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Adiabatic shear band localization in single crystals under dynamic loading processes

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THE MAIN OBJECTIVE of the paper is the investigation of adiabatic shear band localization phenomena in inelastic single crystals under dynamic loading processes. In the first part, a rate-dependent plastic model of single crystals is developed within the thermodynamic framework of the rate-type covariance constitutive structure. This model takes account of the effects as follows: (i) influence of covariance terms, lattice rotations and plastic spin; (ii) thermomechanical coupling; (iii) evolution of the dislocation substructure. An adiabatic process is formulated and examined. The relaxation time is used as a regularization parameter. The viscoplastic regularization assures the stable integration algorithm by using the finite element method. It has been shown that the evolution problem (the initial-boundary value problem) for rate-dependent plastic model of single crystals is well posed. The second part is devoted to the investigation of criteria of localization of plastic deformation in both single slip and symmetric double slip processes. The adiabatic shear band formation in elastic-plastic rate-independent single crystals during dynamic loading processes is investigated. The critical value of the strain hardening rate and the misalignment of the shear band from the active slip systems in the crystal's matrix have been determined. Particular attention is focused on the investigation of synergetic effects. Calculations have been obtained for aluminum single crystals. The results obtained are compared with available experimental observations.

1. Introduction

RECENT EXPERIMENTAL observations and theoretical investigations have shown that the synergetic effects have great influence on the behaviour of inelastic single crystals. Particularly the adiabatic shear band localization in single crystals is affected very much by cooperative phenomena.

Experimental observations of the macroscopic adiabatic shear band localization in single crystals performed by CHANG and ASARO [6, 7], SPITZIG [35] and LISIECKI *et al.* [18] showed that the strain-hardening rate h_{crit} at the inception of shear band localization is positive and the direction of the localized shear band is misaligned by some small angle δ from the active slip system.

On the other hand, the investigations presented by MECKING and KOCKS [21], FOLLANSBEE [12] and FOLLANSBEE and KOCKS [13] showed the great influence of the strain rate sensitivity on the behaviour of inelastic metallic single crystals in dynamic loading processes. To describe the strain rate sensitivity effects, FOLLANSBEE [12] suggested to take into consideration the evolution of the

dislocation substructure.

Experimental study of highly heterogeneous deformations in copper single crystals performed by RASHID *et al.* [33] showed that the strain rate history dependence of the substructure evolution plays an important role, particularly in adiabatic shear band formation phenomena.

ASARO and RICE [3] have clearly shown that the classical theory of crystals based on the Schmid constitutive law does not seem to be appropriate to explain the shear band localization phenomenon in ductile metallic single crystals.

ASARO and RICE [3] have focused attention on the localization criteria for "an assumed class of materials that essentially obey Schmid's rule but display modest departure from it". They proved that the plastic hardening rate h_{crit} at the inception of localization may be positive when there are deviations from the Schmid law, cf. also PEIRCE, ASARO and NEEDLEMAN [21, 22], QIN and BASSANI [32, 33] and BASSANI [5].

To describe the main experimentally observed facts connected with the macroscopic shear band formation, DUSZEK–PERZYNA and PERZYNA [9] have considered the synergetic effects resulting from taking into account spatial covariance effects and thermomechanical couplings. PERZYNA and KORBEL [29] have investigated the influence of the evolution of substructure on the shear band localization phenomena in single crystals for single slip process. DUSZEK–PERZYNA and PERZYNA [10] have examined the influence of thermal expansion, thermal plastic softening and spatial covariance effects on shear band localization criteria for a planar model of an f.c.c. crystal undergoing symmetric primary-conjugate double slip process, cf. also PERZYNA and DUSZEK–PERZYNA [27]. In the paper by PERZYNA and KORBEL [30] the attention is focused on the discussion of the cooperative influence of various effects on criteria for shear band localization in both the symmetric double slip and single slip processes.

It has been proved by previously mentioned theoretical investigations that the main cooperative phenomena which affect the behaviour of metallic single crystals are generated by thermomechanical couplings and the evolution of the dislocation substructure.

To describe the influence of main cooperative phenomena on the behaviour of metallic single crystals, we intend to start from the development of the thermodynamic theory of single crystals with special emphasis on the investigations of thermomechanical couplings and internal dissipative effects. Then this theory is used for the investigations of the adiabatic shear band formation in single crystals under dynamic loading processes.

In Sec. 2 the constitutive rate-dependent model and the formulation of the initial-boundary value problem (evolution problem) are presented. Section 3 is devoted to the rate-independent model of inelastic single crystals. In Secs. 4 and 5 the investigation of the adiabatic shear band localization is given. Single slip and symmetric double slip processes are considered. The identification procedure for the material functions and constants is presented in Sec. 6.

In Sec. 7 the numerical investigation for the localization criteria is given. Discussion of the results and final comments are presented in Sec. 8.

2. Formulation of the initial-boundary value problem

2.1. General postulates

To formulate the initial-boundary value problem which describes an adiabatic plastic deformation process for an elastic-viscoplastic model of single crystals, we take advantage of the results obtained previously in the following papers: DUSZEK–PERZYNA and PERZYNA [9, 10], PERZYNA [25, 28].

Let us assume that the regular motion of a body $\mathcal{B}$ is described by the mapping

$$\mathbf{x} = \phi(\mathbf{X}, t), \tag{2.1}$$

where points in $\mathcal{B}$ are denoted by $\mathbf{X}$ and those in the actual configuration $\mathcal{S}$ of a body $\mathcal{B}$ at time t by $\mathbf{x}$. Then *the kinematic equation* has the form

$$\boldsymbol{\upsilon} = \dot{\phi}(\mathbf{X}, t) \mid_{\mathbf{X}=\phi^{-1}(\mathbf{x},t)}, \tag{2.2}$$

where $\boldsymbol{\upsilon}$ denotes the spatial velocity and the dot – the material differentiation with respect to time t.

Let $\varrho(\mathbf{x}, t)$ be the mass density of the deformed body $\mathcal{B}$ at time t. Then *the conservation of mass* states that the equation of continuity

$$\dot{\varrho} = -\varrho \operatorname{div} \boldsymbol{\upsilon} \tag{2.3}$$

is satisfied.

Assume that conservation of mass (2.3) holds, then *the balance of momentum* is equivalent to (provided there is no body force field)

$$\dot{\boldsymbol{\upsilon}} = \frac{1}{\varrho} \operatorname{div} \left(\frac{1}{J} \boldsymbol{\tau} \right), \tag{2.4}$$

where J is the Jacobian of a mapping ϕ and $\boldsymbol{\tau}$ is the Kirchhoff stress tensor.

It is postulated that the free energy function is given by

$$\psi = \widehat{\psi}(\mathbf{e}, \mathbf{F}, \vartheta; \boldsymbol{\mu}), \tag{2.5}$$

where $\mathbf{e}$ denotes the Eulerian strain tensor, $\mathbf{F}$ is the deformation gradient, ϑ temperature and $\boldsymbol{\mu}$ is the matrix of the internal state variables.

The form of the free energy function $\psi = \widehat{\psi}(\mathbf{e}, \mathbf{F}, \vartheta)$ is suggested for spatial description in thermoelasticity. To extend the domain of description of the material properties of a single crystal and particularly, to take into consideration the plastic flow effects and the dislocation substructure, we have to introduce a

set of the internal state variables. In our case the matrix $\boldsymbol{\mu}$ is postulated in the form

$$\boldsymbol{\mu} = (\boldsymbol{\gamma}, \boldsymbol{\alpha}_M, \boldsymbol{\alpha}_D), \tag{2.6}$$

where

$$\boldsymbol{\gamma} = \begin{bmatrix} \gamma^{(1)} \\ \vdots \\ \gamma^{(n)} \end{bmatrix}, \qquad \boldsymbol{\alpha}_M = \begin{bmatrix} \alpha_M^{(1)} \\ \vdots \\ \alpha_M^{(n)} \end{bmatrix}, \qquad \boldsymbol{\alpha}_D = \begin{bmatrix} \alpha_D^{(1)} \\ \vdots \\ \alpha_D^{(n)} \end{bmatrix}, \tag{2.7}$$

$\boldsymbol{\gamma}$ defines the shearing, $\boldsymbol{\alpha}_M$ the density of mobile dislocations and $\boldsymbol{\alpha}_D$ the density of obstacle dislocations in the slip system of a crystal.

Let us postulate evolution equations for the internal state variables $\boldsymbol{\gamma}$, $\boldsymbol{\alpha}_M$ and $\boldsymbol{\alpha}_D$ as follows

$$\dot{\boldsymbol{\gamma}} = \begin{bmatrix} \dot{\gamma}^{(1)} \\ \vdots \\ \dot{\gamma}^{(n)} \end{bmatrix} \equiv \mathbf{G}, \tag{2.8}$$

where $$\dot{\gamma}^{(\beta)} = \frac{1}{T^{(\beta)}} \left\langle \Phi \left[\frac{\tau^{(\beta)}}{\tau_c^{(\beta)}(\boldsymbol{\gamma}, \boldsymbol{\alpha}_D, \vartheta) + \boldsymbol{\kappa}^{(\beta)} : \boldsymbol{\tau}} - 1 \right] \right\rangle \operatorname{sgn} \tau^{(\beta)},$$

$$\begin{aligned} \dot{\boldsymbol{\alpha}}_M &= \mathbf{a}_1 \cdot \dot{\boldsymbol{\gamma}} + \mathbf{a}_2 \cdot \dot{\vartheta} + \mathbf{a}_3 \cdot \dot{\boldsymbol{\alpha}}_D, \\ \dot{\boldsymbol{\alpha}}_D &= \mathbf{b}_1 \cdot \dot{\boldsymbol{\gamma}} + \mathbf{b}_2 \cdot \dot{\vartheta} + \mathbf{b}_3 \cdot \dot{\boldsymbol{\alpha}}_M, \end{aligned} \tag{2.9}$$

where $T^{(\beta)}$ denotes the relaxation time, Φ is the overstress empirical viscoplastic function, $\tau^{(\beta)}$ defines the Schmid resolved stress on the slip system β ($\beta = 1, 2, \ldots, n$), $\tau_c^{(\beta)}$ is the critical Schmid resolved stress on the slip system β, $\boldsymbol{\kappa}^{(\beta)}$ denotes the symmetric tensor of the non-Schmid effects, and the matrices $\mathbf{a}_i$, $\mathbf{b}_i$ ($i = 1, 2, 3$) are the material functions of $\boldsymbol{\gamma}$, ϑ, $\boldsymbol{\alpha}_D$ and $\boldsymbol{\alpha}_M$.

Consistency condition for the evolution equations (2.9) needs the assertions

$$\det[\mathbf{1} - \mathbf{a}_3 \cdot \mathbf{b}_3] \neq 0 \qquad \text{and} \qquad \det[\mathbf{1} - \mathbf{b}_3 \cdot \mathbf{a}_3] \neq 0. \tag{2.10}$$

We postulate that the balance of energy and the entropy production inequality hold. Then we obtain two fundamental evolution equations for the Kirchhoff stress tensor $\boldsymbol{\tau}$ and for temperature ϑ in the form

$$\begin{aligned} \mathrm{L}_{\mathbf{v}} \boldsymbol{\tau} &= \mathcal{L}^e : \mathbf{d} - \mathcal{L}^{\mathrm{th}} \dot{\vartheta} - (\mathcal{L}^e : \mathbf{N} + \mathbf{b}) \cdot \dot{\boldsymbol{\gamma}}, \\ \varrho c_p \dot{\vartheta} &= -\operatorname{div} \mathbf{q} + \vartheta \frac{\varrho}{\varrho_{\mathrm{Ref}}} \frac{\partial \boldsymbol{\tau}}{\partial \vartheta} : \mathbf{d} + \chi \sum_{\beta=1}^{n} \tau^{(\beta)} \dot{\gamma}^{(\beta)} \\ &\quad + \chi^* \sum_{\beta=1}^{n} \sum_{\delta=1}^{n} \left(a_1^{-1} \right)^{(\beta\delta)} \tau^{(\delta)} \dot{\alpha}_M^{(\beta)} + \chi^{**} \sum_{\beta=1}^{n} \sum_{\delta=1}^{n} \left(b_1^{-1} \right)^{(\beta\delta)} \tau^{(\delta)} \dot{\alpha}_D^{(\beta)}, \end{aligned} \tag{2.11}$$

where $\mathrm{L}_{\mathbf{v}}$ denotes the Lie derivative of $\boldsymbol{\tau}$ with respect to $\mathbf{v}$, $(a_1^{-1})^{(\beta\delta)}$ and $(b_1^{-1})^{(\beta\delta)}$ are components of $\mathbf{a}_1^{-1}$ and $\mathbf{b}_1^{-1}$, and

$$\mathcal{L}^e = \varrho_{\mathrm{Ref}} \frac{\partial^2 \widehat{\psi}}{\partial \mathbf{e}^2}, \qquad \mathcal{L}^{\mathrm{th}} = -\varrho_{\mathrm{Ref}} \frac{\partial^2 \widehat{\psi}}{\partial \mathbf{e} \partial \vartheta},$$

$$\mathbf{N} = \begin{bmatrix} \mathbf{N}^{(1)} \\ \vdots \\ \mathbf{N}^{(n)} \end{bmatrix}, \qquad \mathbf{N}^{(\beta)} = \frac{1}{2}\left[\mathbf{s}^{(\beta)}\mathbf{m}^{(\beta)} + \mathbf{m}^{(\beta)}\mathbf{s}^{(\beta)}\right],$$

$$\mathbf{W} = \begin{bmatrix} \mathbf{W}^{(1)} \\ \vdots \\ \mathbf{W}^{(n)} \end{bmatrix}, \qquad \mathbf{W}^{(\beta)} = \frac{1}{2}\left[\mathbf{s}^{(\beta)}\mathbf{m}^{(\beta)} - \mathbf{m}^{(\beta)}\mathbf{s}^{(\beta)}\right],$$

(2.12)

$$\mathbf{b} = \begin{bmatrix} \mathbf{b}^{(1)} \\ \vdots \\ \mathbf{b}^{(n)} \end{bmatrix}, \qquad \mathbf{b}^{(\beta)} = (\mathbf{N}^{(\beta)} + \mathbf{W}^{(\beta)})\cdot\boldsymbol{\tau} + \boldsymbol{\tau}(\mathbf{N}^{(\beta)} - \mathbf{W}^{(\beta)}),$$

$$c_p = -\vartheta \frac{\partial^2 \widehat{\psi}}{\partial \vartheta^2}, \qquad \chi\tau^{(\beta)} = -\varrho \frac{\partial \widehat{\psi}}{\partial \gamma^{(\beta)}},$$

$$\chi^* \tau^{(\beta)} = -\varrho \sum_{\delta=1}^{n} a_1^{(\beta\delta)} \frac{\partial \widehat{\psi}}{\partial \alpha_M^{(\delta)}},$$

$$\chi^{**} \tau^{(\beta)} = -\varrho \sum_{\delta=1}^{n} b_1^{(\beta\delta)} \frac{\partial \widehat{\psi}}{\partial \alpha_D^{(\delta)}}.$$

2.2. Adiabatic process

For an adiabatic process ($\mathbf{q} = 0$) from $(2.11)_2$ we obtain

$$\dot{\vartheta} = \mathcal{F} : \mathbf{d} + K\mathbf{G}, \tag{2.13}$$

where

$$\mathcal{F} = \frac{\varrho}{\varrho_{\mathrm{Ref}}} \frac{\vartheta}{\varrho c_p - D} \frac{\partial \boldsymbol{\tau}}{\partial \vartheta},$$

$$K = \frac{\boldsymbol{\tau} : \mathbf{N}}{\varrho c_p - D}\left(\chi + \chi^* \mathbf{a}_1^{-1}\cdot\mathbf{A}_1 + \chi^{**}\mathbf{b}_1^{-1}\cdot\mathbf{B}_1\right),$$

$$D = \boldsymbol{\tau} : \mathbf{N}\cdot\left(\chi^* \mathbf{a}_1^{-1}\cdot\mathbf{A}_2 + \chi^{**}\mathbf{b}_1^{-1}\cdot\mathbf{B}_2\right), \tag{2.14}$$

$$\mathbf{A}_1 = (\mathbf{a}_1 + \mathbf{a}_3\cdot\mathbf{b}_1)(1 - \mathbf{a}_3\cdot\mathbf{b}_3)^{-1},$$

$$\mathbf{B}_1 = (\mathbf{b}_1 + \mathbf{b}_3\cdot\mathbf{a}_1)(1 - \mathbf{b}_3\cdot\mathbf{a}_3)^{-1}.$$

To guarantee the existence of $\mathcal{F}$ and K we have to assume $D \neq \varrho c_p$.

Taking into account (2.13) we can write the evolution equations (2.9) in the form

$$\begin{aligned} \dot{\boldsymbol{\alpha}}_M &= (\mathbf{A}_1 + \mathbf{A}_2 K)\cdot\mathbf{G} + \mathbf{A}_2\mathcal{F} : \mathbf{d}, \\ \dot{\boldsymbol{\alpha}}_D &= (\mathbf{B}_1 + \mathbf{B}_2 K)\cdot\mathbf{G} + \mathbf{B}_2\mathcal{F} : \mathbf{d}, \end{aligned} \tag{2.15}$$

and the rate-type constitutive relation for the Kirchhoff stress tensor $\boldsymbol{\tau}$ as follows,

$$\mathrm{L}_{\boldsymbol{\upsilon}}\boldsymbol{\tau} = \left(\mathcal{L}^e - \mathcal{L}^{\mathrm{th}}\mathcal{F}\right) : \mathbf{d} - \left(\mathcal{L}^e : \mathbf{N} + \mathbf{b} + \mathcal{L}^{\mathrm{th}}K\right)\cdot\mathbf{G}. \tag{2.16}$$

2.3. An abstract form of the evolution problem

In an abstract form Eqs. (2.2), (2.3), (2.4), (2.16), (2.8), (2.15) and (2.13) can be written as follows:

$$\dot{\boldsymbol{\varphi}} = \mathcal{A}(t,\boldsymbol{\varphi})\boldsymbol{\varphi} + \mathrm{f}(t,\boldsymbol{\varphi}) \tag{2.17}$$

where

$$\boldsymbol{\varphi} = \begin{bmatrix} \phi \\ \boldsymbol{\upsilon} \\ \varrho \\ \boldsymbol{\tau} \\ \boldsymbol{\gamma} \\ \boldsymbol{\alpha}_M \\ \boldsymbol{\alpha}_D \\ \vartheta \end{bmatrix}, \qquad \mathrm{f} = \begin{bmatrix} \boldsymbol{\upsilon} \\ 0 \\ 0 \\ (\mathcal{L}^e : \mathbf{N} + \mathbf{b} + \mathcal{L}^{\mathrm{th}}K)\cdot\mathbf{G} \\ \mathbf{G} \\ (\mathbf{A}_1 + \mathbf{A}_2 K)\cdot\mathbf{G} \\ (\mathbf{B}_1 + \mathbf{B}_2 K)\cdot\mathbf{G} \\ K\mathbf{G} \end{bmatrix},$$

(2.18)

$$\mathcal{A} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0\,0\,0\,0 \\ 0 & 0 & \dfrac{\tau}{\varrho_{\mathrm{Ref}}}\mathrm{grad} & \dfrac{\varrho}{\varrho_{\mathrm{Ref}}}\mathrm{div} & 0\,0\,0\,0 \\ 0 & \varrho\mathrm{div} & 0 & 0 & 0\,0\,0\,0 \\ 0 & (\mathcal{L}^e - \mathcal{L}^{\mathrm{th}}\mathcal{F}) : \mathrm{sym}\left[\dfrac{\partial}{\partial\mathbf{x}}\right] - 2\mathrm{sym}\left[\boldsymbol{\tau}\cdot\dfrac{\partial}{\partial\mathbf{x}}\right] & 0 & 0 & 0\,0\,0\,0 \\ 0 & 0 & 0 & 0 & 0\,0\,0\,0 \\ 0 & \mathbf{A}_2\mathcal{F} : \mathrm{sym}\left[\dfrac{\partial}{\partial\mathbf{x}}\right] & 0 & 0 & 0\,0\,0\,0 \\ 0 & \mathbf{B}_2\mathcal{F} : \mathrm{sym}\left[\dfrac{\partial}{\partial\mathbf{x}}\right] & 0 & 0 & 0\,0\,0\,0 \\ 0 & \mathcal{F} : \mathrm{sym}\left[\dfrac{\partial}{\partial\mathbf{x}}\right] & 0 & 0 & 0\,0\,0\,0 \end{bmatrix}.$$

To investigate the behaviour of rate-dependent elasto-plastic single crystal during an adiabatic process and particularly, to examine the shear band formation, let us formulate the initial-boundary value problem (the evolution problem) as follows.

Find $\boldsymbol{\varphi}$ as a function of t and $\mathbf{x}$ such that the following assertions are satisfied:

(i) the differential equations in an abstract form (2.17) are fulfilled;

(ii) boundary conditions:

(a) displacement ϕ is prescribed on a part ∂_ϕ of $\partial\phi(\mathcal{B})$ and tractions $(\boldsymbol{\tau}\cdot\mathbf{n})^a$ are prescribed on a part $\partial_{\boldsymbol{\tau}}$ of $\partial\phi(\mathcal{B})$, where $\partial_\phi \cap \partial_{\boldsymbol{\tau}} = 0$ and $\overline{\partial_\phi \cup \partial_{\boldsymbol{\tau}}} = \partial\phi(\mathcal{B})$;

(b) heat flux $(\mathbf{q}\cdot\mathbf{n}) = 0$ is prescribed on $\partial\phi(\mathcal{B})$;

(iii) the initial conditions: $\boldsymbol{\varphi}$ is given at $X \in \mathcal{B}$ at $t = 0$.

3. Rate-independent response of single crystals

Assuming in (2.8) $T^{(\beta)} = 0$ we obtain

$$\tau^{(\beta)} = \tau_c^{(\beta)}(\gamma, \alpha_D, \vartheta) + \boldsymbol{\kappa}^{(\beta)} : \boldsymbol{\tau}. \tag{3.1}$$

Material differentiation with respect to time of (3.1) yields

$$\dot{\gamma}^{(\beta)} = \sum_{\delta=1}^{n} \hat{h}_{\beta\delta}^{-1} \left(\dot{\tau}^{(\delta)} - \boldsymbol{\kappa}^{(\delta)} : \dot{\boldsymbol{\tau}} \right) + \pi^{(\beta)}\dot{\vartheta} - \sum_{\delta=1}^{n} g_{\beta\delta}\dot{\alpha}_D^{(\delta)}, \tag{3.2}$$

where

$$\hat{h}_{\beta\delta} = \frac{\partial \tau_c^{(\beta)}}{\partial \gamma^{(\delta)}}, \qquad \pi^{(\beta)} = -\sum_{\delta=1}^{n} \frac{\partial \tau_c^{(\delta)}}{\partial \vartheta} \hat{h}_{\beta\delta}^{-1}, \qquad g_{\beta\delta} = \sum_{\nu=1}^{n} \frac{\partial \tau_c^{(\nu)}}{\partial \alpha_D^{(\delta)}} \hat{h}_{\beta\nu}^{-1}. \tag{3.3}$$

For rate-independent process the evolution equation for shearing $\boldsymbol{\gamma}$ has to be replaced by

$$\dot{\boldsymbol{\gamma}} = \mathbf{M}^{-1} \Big[\mathbf{N} : \mathcal{L}^e : \mathbf{N} + \mathbf{b} : \mathbf{N} - \mathcal{F} \left(\mathcal{L}^{\mathrm{th}} : \mathbf{N} + \frac{\partial \tau_c}{\partial \vartheta} + \frac{\partial \tau_c}{\partial \boldsymbol{\alpha}_D} \cdot \mathbf{B}_2 \right) - \boldsymbol{\kappa} : \mathcal{L}^e \Big] : \mathbf{d}, \tag{3.4}$$

where

$$\mathbf{M} = \mathbf{h} + (\mathbf{N} - \boldsymbol{\kappa}) : \mathcal{L}^e : \mathbf{N} + \mathbf{b} : \mathbf{N} + \left(\mathcal{L}^{\mathrm{th}} : \mathbf{N} + \frac{\partial \tau_c}{\partial \vartheta} \right) K. \tag{3.5}$$

4. Analysis of acceleration waves

4.1. General consideration

To investigate the intrinsic mathematical structure of the set of the field equations which determine the adiabatic inelastic flow processes, let us analyse the problem of propagation of acceleration waves. We shall show that the theory of acceleration waves in materials considered can be based on the notion of an instantaneous adiabatic acoustic tensor.

Let $\sum(t)$ denote a smooth surface with outward normal $\mathbf{n}$ which is moving through the solid body with velocity $\mathbf{w}(t, \mathbf{x})$. Some field quantities or their derivatives may be discontinuous across $\sum(t)$ which is then called a singular surface. If the surface $\sum(t)$ is composed of the same material points at all times, one then refers to $\sum(t)$ as a stationary discontinuity. Otherwise, the surface $\sum(t)$ is called a propagating singular surface or wave, cf. HILL [15].

Let c denote the normal speed of propagation of $\sum(t)$ with respect to the material in its current configuration. It is related to the spatial velocity $\mathbf{v}(t, \mathbf{x})$ and to the normal wave speed $w = \mathbf{w} \cdot \mathbf{n}$, by the following equation: $c = w - \mathbf{v} \cdot \mathbf{n}$.

It is said that $\sum(t)$ is an acceleration wave if the fields ϕ, $\mathbf{v}$, $\mathbf{F}$, $\boldsymbol{\mu}$ and ϑ are continuous functions of t and $\mathbf{x}$ while $\dot{\mathbf{v}}$, $\nabla \mathbf{v}$, $\dot{\mathbf{F}}$, $\nabla \mathbf{F}$, $\dot{\boldsymbol{\mu}}$, $\nabla \boldsymbol{\mu}$, $\dot{\vartheta}$, $\nabla \vartheta$ have (at most) jump discontinuities across $\sum(t)$ but are continuous in t and $\mathbf{x}$ jointly everywhere else ($\boldsymbol{\mu}$ denotes a set of the internal state variables).

An acceleration wave in which $\dot{\vartheta}$ and $\nabla \vartheta$ are continuous functions of t and $\mathbf{x}$ is called homothermal.

From the definition of an acceleration wave and the constitutive assumption

$$\psi = \hat{\psi}(\mathbf{e}, \mathbf{F}, \vartheta, \boldsymbol{\mu}) \tag{4.1}$$

we have

$$[\![\psi]\!] = [\![\boldsymbol{\sigma}]\!] = 0, \tag{4.2}$$

where $[\![\cdot]\!]$ denotes the jump of a quantity across $\sum(t)$ in the direction of its local normal $\mathbf{n}(t, \mathbf{x})$.

Hadamard's compatibility conditions require that jumps in velocity and stress derivatives be related as follows (cf. HADAMARD [14] and HILL [15]):

$$\begin{aligned} [\![\nabla \mathbf{v}]\!] &= -\frac{1}{c}[\![\mathbf{a}]\!]\mathbf{n}, \\ [\![\nabla \boldsymbol{\sigma}]\!] &= -\frac{1}{c}[\![\dot{\boldsymbol{\sigma}}]\!]\mathbf{n}, \end{aligned} \tag{4.3}$$

where ∇ denotes the spatial gradient, $\boldsymbol{\sigma} = (1/J)\boldsymbol{\tau}$ is the Cauchy tensor, and $\mathbf{a} = \dot{\mathbf{v}}$.

Balance of momentum requires that

$$\operatorname{div}\boldsymbol{\sigma} = \varrho \mathbf{a}. \tag{4.4}$$

Finally we have

$$\mathbf{n}\cdot[\![\dot{\boldsymbol{\sigma}}]\!] = -\varrho c[\![\mathbf{a}]\!]. \tag{4.5}$$

From the last result it becomes clear that the existence and propagation speed of acceleration waves in solids is directly related to the assumed constitutive structure of the material.

Since ϑ is continuous across $\sum(t)$, we have

$$[\![\dot{\vartheta}]\!] = -c[\![\nabla\vartheta]\!]\cdot\mathbf{n}. \tag{4.6}$$

For an acceleration wave in an adiabatic process we have (cf. PERZYNA [26])

$$[\![\mathbf{q}]\!] = 0, \qquad [\![\dot{\mathbf{q}}]\!] = 0, \qquad [\![\dot{\vartheta}]\!] \neq 0, \qquad [\![\nabla\vartheta]\!] \neq 0, \tag{4.7}$$

where $\mathbf{q}$ denotes the heat flux vector field.

Hence an acceleration wave in inelastic solids for an adiabatic process is not homothermal.

This conclusion will play an important role in an analysis of acceleration waves in particular material models for adiabatic process of a crystal.

4.2. Rate-dependent adiabatic process

For rate-dependent adiabatic process we have

$$[\![\mathrm{L}_{\mathfrak{v}}\boldsymbol{\tau}]\!] = \mathbb{E} : [\![\mathbf{d}]\!]. \tag{4.8}$$

where

$$\mathbb{E} = \mathcal{L}^{e} - \mathcal{L}^{\mathrm{th}}\mathcal{F}. \tag{4.9}$$

THEOREM 1. *For an adiabatic rate-dependent plastic flow process of single crystal described by* Eq. (2.17), *the acceleration discontinuity* $[\![\mathbf{a}]\!]$ *is the solution of the eigenvalue problem*

$$\mathbf{A}\cdot[\![\mathbf{a}]\!] = \varrho_{\mathrm{Ref}}c^2[\![\mathbf{a}]\!], \tag{4.10}$$

where

$$\mathbf{A} = \mathbf{n}\cdot(\mathbb{E}\cdot\mathbf{n} + \boldsymbol{\tau}\cdot\mathbf{n}\mathbf{g}) \tag{4.11}$$

denotes the instantaneous adiabatic acoustic tensor and $\mathbf{g}$ *is the metric tensor.*

4.3. Rate-independent adiabatic process

For rate-independent adiabatic process we obtain

$$[\![\mathrm{L}_{\mathfrak{v}}\boldsymbol{\tau}]\!] = \mathbb{L} : [\![\mathbf{d}]\!], \tag{4.12}$$

where

$$\mathbb{L} = \mathcal{L}^e - \mathcal{L}^{\mathrm{th}}\mathcal{F} - [\mathcal{L}^e : \mathbf{N} + \mathbf{b} + \mathcal{L}^{\mathrm{th}}K]\cdot\mathbf{M}^{-1}\cdot\Big[\mathbf{N} : \mathcal{L}^e : \mathbf{N} + \mathbf{b} : \mathbf{N} - \mathcal{F}\left(\mathcal{L}^{\mathrm{th}} : \mathbf{N} + \frac{\partial\tau_c}{\partial\vartheta} + \frac{\partial\tau_c}{\partial\boldsymbol{\alpha}_D}\cdot\mathbf{B}_2\right) - \boldsymbol{\kappa} : \mathcal{L}^e\Big], \tag{4.13}$$

$$h^{(\alpha\beta)} = \frac{\partial\tau_c^{(\alpha)}}{\partial\gamma^{(\beta)}}, \qquad \left(\frac{\partial\tau_c}{\partial\boldsymbol{\alpha}_D}\right)^{(\beta\delta)} = \frac{\partial\tau_c^{(\beta)}}{\partial\alpha_D^{(\delta)}}, \qquad \frac{\partial\tau_c}{\partial\vartheta} = \begin{bmatrix} \dfrac{\partial\tau_c^{(1)}}{\partial\vartheta} \\ \vdots \\ \dfrac{\partial\tau_c^{(n)}}{\partial\vartheta} \end{bmatrix}.$$

THEOREM 2. *For an adiabatic rate-independent plastic flow process of single crystal, the acceleration discontinuity* $[\![\mathbf{a}]\!]$ *is the solution of the eigenvalue problem*

$$\widehat{\mathbf{A}}\cdot[\![\mathbf{a}]\!] = \varrho_{\mathrm{Ref}}c^2[\![\mathbf{a}]\!], \tag{4.14}$$

where

$$\widehat{\mathbf{A}} = \mathbf{n}\cdot(\mathbb{L}\cdot\mathbf{n} + \boldsymbol{\tau}\cdot\mathbf{ng}) \tag{4.15}$$

denotes the instantaneous adiabatic acoustic tensor.

4.4. Analysis of eigenvalues of acoustic tensors

In the case of a rate-dependent process, all eigenvalues of the instantaneous adiabatic acoustic tensor $\mathbf{A}$ are positive. This of course is implied by hyperbolicity of the initial-boundary value problem.

For simplicity let us introduce rectangular Cartesian coordinates $\{x^i\}$ in such a way that $\mathbf{n}$ is in x^2-direction. We can assume, without loss of generality, $a_3 = 0$, and consider the reduced problem

$$\det[\mathbf{A}^{jk} - \zeta\delta^{jk}] = 0 \qquad \text{for} \quad j,k = 1,2, \tag{4.16}$$

where

$$\zeta = \varrho_{\mathrm{Ref}}c^2. \tag{4.17}$$

This leads to the result

$$\zeta_{1,2} = \frac{1}{2}(A^{11} + A^{22}) \pm \frac{1}{2}\sqrt{(A^{11} - A^{22})^2 + 4A^{12}A^{21}}\,. \tag{4.18}$$

Assuming the linear behaviour of the crystal and linear thermal expansion, i.e.

$$(\mathcal{L}^e)^{ijkl} = \tau^{jl}\delta^{ik} + \mu\left(\delta^{ik}\delta^{jl} + \delta^{il}\delta^{jk}\right) + \lambda\delta^{ij}\delta^{kl},$$
$$(\mathcal{L}^e)^{-1} : \mathcal{L}^{\mathrm{th}} = \theta\mathbf{I}, \tag{4.19}$$

where μ and λ are Lamé moduli and θ denotes the thermal expansion coefficient, we can find

$$\zeta_{1,2} = \frac{1}{2}(3\mu + \lambda + 3\tau^{22}) - \frac{1}{2}\theta\frac{\varrho}{\varrho_{\mathrm{Ref}}}\frac{\vartheta}{\varrho c_p - D}\left[\tau^{12}\cdot\frac{\partial\tau^{12}}{\partial\vartheta} + (2\mu + 2\lambda + \tau^{22})\frac{\partial\tau^{22}}{\partial\vartheta}\right]$$
$$\pm\frac{1}{2}\left\{\left[\mu + \lambda + \tau^{22} - \frac{\varrho}{\varrho_{\mathrm{Ref}}}\frac{\theta\vartheta}{\varrho c_p - D}\left((2\mu + 2\lambda + \tau^{22})\frac{\partial\tau^{22}}{\partial\vartheta} - \tau^{12}\frac{\partial\tau^{12}}{\partial\vartheta}\right)\right]^2\right.$$
$$\left. - 4\frac{\varrho}{\varrho_{\mathrm{Ref}}}\frac{\theta\vartheta}{\varrho c_p - D}\left[\frac{4}{3}\mu + \lambda + \tau^{22}\right]\cdot\left[1 - \frac{\varrho}{\varrho_{\mathrm{Ref}}}\frac{\theta\vartheta}{\varrho c_p - D}\frac{\partial\tau^{22}}{\partial\vartheta}\right]\tau^{12}\frac{\partial\tau^{12}}{\partial\vartheta}\right\}^{1/2}. \tag{4.20}$$

Neglecting thermal effects and the evolution of the dislocation substructure we have

$$\zeta_1 = 2\mu + \lambda + 2\tau^{22}, \qquad \zeta_2 = \mu + \tau^{22}. \tag{4.21}$$

In the case of a rate-independent process it may happen that some eigenvalues of the instantaneous adiabatic acoustic tensor $\widehat{\mathbf{A}}$ are equal zero. Then the associated discontinuity does not propagate ($c = 0$). This situation is referred to as the strain localization condition, i.e.

$$\det\widehat{\mathbf{A}} = 0. \tag{4.22}$$

5. Shear band formation

5.1. Single slip process ($n = 1$)

Mathematical analysis of the governing equations and the perturbation method give the hardening modulus rate h and the direction of the shear band $\mathbf{n}$ at the initiation of localization (cf. DUSZEK–PERZYNA and PERZYNA [9, 10], PERZYNA and DUSZEK–PERZYNA [28] and PERZYNA and KORBEL [29, 30])

$$\left(\frac{h}{\tau}\right)_{\mathrm{crit}} = \Pi + \frac{\Gamma}{\tau} - \Omega + \frac{\tau}{\mu}\left(\Theta^2\nu + \Theta + \frac{1}{4\nu}\right) + \frac{1}{4}\kappa^2\frac{\mu}{\tau},$$
$$\mathbf{n} = \mathbf{m} + \left(\frac{\Theta\tau}{2\mu} + \frac{\tau}{4\mu\nu}\right)\mathbf{s} - \frac{1}{2}\kappa\mathbf{z}, \tag{5.1}$$

where $\mathbf{z}$ is a unit vector perpendicular to $\mathbf{s}$ and $\mathbf{m}$, so that $\mathbf{s}$, $\mathbf{m}$, $\mathbf{z}$ form a right-handed triad

$$\Theta = \Delta\theta\mu, \qquad \Pi = \Delta\pi h, \qquad \Gamma = b_1 \frac{\partial \tau_c}{\partial \alpha_D},$$

$$\Omega = b_2 \Delta \frac{\partial \tau_c}{\partial \alpha_D}, \qquad \Delta = \frac{\chi + \chi^* + \chi^{**}}{\varrho c_p}, \qquad \nu = \frac{\lambda + \mu}{\lambda + 2\mu},$$

μ and λ are Lamé moduli, and

$$\boldsymbol{\kappa}^{(1)} = \boldsymbol{\kappa}^{(2)} = \begin{bmatrix} 0 & \frac{1}{2}\kappa \\ \frac{1}{2}\kappa & 0 \end{bmatrix}. \tag{5.2}$$

It is assumed that $\kappa = 0.0017$, $a_1 = 6.5 \cdot 10^{16}$, $b_1 = -6.85 \cdot 10^{13}$ and $b_2 = 0$. All other material parameters are given in Table 1.

Table 1. Material parameters.

	Parameter	Unit	Aluminium
ϱ	density	Kg m^{-3}	2702
c_p	specific heat	J Kg^{-1} K^{-1}	896
μ	shear modulus	G Pa	26.0
E	Young's modulus	G Pa	71.0
K	bulk modulus	G Pa	73.2
θ	coefficient of thermal expansion	K^{-1}	$23.8 \cdot 10^{-6}$
χ	irreversibility coefficient	-	0.65 – 0.85

5.2. Symmetric double slip process ($n = 2$)

It is assumed that the crystal has two active slip systems, symmetrically oriented with respect to the maximum principal stress τ^{22} (the tensile axis is x^2) at the angle φ.

The condition for localization is reduced to the equation

$$A\left(\frac{n_1}{n_2}\right)^4 + B\left(\frac{n_1}{n_2}\right)^3 + C\left(\frac{n_1}{n_2}\right)^2 + D\left(\frac{n_1}{n_2}\right) + E = 0, \tag{5.3}$$

where

$$
\begin{aligned}
A &= (\mathbb{L}^{2222} + \tau^{22})(\mathbb{L}^{2112} + \tau^{22}),\\
B &= (\mathbb{L}^{2222} + \tau^{22})(\mathbb{L}^{1112} + \mathbb{L}^{2111}) + (\mathbb{L}^{2112} + \tau^{22})(\mathbb{L}^{1222} + \mathbb{L}^{2221})\\
&\qquad - \mathbb{L}^{2212}(\mathbb{L}^{1122} + \mathbb{L}^{2121}),\\
C &= (\mathbb{L}^{1111} + \tau^{11})(\mathbb{L}^{2222} + \tau^{22}) + (\mathbb{L}^{1222} + \mathbb{L}^{2221})(\mathbb{L}^{1112} + \mathbb{L}^{2111})\\
&\qquad + (\mathbb{L}^{1221} + \tau^{11})(\mathbb{L}^{2112} + \tau^{22}) - (\mathbb{L}^{1122} + \mathbb{L}^{2121})(\mathbb{L}^{1212} + \mathbb{L}^{2211})\\
&\qquad - \mathbb{L}^{1121}\mathbb{L}^{2212},\\
D &= (\mathbb{L}^{1111} + \tau^{11})(\mathbb{L}^{1222} + \mathbb{L}^{2221}) + (\mathbb{L}^{1221} + \tau^{11})(\mathbb{L}^{1112} + \mathbb{L}^{2111})\\
&\qquad - \mathbb{L}^{1121}(\mathbb{L}^{1212} + \mathbb{L}^{2211}),\\
E &= (\mathbb{L}^{1111} + \tau^{11})(\mathbb{L}^{1221} + \tau^{11}).
\end{aligned}
\tag{5.4}
$$

The ratio $(n_2/n_1) = \tan\beta$ gives us the direction of the macroscopic shear band. Solving the fourth order algebraic equation (5.3) we have to choose the real and positive solutions for (n_2/n_1), and next to take such value of the angle β that maximizes the value of the hardening modulus rate h/τ^{22}. Then the misalignment angle $\delta = \beta - \varphi$. We shell denote

$$
\mathbf{h} = \begin{bmatrix} h & h_1 \\ h_1 & h \end{bmatrix}, \tag{5.5}
$$

and assume $h_1/h = q = 1.2$.

In such a way we obtain the critical value of the hardening modulus rate and the misalignment angle between the shear band and the slip plane in point of the inception of the shear band formation.

6. Physical identification of introduced coefficients

For better presentation of theoretical results we have performed numerical estimations of the considered quantities for two particular cases of uniaxial tensile test.

The paper of CHANG and ASARO [7] for Al–Cu single crystals tested at 298 K was taken as the experimental base for calculations.

For simplicity we have made some additional assumptions about the process and we have to write the specific evolution equations for density of dislocation parameters. We used the evolution equations proposed by BALKE and ESTRIN [4] in the form

$$
\begin{aligned}
&\dot{\alpha}_M = A_1\dot{\gamma}, \qquad A_1^{(\beta\beta)} = \frac{c_1}{b^2}\frac{\alpha_D^{(\beta)}}{\alpha_M^{(\beta)}} - c_2\alpha_M^{(\beta)} - \frac{c_3}{b}\sqrt{\alpha_D^{(\beta)}}, \qquad A_1^{(\beta\delta)} = -\xi\alpha_M^{(\beta)},\\
&\dot{\alpha}_D = B_1\dot{\gamma}, \qquad B_1^{(\beta\beta)} = c_2\alpha_M^{(\beta)} + \frac{c_3}{b^2}\sqrt{\alpha_D^{(\beta)}} - c_4\alpha_D^{(\beta)}, \qquad B_1^{(\beta\delta)} = \xi\alpha_M^{(\beta)},\\
&\qquad\qquad \beta, \delta = 1, 2.
\end{aligned}
\tag{6.1}
$$

Preserving proportional dependence of generated and annihilated dislocations proposed by the authors we have been able to estimate coordinates of matrices $\mathbf{A}_1$, $\mathbf{B}_1$ in the point of inception of the shear band formation.

For the considered process we have obtained

$$A_1^{(\beta\beta)} \sim 4.2 \times 10^{16}\ \mathrm{m}^{-2}, \qquad A_1^{(\beta\delta)} \sim -1.6 \times 10^{14}\ \mathrm{m}^{-2},$$
$$B_1^{(\beta\beta)} \sim -2.45 \times 10^{14}\ \mathrm{m}^{-2}, \qquad B_1^{(\beta\delta)} \sim 1.6 \times 10^{14}\ \mathrm{m}^{-2}.$$

From the experimental data we have $\partial\tau_2/\partial\vartheta = -0.06$ MPa/K, $\tau_c = 195$ MPa, $\gamma_c = 0.4$ and $\xi = 0.01$.

When we assume the linear elastic behaviour of the crystal and linear thermal expansion cf. (4.19), we can estimate influence of various effects on the value of the fundamental matrix $\mathbb{L}$.

For example the non-dissipative thermal effects are introduced by $\mathcal{F}$, the non-Schmid effects by the matrix $\boldsymbol{\kappa}$, and the substructure evolution effects by coefficient K.

7. Numerical results

Analysing the localization conditions we can observe that these various effects cooperate and then some synergetic effects are generated (cf. Figs. 4 – 7). The synergetic effect is defined as the difference between the result obtained for two cooperative phenomena and the sum of the results obtained when these two phenomena are active separately. For the considered process in single slip case we may say that most significant are the evolution of the dislocation substructure and the non-Schmid synergetic effects, while in double slip case the non-Schmid effects can be neglected. However, both cases indicate that the evolution of the dislocation substructure effects should be taken into consideration in entire analysis of simple crystal deformation process.

Besides the synergetic effects we obtain also the values of critical hardening modulus and misalignment angle between the shear band and the slip planes for processes in which different effects were considered (Figs. 1 – 3).

We can observe that in the processes, in which non-dissipative thermal effect is included, the value of hardening modulus is only slightly higher than in the process without this effect.

Next, the two processes in which one of them has the non-Schmid effect but the other not, show more significant difference in value of hardening modulus, but this difference is not so high as that introduced by thermal couplings and the evolution of substructure.

Very important observation is that for both cases: single slip and double slip processes, the value of misalignment angle does not depend on the fact whether the various effects are considered or not. Of course, the value of this angle is more reasonable for double slip process (Fig. 3).

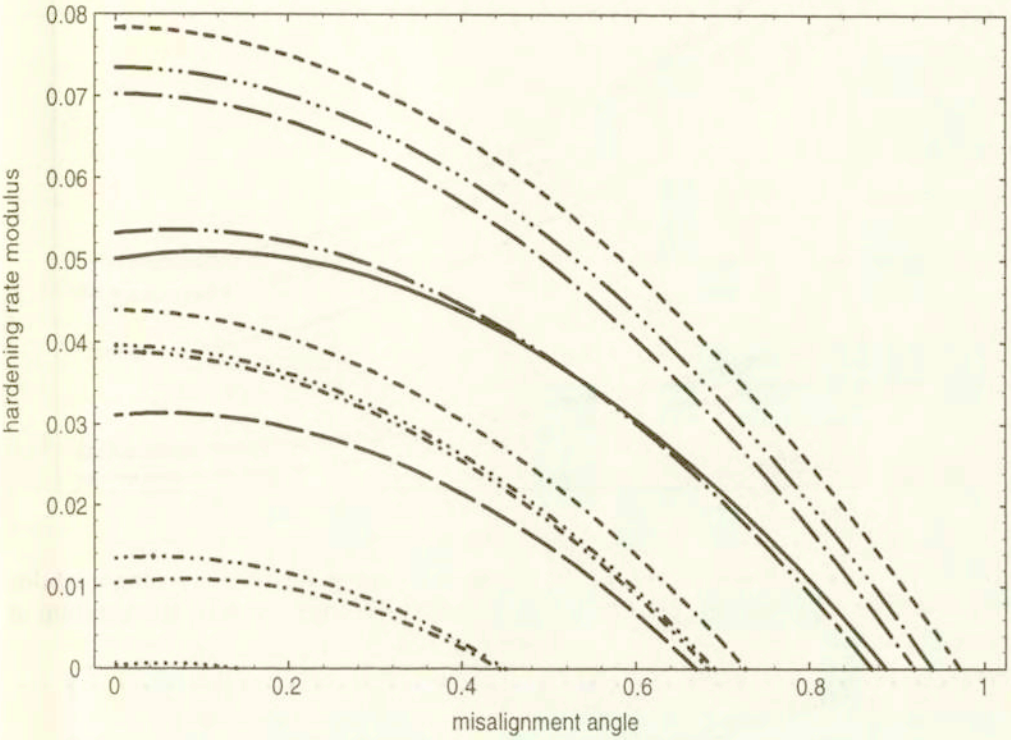

FIG. 1. Numerical results for single slip process for the hardening modulus rate h/τ^{22} as a function of the misalignment angle δ for Al–Cu single crystal.

- adiabatic process with substructure and non-Schmid effects,
- adiabatic process with substructure, non-dissipative thermal term and non-Schmid effects,
- isothermal process with substructure and non-Schmid effects,
- adiabatic process with substructure and non-dissipative thermal term,
- adiabatic process with substructure,
- adiabatic process with non-Schmid effects,
- isothermal process with non-Schmid effects,
- adiabatic process with non-dissipative thermal term and non-Schmid effects,
- isothermal process with substructure,
- adiabatic process with non-dissipative thermal term,
- adiabatic process,
- isothermal process.

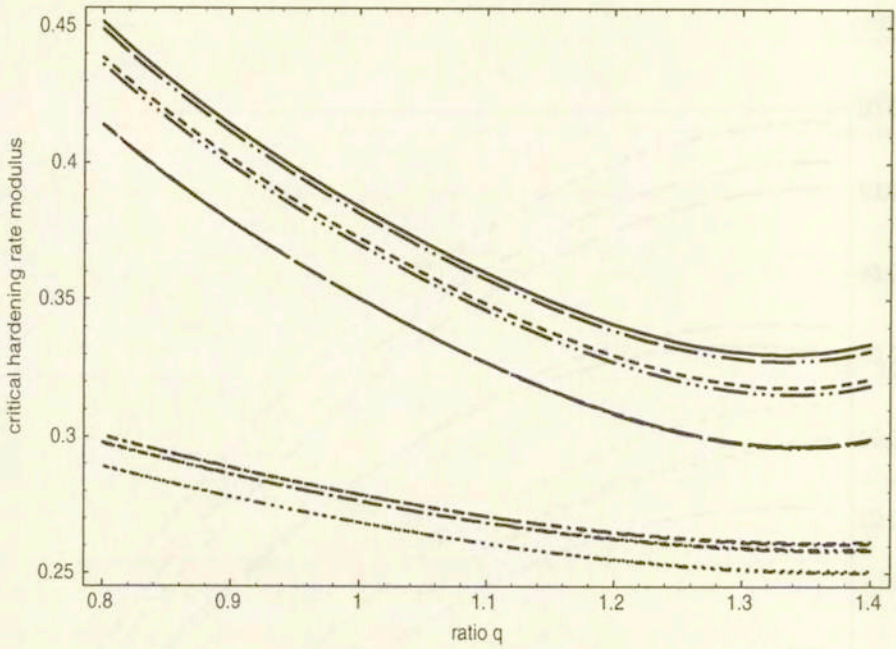

FIG. 2. Numerical results for symmetric double slip process for the hardening modulus rate h/τ^{22} as a function of the ratio $q = h_1/h$ for Al–Cu single crystal. For notation of lines see Fig. 1.

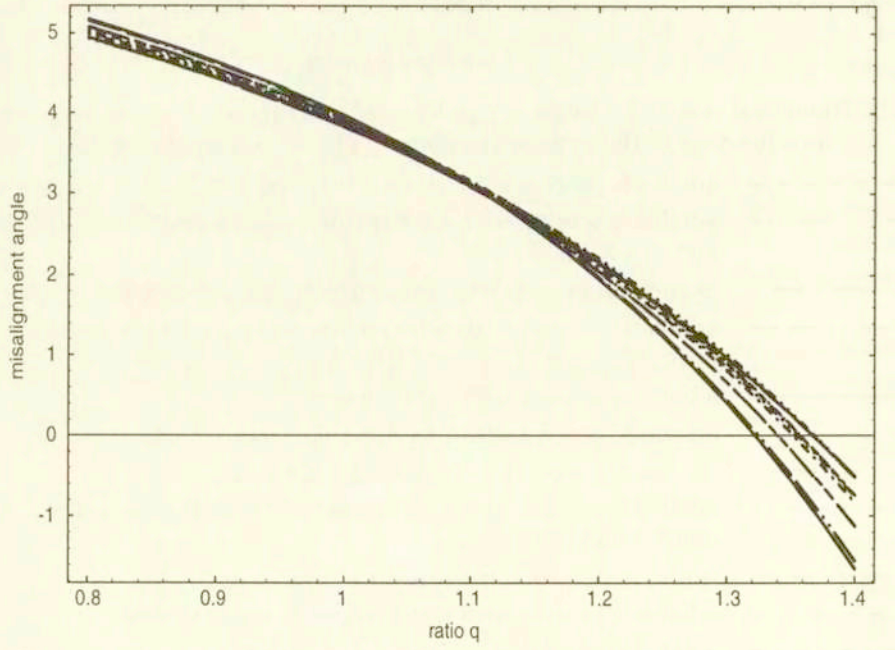

FIG. 3. Numerical results for symmetric double slip process for the misalignment angle δ as a function of the ratio $q = h_1/h$ for Al–Cu single crystal. For notation of lines see Fig. 1.

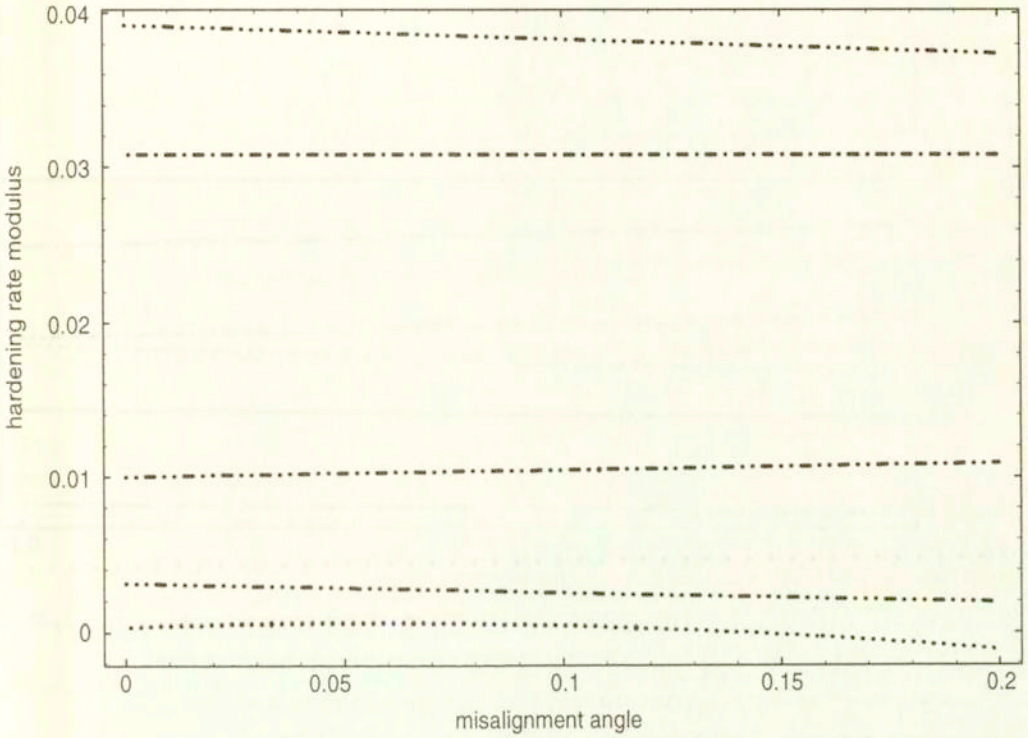

FIG. 4. Synergetic effects for single slip process for the hardening modulus rate h/τ^{22} as a function of the misalignment angle δ for Al–Cu single crystal.

– · · · · – · · · · – spatial covariance and non-Schmid effects,
– · – · – · – · – spatial covariance and substructure effects,
– · · – · · – · · – spatial covariance and thermomechanical effects,
– · · · – · · · – · spatial covariance and non-dissipative thermal effects,
· · · · · · · · · · · · isothermal process (spatial covariance effect).

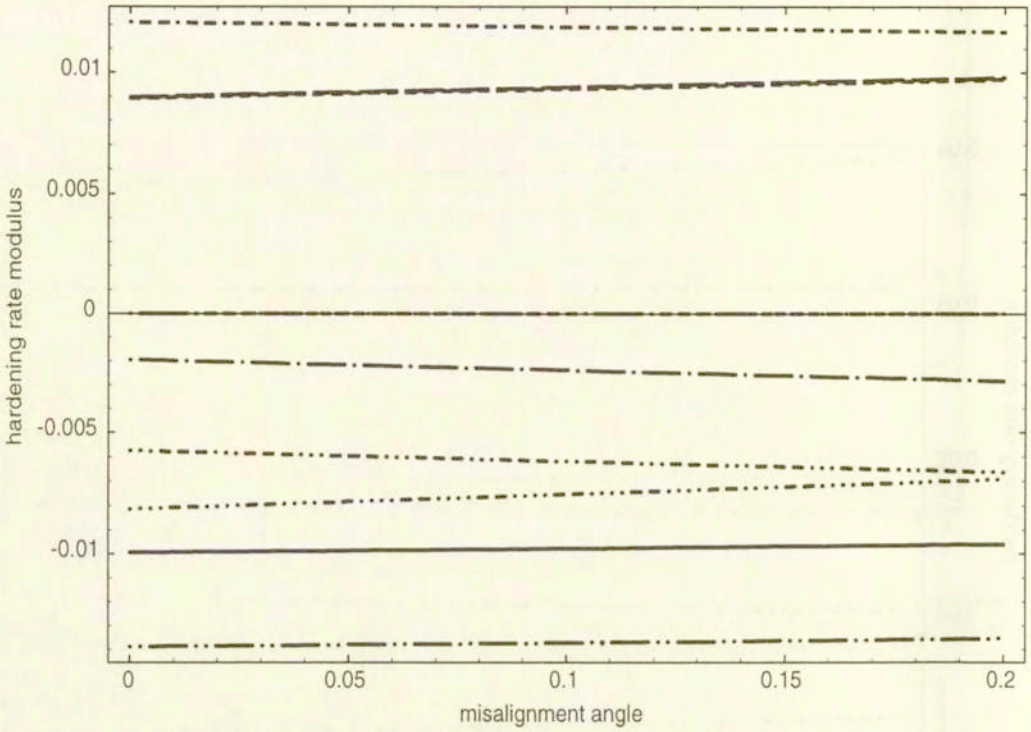

FIG. 5. Synergetic effects for single slip process for the hardening modulus rate h/τ^{22} as a function of the misalignment angle δ for Al–Cu single crystal.

- substructure and non-dissipative thermal effects,
- substructure and thermomechanical effects,
- substructure, thermomechanical and non-dissipative thermal effects,
- substructure and non-Schmid effects,
- thermomechanical and non-dissipative thermal effects,
- substructure, thermomechanical and non-Schmid effects,
- thermomechanical and non-Schmid effects,
- non-dissipative thermal and non-Schmid effects,
- substructure, thermomechanical, non-dissipative thermal and non-Schmid effects,
- thermomechanical, non-dissipative thermal and non-Schmid effects.

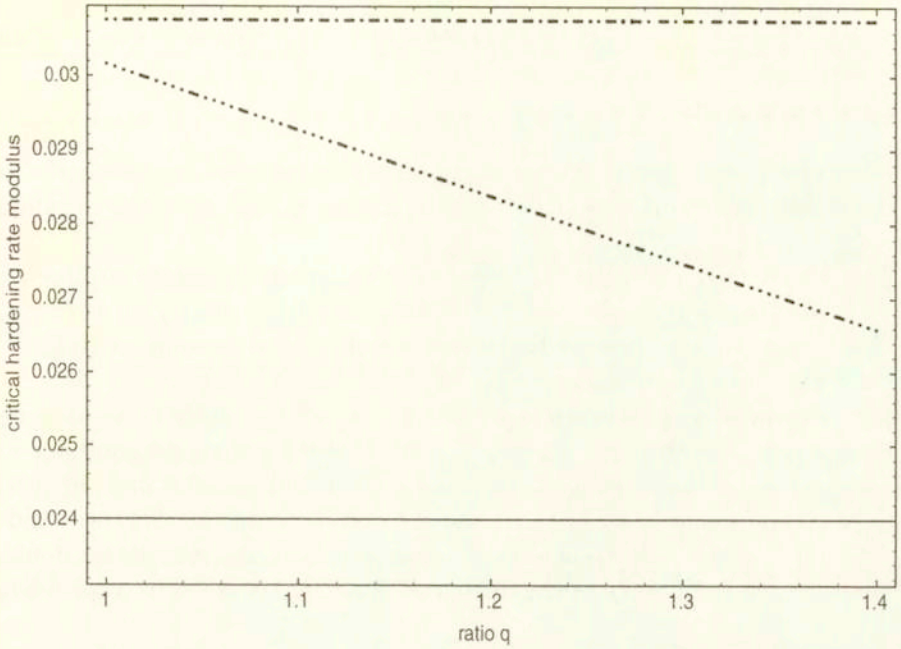

FIG. 6. Synergetic effects for symmetric double slip process for the hardening modulus rate h/τ^{22} as a function of the ratio $q = h_1/h$ for Al–Cu single crystal. For notation of lines see Fig. 4.

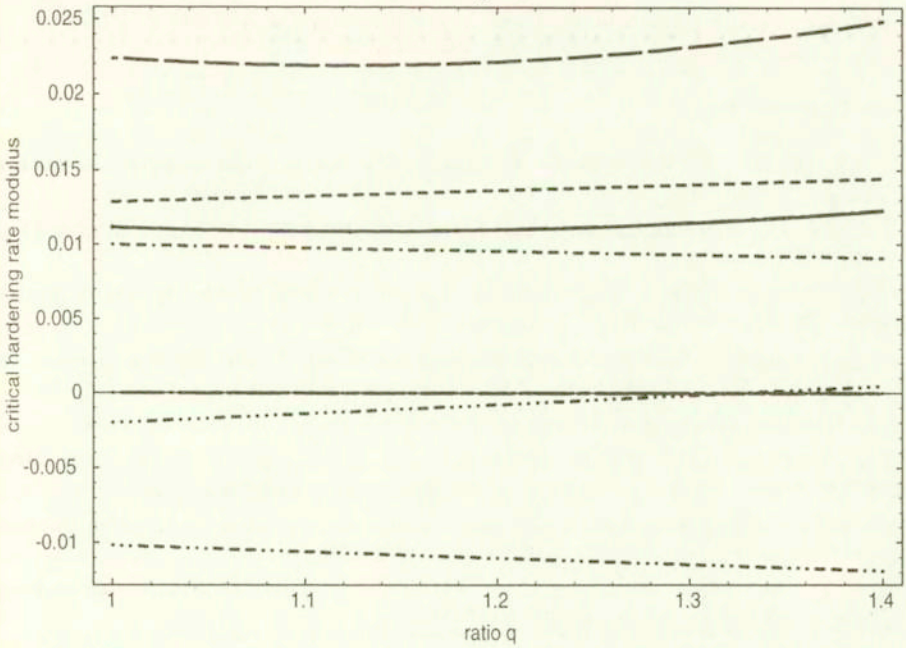

FIG. 7. Synergetic effects for symmetric double slip process for the hardening modulus rate h/τ^{22} as a function of the ratio $q = h_1/h$ for Al–Cu single crystal. For notation of lines see Fig. 5.

8. Final comments

The evolution of the dislocation substructure affects very much the results for the critical modulus rate $(h/\tau^{22})_{\text{crit}}$. It has no influence on the misalignment angle δ.

Two cooperative phenomena, namely the thermomechanical coupling and the dislocation substructure give distinct synergetic effect (mostly on $(h/\tau^{22})_{\text{crit}}$).

The change of the irreversibility coefficient χ in the range of $(0.65 - 0.85)$ does not give important influence on the localization results.

Comparison of the theoretical results for $(h/\tau^{22})_{\text{crit}}$ with those obtained experimentally by CHANG and ASARO [7] and SPITZIG [35] shows good agreement.

Comparison of the theoretical results for the misalignment angle δ with those obtained experimentally by CHANG and ASARO [7], LISIECKI, NELSON and ASARO [18] and SPITZIG [35] shows good agreement only for symmetric double slip process when the geometry of the deformed specimen is taken into consideration.

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