place at a relative end-displacement $u/l_0 = 0.1405$ when the tangent stiffness matrix corresponding to uniform straining, $[\hat{K}^0]$, ceases to be positive definite. The respective theoretical value for a continuum is 0.1402.‡ It can be shown [cf. Petryk (1989), Section 8] that the inequality (6) is satisfied for the assumed material model up to this critical point so that Theorem 3 applies. As soon as $[\hat{K}^0]$ has become indefinite, the computer program has automatically found another velocity solution corresponding to necking initiation and left the (unstable) fundamental path, in full agreement with the theory. Further deformations take place at a positive definite tangent stiffness

† In our computations we have used an analytic expression in which the only time derivatives approximated by a differential quotient are those of $f(\Theta)$ and of $f'(\Theta)$ at fixed Θ.

‡ With the slight degree of compressibility of the material neglected, the bifurcation point is found at 0.1407 from Hill and Hutchinson's (1975) analysis for an incompressible solid.

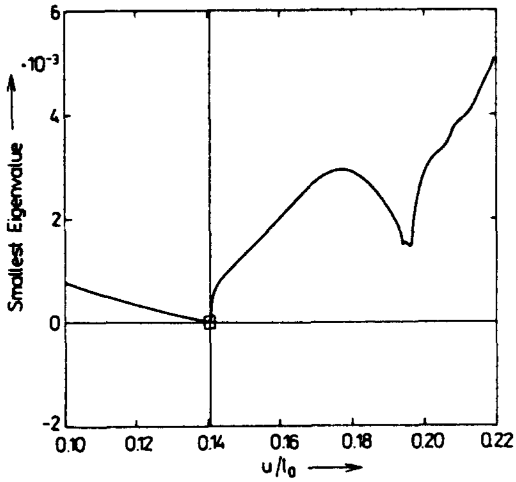

Fig. 1. The smallest eigenvalue of the tangent stiffness matrix versus relative end-displacement in the calculation of plane strain tension of an initially perfect specimen for the power hardening law.

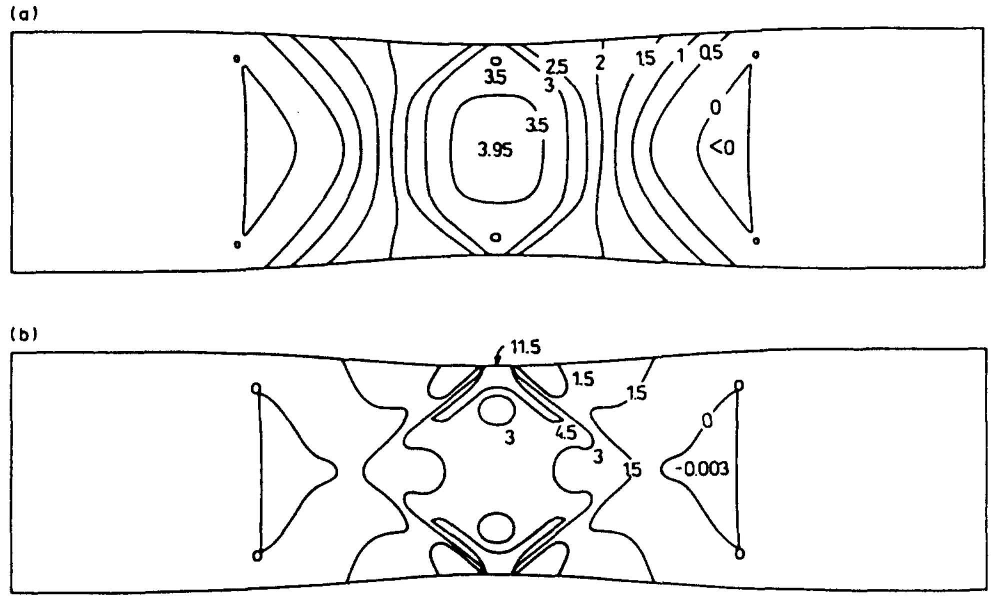

Fig. 2. Current distribution of maximum principal strain-rate (normalized by end-velocity/initial length) for the power hardening law. (a) at $u/l_0 = 0.192$, (b) at $u/l_0 = 0.196$.

matrix $[\hat{K}]$,† as illustrated in Fig. 1, although definite decrease of the smallest eigenvalue of $[\hat{K}]$ can be observed in correlation with concentration of the deformation rate in the central elements at lateral surfaces and in shear bands propagating from these elements (Fig. 2). In passing, it may be remarked that shear bands can develop at positive definite $[\hat{K}]$ so long as stability of *equilibrium* is maintained. In Fig. 3 the deformed mesh (obtained by symmetric reflections of that actually computed for one quadrant) is shown at $u/l_0 = 0.192$ and $u/l_0 = 0.220$, while the respective distributions of the maximum principal logarithmic strain are given in Fig. 4. In comparison with the results for imperfect specimens (Tvergaard *et al.*, 1981), the shear band pattern becomes visible at clearly larger elongations.

† Since the effect of partial unloading on the constitutive potential is neglected in the material model, the inequality (6) is not satisfied along the secondary path and spurious bifurcations at positive definite $[\hat{K}]$ are not excluded. It should also be mentioned that a kind of hourglass instability has been detected between the partially unloaded and fully loaded zones but this appears to have no visible influence on the mesh deformation.

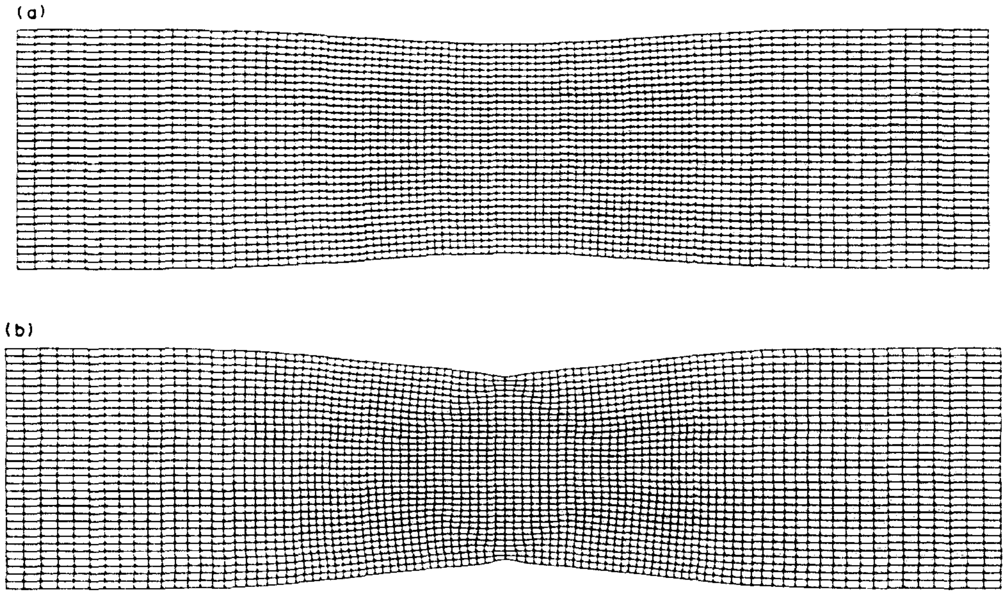

Fig. 3. Deformed finite element mesh at two stages of the deformation for the power hardening law. (a) $u/l_0 = 0.192$, (b) $u/l_0 = 0.220$.

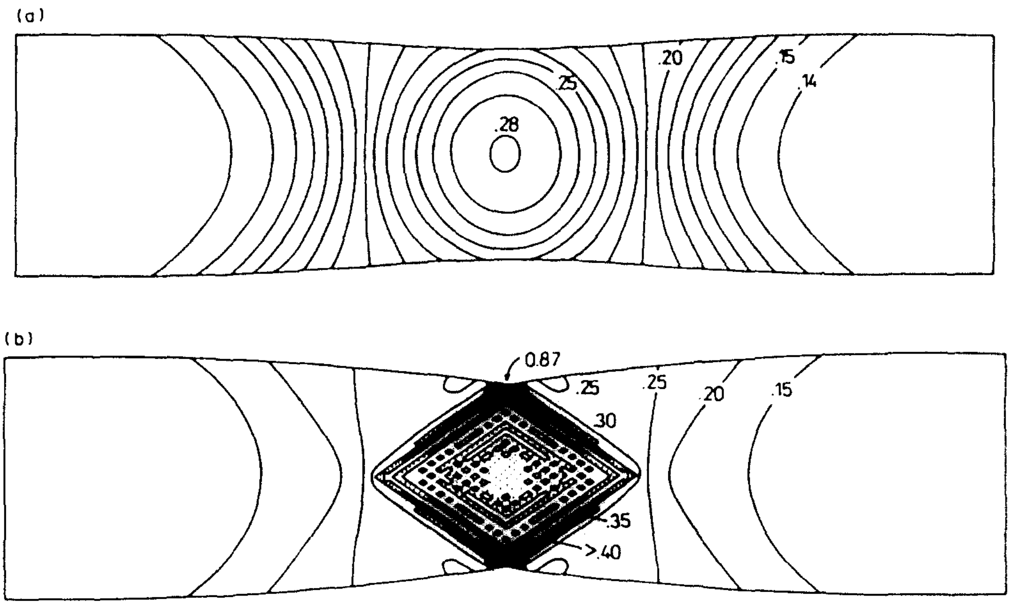

Fig. 4. Distribution of maximum principal logarithmic strain for the power hardening law. (a) at $u/l_0 = 0.192$, (b) at $u/l_0 = 0.220$.

This may be attributed to imperfection sensitivity (the onset of unloading in an imperfect specimen has been reported at $u/l_0 = 0.123$ in contrast to 0.140 in the present case), although the use of a different computational algorithm might also have an influence in the numerical results. An interesting deformation pattern in the central part of the specimen in Fig. 4b appears to be related to instability of uniform deformation at the level of a material element.

(ii) *Piecewise-linear hardening law*. To illustrate the possibility of calculating bifurcations induced by a discontinuous change of the tangent modulus (which relates the right-hand rates of the equivalent stress and strain), a relationship between Kirchhoff stress τ and logarithmic strain e at uniaxial monotonic tension is taken in the form

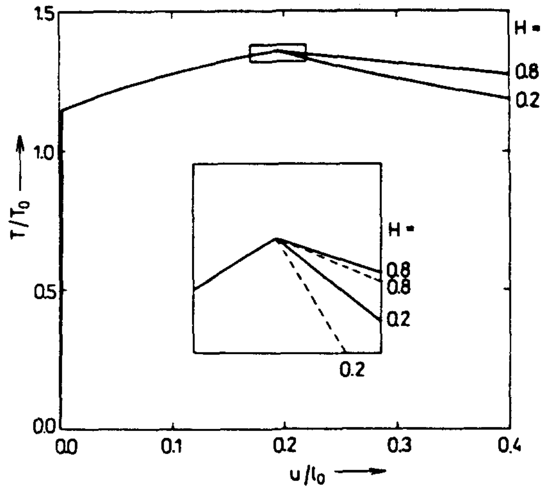

Fig. 5. Normalized load ($T_0 = \tau_y h_0$) versus end-displacement at uniform plane strain tension for two versions of the piecewise-linear hardening law. The broken lines indicate the initial slopes for secondary post-bifurcation paths for $H = 0.8$ and $H = 0.2$.

$$e = \begin{cases} \tau_y/E + (\tau - \tau_y)/(2\tau_y) & \text{for } \tau_y \leqslant \tau \leqslant 1.4\tau_y \\ \tau_y/E + 0.2 + (\tau - 1.4\tau_y)/(H\tau_y) & \text{for } 1.4\tau_y \leqslant \tau \end{cases} \tag{51}$$

where τ_y denotes the initial yield stress, $E = 500\tau_y$ is the Young modulus, and $H\tau_y$ is the constant hardening modulus at strain $e > 0.202$. Two values of H have been examined: $H = 0.8$ and 0.2. The respective variations of normalized load versus relative end-displacement at uniform plane strain tension are shown in Fig. 5. All other parameters characterizing the material response at a yield-surface vertex are taken to be the same as in the previous example (op. cit.). The uniform (48 × 16) mesh is employed throughout a quadrant of the specimen whose initial aspect ratio l_0/h_0 is taken again as 3.

No bifurcation takes place up to the load peak at $u/l_0 = 0.192$ beyond which the tangent stiffness matrix corresponding to uniform straining becomes abruptly indefinite for the values of H examined. Accordingly, the fundamental path has not been followed further

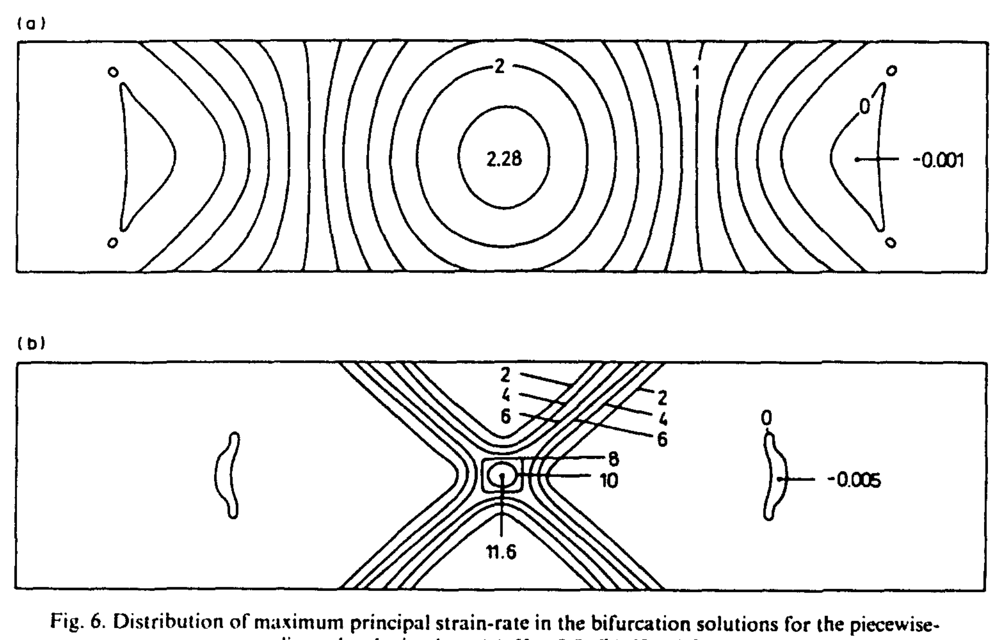

Fig. 6. Distribution of maximum principal strain-rate in the bifurcation solutions for the piecewise-linear hardening law. (a) $H = 0.8$, (b) $H = 0.2$.

by the computer program. Immediately beyond the load peak secondary paths are initiated with velocity fields which have been selected automatically by the minimization procedure. This has created no numerical difficulty (except that more iterations were needed to approach the minimum point), also for $H = 0.2$ when at the starting point of minimization (i.e. for the fundamental velocity field) 21 diagonal elements of the factorized tangent stiffness matrix were negative from a total number of 3119 degrees of freedom in the examined quadrant. The respective initial slopes of secondary load/end-displacements curves are indicated in Fig. 5 by broken lines. The strain rate distribution at the instant of bifurcation for $H = 0.8$ (cf. Fig. 6a) resembles closely the incipient necking mode for the smooth hardening law. At the bifurcation point for $H = 0.2$ (Fig. 6b) a shear band mode is clearly activated.

Acknowledgement—This paper was written when H.P. stayed at the Department of Mechanical Engineering, Dortmund University, as a Fellow of the Alexander von Humboldt Foundation. The support of the AvH Foundation is gratefully acknowledged.

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APPENDIX

Proof of Theorem 1. Consider the quantity

$$I(\bar{v}) \equiv \int_V U(\nabla v)\,dV = \tfrac{1}{2}\dot{Q}_\alpha(\bar{v})v_\alpha \tag{A1}$$

defined for all $\bar{v} \in R^N$. By (4) and the assumed continuity and homogeneity of the constitutive relationship, the function $I(\cdot)$ is continuous, continuously differentiable and positively homogeneous of degree two.

Let $|\cdot|$ denote a norm in R^N, for instance, let $|\bar{v}| = (v_\alpha v_\alpha)^{1/2}$. Let $\bar{v}^0 \in \mathscr{V}$ be a non-zero fixed vector. Every $\bar{v} \in \mathscr{V}$ can be expressed as

$$\bar{v} = \bar{v}^0 + \gamma\bar{w}^*, \quad \text{where} \quad \bar{w}^* \in \mathscr{W}, \quad |\bar{w}^*| = 1, \quad \gamma = |\bar{v} - \bar{v}^0|. \tag{A2}$$

On substituting (A1) and (A2) into (20) and rearranging with the help of the homogeneity of I, we obtain

$$\begin{aligned} J(\bar{v}) &= I(\bar{v}^0 + \gamma\bar{w}^*) - \sum_{\alpha=1}^{M} \dot{P}_\alpha v_\alpha \\ &= \gamma^2(I(\bar{v}^0/\gamma + \bar{w}^*) - I(\bar{w}^*)) + \gamma^2 I(\bar{w}^*) - \sum_{\alpha=1}^{M} \dot{P}_\alpha(v_\alpha^0 + \gamma w_\alpha^*). \end{aligned} \tag{A3}$$

As a continuously differentiable function, I is Lipschitz continuous in any ball, so that there is a constant C such that

$$|I(\bar{w} + \bar{v}) - I(\bar{w})| \leqslant C|\bar{v}| \quad \text{if} \quad |\bar{v}| \leqslant 1, \quad |\bar{w}| \leqslant 1.$$

Consequently,

$$I(\bar{w} + \bar{v}) - I(\bar{w}) \geqslant -C|\bar{v}| \quad \text{if} \quad |\bar{v}| \leqslant 1, \quad |\bar{w}| \leqslant 1. \tag{A4}$$

From (A3), (A4) and homogeneity of a norm it follows that for $\gamma > |\bar{v}^0|$ we have

$$\begin{aligned} J(\bar{v}) &\geqslant \gamma^2 I(\bar{w}^*) - \left(C|\bar{v}^0| + \sum_{\alpha=1}^{M} \dot{P}_\alpha w_\alpha^*\right)\gamma - \sum_{\alpha=1}^{M} \dot{P}_\alpha v_\alpha^0 \\ &\geqslant \gamma^2 I(\bar{w}^*) - \gamma A - B, \quad A, B = \text{const.}; \end{aligned} \tag{A5}$$

the last estimation is obvious since w_α^* are uniformly bounded.

An infimum of $I(\bar{w}^*)$ on the sphere $|\bar{w}^*| = 1$ must be reached at some minimum point since the space $\mathscr{W}$ is finite-dimensional and I is continuous. The minimum value must be positive, by the assumed directional stability of equilibrium, so that $I(\bar{w}^*) \geqslant \frac{1}{2}\mu > 0$, where μ is defined by (45). On substituting this into (A5) we arrive finally at the result that $J(\bar{v}) \to +\infty$ when the distance $\gamma = |\bar{v} - \bar{v}^0|$ increases to infinity while $\bar{v} \in \mathscr{V}$.

It remains to apply the known argument to complete the proof. From the final property of $J(\bar{v})$ we obtain that $J(\bar{v}) > J(\bar{v}^0)$ if $\bar{v} \in \mathscr{V}$ and $|\bar{v} - \bar{v}^0| \geqslant c$, where c is a sufficiently large number. Since J is continuous, it follows that the absolute minimum of $J(\bar{v})$ in $\mathscr{V}$ is attained at some $\bar{v}$ such that $|\bar{v} - \bar{v}^0| < c$. Since J is continuously differentiable, the stationarity condition (19) must be satisfied at a minimum point, so that the minimizer represents a solution to (14). The theorem has been proven.