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Analysis of the fundamental equations describing thermoplastic flow process in solid body(*)

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THE AIM of this paper is to investigate the influence of thermomechanical couplings and thermal softening effects on shear band localization during a dynamic deformation process. The structure of the system of equations describing the behaviour of a material is analyzed. This analysis gives the answer to the question what are the conditions for the material functions, thanks to which we obtain different type of the system of equations — hyperbolic or parabolic. Two thermodynamic descriptions of the material were compared: the first, by a material derivative, the second, by the Lie derivative. It was shown that covariance terms which appear in the equations after assuming the invariance under arbitrary spatial diffeomorphism, have a significant influence on the hyperbolicity conditions. Thus we must be very careful in choosing a proper description of the thermomechanical behaviour of a material.

Celem pracy jest zbadanie wpływu termomechanicznych sprzężeń i efektów termicznego osłabienia na lokalizację wzdłuż pasm ścinania podczas procesu dynamicznych deformacji. Zanalizowano strukturę układu równań opisujących zachowanie się materiału. Analiza ta daje odpowiedź na pytanie jakie są warunki dla funkcji materiałowych, dzięki którym otrzymujemy różne typy układu równań — hiperboliczny bądź paraboliczny. Porównano dwa termodynamiczne opisy materiału, pierwszy za pomocą pochodnej materialnej, drugi za pomocą pochodnej Liego. Wykazano, że człony kowariantne pojawiające się w równaniach po założeniu niezmienniczości procesu względem dowolnego dyfeomorfizmu mają istotny wpływ na warunek hiperboliczności układu równań. Tak więc, sprawa wyboru właściwego opisu termomechanicznego zachowania się materiału jest niezmiernie ważna.

Целью работы является исследование влияния термомеханических сопряжений и эффектов термического ослабления на локализацию вдоль полос свига во время процесса динамических деформаций. Анализируется структура системы уравнений, описывающих поведение материала. Этот анализ дает ответ на вопрос, какими являются условия локализации для материальных функций, благодаря которым получаем разного типа системы уравнений — гиперболический или параболический. Получены два термодинамических описания матерала, первое при помощи материальной производной, второе при помощи производной Ли. Показано, что ковариантные члены, появляющиеся в уравнениях после принятия инвариантности по отношению к произвольному диффеоморфизму, имеют существенное влияние на условие гиперболичности системы уравнений. И так, вопрос выбора правильного термомеханического описания поведения материала является неизмерно важным.

1. Introduction

EXPERIMENTAL investigations of different types of materials have shown that in dynamic processes thermal effects play an important role in the initiation and

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formation of shear band localization. From the theoretical point of view, the criteria of localization can be found by analyzing the type of equations describing the thermomechnical process. These equations are formulated within the framework of the thermodynamic theory with internal state variables. The displacement and temperature fields are coupled and the transport of heat takes place with finite velocity. By introducing the Lie derivative to define all objective rates of stress, heat flux, temperature and velocity (MARSDEN and HUGHES [7]), the invariance under arbitrary spatial diffeomorphism was obtained.

The main objective of this paper is to investigate the propagation of discontinuities of stress and temperature in an elastic-plastic material under dynamic loading. We derived the conditions under which the uncoupled mechanical and thermal waves propagate and we also determined their velocities in two cases: first, in the material description, then, the same procedure was applied for the case of the Lie derivative.

Constitutive equations for an elastic-plastic material in the thermodynamic theory were proposed by PERZYNA [9]. They are very general and they describe many different additional effects such as thermal softening, isotropic and kinematic hardening, the micro-damage process.

This paper provides the first step and introduction for future investigations in this subject; this is why it contains some simplifications. Our analysis is restricted to the one-dimensional case and not all of the additional phenomena are taken into account. In the future we would like to extend the presented methods to other states and analyze the influence of such effects as porosity, kinematic hardening, etc.

2. General description of thermomechanical couplings

The thermomechanical state of the material particle for a given time t is described by the constitutive functions which characterize the mechanical and thermal properties of the material.

We assume that this state is represented by a set of variables as follows:

$$s = (\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}), \tag{2.2}$$

where $\mathbf{F}$ denote the deformation gradient, $\mathbf{e}$ — Eulerian strain tensor, ϑ — the absolute temperature and $\boldsymbol{\mu}$ — a set of internal state variables which describe all dissipation effects occurring during the thermal process, the plastic flow phenomenon, isotropic and kinematic hardening and porosity.

The response of the material for an intrinsic state is described by the following set of variables:

(2.2) $$\{\boldsymbol{\tau},\ \psi,\ \eta,\ \mathbf{q}\},$$

where $\boldsymbol{\tau}$ denotes the Kirchhoff stress tensor, ψ is the free energy function, η is the entropy and $\mathbf{q}$ the heat flux. It is postulated that there exists the free energy function and it has the form

(2.3) $$\psi = \hat{\psi}(s).$$

Thus stress, entropy and heat flux are determined by the free energy function which is a consequence of the second law of thermodynamics:

$$\begin{aligned}
\boldsymbol{\tau} &= \tau(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}) = \rho_0 \partial_e \hat{\psi}(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}),\\
\eta &= \eta(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}) = -\partial_\vartheta \hat{\psi}(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}),\\
\mathbf{q} &= \mathbf{q}(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}) = -\rho\vartheta\partial_{\mu_q}\hat{\psi}(\mathbf{e},\ \mathbf{F},\ \vartheta,\ \boldsymbol{\mu}),
\end{aligned}$$

where μ_q — thermal internal state variables.

Let us discuss the general equations describing the thermomechanical process for an elastic-plastic solid, (see DUSZEK, PERZYNA [3])

1. The energy balance equation which includes thermomechanical couplings and dissipation effects

(2.5) $$\rho c_p \dot{\vartheta} = -\operatorname{div}\mathbf{q} + \vartheta \frac{\rho}{\rho_0}\frac{\partial \boldsymbol{\tau}}{\partial \vartheta} : \mathbf{d} + \rho\chi \left\langle \frac{1}{H}[\mathbf{P}:\dot{\boldsymbol{\tau}} + \pi\dot{\vartheta}]\right\rangle,$$

where

$c_p = -\vartheta \dfrac{\partial^2 \hat{\psi}}{\partial \vartheta^2}$ specific heat,

$\chi = -\left(\dfrac{\partial \hat{\psi}}{\partial \boldsymbol{\mu}} - \vartheta \dfrac{\partial^2 \hat{\psi}}{\partial \vartheta \partial \boldsymbol{\mu}}\right)\mathbf{m}(\mathbf{s})$ describes dissipation effects,

$\varphi = f(\boldsymbol{\tau}) - \varkappa,\ f(\cdot) = J_2,$

$\varkappa =$ temperature dependent work-hardening-softening parameter,

$\mathbf{P} = \dfrac{1}{2\sqrt{J_2}}\dfrac{\partial \varphi}{\partial \boldsymbol{\tau}},$

$\pi = \dfrac{1}{2\sqrt{J_2}}\dfrac{\partial \varphi}{\partial \vartheta}$ describes thermal softening of the material caused by the increasing temperature,

$H = \dfrac{1}{2\sqrt{3J_2}}\dfrac{\partial \varkappa}{\partial \varepsilon^p},$ ε^p is the equivalent plastic deformation,

$\mathbf{d} = \dfrac{1}{2}[\operatorname{grad}\mathbf{v} + (\operatorname{grad}\mathbf{v})^T].$

The cross-coupling effects are described in Eq. (2.5) by two terms. The first one, which has not dissipative character, evaluates the temperature dependence of the stress tensor and is proportional to $\partial\boldsymbol{\tau}/\partial\vartheta:\mathbf{d}$. The second term, proportional to $\frac{\partial^2\hat{\psi}}{\partial\vartheta\partial\boldsymbol{\mu}}\, m(s)$, is implied by the temperature denpendence of the generalized force conjugates to the internal state vector $\boldsymbol{\mu}$. This one is very dissipative in its nature.

2. The constitutive equation for the heat flux $\mathbf{q}$

$$TL_{\mathbf{v}}\mathbf{q} + \mathbf{q} = -k\,\mathrm{grad}\,\vartheta. \tag{2.6}$$

where T denotes relaxation time, k is the coefficient of thermal conductivity (positive constant), $L_{\mathbf{v}}\mathbf{q}$ is the Lie derivative of the vector $\mathbf{q}$ with respect to the velocity field $\mathbf{v}$ and

$$L_{\mathbf{v}}\mathbf{q} = \left(\frac{\partial q^a}{\partial t} + \frac{\partial q^a}{\partial x_b} v^b - q^b \frac{\partial v^a}{\partial x^b}\right)\mathbf{e}_a. \tag{2.7}$$

Equation (2.6) provides the generalization for non-equilibrium states of the well-known Fourier law. It was postulated by CATTANEO [2] and MAXWELL [8] to correct unacceptable properties of the Fourier theory of diffusion of heat (Eq. (2.6) is called the Maxwell–Cattaneo relation). The classical theory rests upon the hypothesis that the flux of heat is proportional to the gradient of temperature. Thus the temperature distribution in the body is governed by a parabolic partial differential equation and the consequence of it is that the heat impulse given in the surface of the body is felt immediately in all parts of the body, no matter how distant they are from the source. The Maxwell–Cattaneo modification of Fourier's law changes the type of the heat conduction equation to hyperbolic and the finite speeds of waves are possible. It can be seen that for $T = 0$ it reduces to the classical theory.

3. Constitutive equation for the Kirchhoff stress tensor:

$$L_{\mathbf{v}}\boldsymbol{\tau} = \mathscr{L}\cdot\mathbf{d} - \mathbf{z}\dot{\vartheta}, \tag{2.8}$$

where

$$\mathscr{L} = \left[I + \frac{1}{H}\mathscr{L}^e\cdot\mathbf{P}\mathbf{P}\right]^{-1}\left[\mathscr{L}^e - \frac{1}{H}\mathscr{L}^e\cdot\mathbf{P}(\mathbf{P}\cdot\boldsymbol{\tau} + \boldsymbol{\tau}\cdot\mathbf{P})\right],$$

$$\mathbf{z} = \left[I + \frac{1}{H}\mathscr{L}^e\cdot\mathbf{P}\mathbf{P}\right]^{-1}\left[\frac{1}{H}\pi\,\mathscr{L}^e\cdot\mathbf{P} + \mathscr{L}^{\mathrm{th}}\right],$$

$$\mathscr{L}^e = \rho_0\frac{\partial^2\hat{\psi}}{\partial\mathbf{e}^2}, \tag{2.9}$$

$\mathscr{L}^{\mathrm{th}} = -\rho_0\frac{\partial^2\hat{\psi}}{\partial\mathbf{e}\partial\vartheta}$ the coefficient of thermal expansion,

$L_{\mathbf{v}}\boldsymbol{\tau}$ — Lie derivative of a tensor field $\boldsymbol{\tau}$ with respect to the velocity field $\mathbf{v}$.

4. Equation of motion

$$\rho \dot{\mathbf{v}} = \operatorname{div}\left(\frac{1}{J}\boldsymbol{\tau}\right) \text{ and } J = \frac{\rho_0}{\rho}. \tag{2.10}$$

Generally, the presented system of equations consists of 13 equations with 13 unknown variables, but to simplifty the calculations we analyze the one-dimensional case so the number of equations and unknown functions is reduced to four. Of course, this is not a sufficient analysis, but there are some cases when the three-dimensional state can be approximated by the results derived from the one-dimensional theory.

3. Analysis of wave propagation — Material derivative formulation

First, an analysis of the hiperbolicity of the system of Eqs. (2.5), (2.6), (2.8), (2.10) was made in the case when the covariance terms are neglected (that means for a material description). Thus the complete system of partial differential equations governing the one-dimensional thermomechanical process is as follows:

$$\begin{aligned} A_1\dot{\tau} + A_2\dot{\vartheta} - \frac{\partial q}{\partial x} + A_3\frac{\partial v}{\partial x} &= 0,\\ T\dot{q} + k\frac{\partial \vartheta}{\partial x} + q &= 0,\\ \dot{\tau} + z\dot{\vartheta} - \mathscr{L}\frac{\partial v}{\partial x} &= 0,\\ \rho_0\dot{v} - \frac{\partial \tau}{\partial x} - \tau C &= 0, \end{aligned} \tag{3.1}$$

where

$$A_1 = \frac{\rho\chi P}{H},\quad A_2 = \frac{\rho\chi\pi}{H} - \rho c_p,\quad A_3 = \frac{\rho}{\rho_0}\frac{\partial \tau}{\partial \vartheta},\quad C = \frac{\partial \rho}{\partial x},$$

the Lagrangian derivative is denoted by a dot.

To derive the conditions for the hyperbolicity of Eqs. (3.1), we have to find four real characteristic speeds and corresponding characteristic vectors which are linearly independent. In order to evaluate the characteristic values λ, we make the following formal change of operators:

$$\begin{aligned} \partial_t &\longrightarrow -\lambda\Delta,\\ \partial_x &\longrightarrow \Delta, \end{aligned} \tag{3.2}$$

where Δ is a linear differential operator.

After the transformation of the system (3.1), we obtain four algebraic equations with four unknowns ($\Delta\tau$, Δq, $\Delta\vartheta$, Δv):

$$
\begin{aligned}
&A_1\lambda\,\Delta\tau + A_2\lambda\,\Delta\vartheta + \Delta q - A_3\Delta v = 0,\\
&\lambda\,\Delta q - \frac{k}{T}\Delta\vartheta - \frac{1}{T}q = 0,\\
&\lambda\,\Delta\tau + \lambda\, z\,\Delta\vartheta + \mathscr{L}\,\Delta v = 0,\\
&\rho_0\lambda\,\Delta v + \Delta\tau + \tau C = 0.
\end{aligned}
\tag{3.3}
$$

This system has non-zero solutions in the case when the determinant of the matrix formed by the coefficients standing with the unknowns is equal to zero. Its development gives the following characteristic polynomial of the fourth degree:

$$
(A_1 z - A_2)\rho_0\lambda^4 + \left(A_2\mathscr{L} + A_3 z - \frac{k}{T}\rho_0\right)\lambda^2 + \mathscr{L}\frac{k}{T} = 0.
\tag{3.4}
$$

The general solution of this equation has the form

$$
\lambda_i = \pm\left[\frac{\frac{k}{T}\rho_0 - A_3 z - A_2\mathscr{L} \pm \sqrt{\left(A_2\mathscr{L} + A_3 z - \frac{k}{T}\rho_0\right)^2 - \frac{4k\mathscr{L}}{T}(A_1 z - A_2)\rho_0}}{2(A_1 z - A_2)\rho_0}\right]^{\frac{1}{2}},
\tag{3.5}
$$

where $i = 1, 2, 3, 4$, and for a given characteristic value correspond the following signs in the above relation $\lambda_1 = (+,+)$, $\lambda_2 = (+,-)$, $\lambda_3 = (-,+)$, $\lambda_3 = (-,-)$.

The conditions for the existence of real solution are as follows:

$$
\begin{aligned}
&\left(A_2\mathscr{L} + A_3 z - \frac{k}{T}\rho_0\right)^2 - \frac{4k\mathscr{L}}{T}(A_1 z - A_2)\rho_0 > 0,\\
&\left[\frac{k}{T}\rho_0 - A_3 z - A_2\mathscr{L} \pm \sqrt{\left[A_2\mathscr{L} + A_3 z - \frac{k}{T}\rho_0\right]^2 - \frac{4k\mathscr{L}}{T}(A_1 z - A_2)\rho_0}\right](A_1 z - A_2) > 0.
\end{aligned}
\tag{3.6}
$$

If these two conditions are fulfilled, we obtain four real characteristic speeds λ and the relating characteristic vectors which are linearly independent, so the system of equations is hyperbolic. In the elastic-plastic material governed by these equations there are four waves with real and symmetric velocities.

Let us discuss some particular cases of the characteristic speeds.

CASE 1

There is no thermomechanical coupling in the material

$$
\lambda_T^2 = \frac{k}{T\rho c_p},
\tag{3.7}
$$

(3.8) $$\lambda_m^2 = \frac{\mathscr{L}}{\rho_0}.$$

In this case we obtain two symmetric thermal waves and two symmetric mechanical waves with the speeds λ_T and λ_m which depend on the material constants. It is worth noting that when the relaxation time, which influences the speed of the thermal wave, is equal to zero (what means that the Maxwell–Cattaneo relation reduces to Fourier's law), the velocity of the propagation of thermal disturbance is infinite:

(3.9) $$T \longrightarrow 0 \Rightarrow \lambda_T^2 \longrightarrow \infty.$$

When the material has no thermomechanical coupling and is a non-conductor, and thus the coefficient of thermal conductivity k vanishes, then the speed of the thermal wave is equal to zero ($\lambda_T = 0$). In this case there is only a pure mechanical wave and the thermal wave does not exist, but there is a static curve (i.e., a point in a one-dimensional case) of thermal jump.

CASE 2 (adiabatic process)

We consider the adiabatic process with thermomechanical coupling. For this case there are only two symmetric coupled thermomechanical waves which propagate with the speed (called adiabatic):

(3.10) $$\lambda_a^2 = \frac{A_2\mathscr{L} + A_3 z}{\rho_0(A_2 - A_1 z)}.$$

4. Analysis of wave propagation — Lie derivative formulation

In the next step we analyze the system of equations with the covariance terms which appear after applying the Lie derivative. This derivative enables to obtain the invariance of the equations under arbitrary spatial diffeomorphism.

The one-dimensional form of the equations describing the thermomechanical process is the following:

(4.1)
$$\begin{aligned}
A_1\dot{\tau} + A_2\dot{\vartheta} - \frac{\partial q}{\partial x} + A_3\frac{\partial v}{\partial x} &= 0,\\
\dot{q} - q\frac{\partial v}{\partial x} + \frac{k}{T}\frac{\partial \vartheta}{\partial x} + \frac{1}{T}q &= 0,\\
\dot{\tau} + z\dot{\vartheta} - (2\tau + \mathscr{L})\frac{\partial v}{\partial x} &= 0,\\
\rho_0\dot{v} - \frac{\partial \tau}{\partial x} - \tau C &= 0.
\end{aligned}$$

In order to find characteristic speeds, characteristic vectors and to evaluate the conditions for their existence, we apply the same procedure as previously. Without going into details, we present the characteristic polynomial for the characteristic value λ:

$$(4.2)\quad (A_1 z - A_2)\rho_0\lambda^4 + \left[A_3 z + A_2(2\tau + \mathscr{L}) - \rho_0\frac{k}{T}\right]\lambda^2 + zq\lambda + \frac{k}{T}(2\tau + \mathscr{L}) = 0.$$

The solution of this algebraic equation was found by the perturbation procedure with the assumption that the process considered is close to the adiabatic state ($q = 0$). The general solution of Eq. (4.2) has the form

$$(4.3)\qquad \lambda_i = \lambda_i^0 + \varepsilon\lambda_i^l,$$

where $\varepsilon = q$, λ_i^0 is the solution of Eq. (4.2) in the case of the adiabatic process ($\varepsilon = q = 0$) and the form of it is as follows:

$$(4.4)\qquad \begin{aligned} \lambda_i^0 &= \pm\left[\frac{\left[\rho_0\frac{k}{T} - A_3 z - A_2(2\tau + \mathscr{L})\right] \pm \sqrt{\Delta}}{2(A_1 z - A_2)\rho_0}\right]^{\frac{1}{2}}, \\ \Delta &= \left[A_3 z + A_2(2\tau + \mathscr{L}) - \rho_0\frac{k}{T}\right]^2 - 4\rho_0\frac{k}{T}(2\tau + \mathscr{L})(A_1 z - A_2). \end{aligned}$$

The term λ_i^l is obtained from the ratio of the polynomials $G(\lambda)$ and $P'(\lambda)$ taken at the point λ_i^0 where

$$(4.5)\qquad \begin{aligned} P(\lambda) &= (A_1 z - A_2)\rho_0\lambda^4 + \left[A_3 z + A_2(2\tau + \mathscr{L}) - \frac{k\rho_0}{T}\right]\lambda^2 + (2\tau + \mathscr{L})\frac{k}{T}, \\ G(\lambda) &= z\lambda. \end{aligned}$$

The final form of the λ_i^l is as follows:

$$(4.6)\qquad \lambda_i^l = \frac{G(\lambda_i^0)}{P'(\lambda_i^0)} = \pm\frac{z}{2\sqrt{\Delta}}.$$

Using the expressions for λ_i^0 and λ_i^l, we obtain the general solution of the perturbed characteristic polynomial:

$$(4.7)\qquad \lambda_i = \pm\left\{\frac{\rho_0\frac{k}{T} - A_3 z - A_2(2\tau + \mathscr{L}) \pm \sqrt{\Delta}}{2(A_1 z - A_2)\rho_0}\right\}^{\frac{1}{2}} \pm \frac{qz}{2\sqrt{\Delta}}.$$

From the relation (4.7), it can be seen how the covariance terms in the system of equations influence the characteristic speeds. We obtained the additional term which depends on the heat flux q. The analysis of the obtained characteristic speeds made in the same cases as previously leads to the following results.

CASE 1

The thermomechanical couplings are neglected so there are still two symmetric mechanical waves and two non-symmetric thermal waves which propagate with the speeds

$$\lambda_m^2 = \frac{\mathscr{L}}{\rho_0} + \frac{2\tau}{\rho_0}, \tag{4.8}$$

$$\lambda_T = \pm\sqrt{\frac{k}{T\rho c_p}} + \frac{Tqz}{2\rho_0 k}. \tag{4.9}$$

For the relaxation time vanishing to 0, the velocity of thermal wave tends to infinity.

CASE 2 (adiabatic process)

The thermomechanical couplings exist but the conductivity of the material is equal to zero, so there are two symmetric coupled thermomechanical waves which propagate with the speeds

$$\lambda_a^2 = \frac{A_3 z + A_2(2\tau + \mathscr{L})}{\rho_0(A_2 - A_1 z)}. \tag{4.10}$$

5. Final comments

We have compared two descriptions of the thermodynamic behaviour of a plastic material. The first one is concerned with the case when all objective rates of stress, temperature, heat flux and velocity are defined by the material derivative. In the second description it is replaced by the Lie derivative. We wanted to find the answer to the question how the additional terms which appear in the equations after applying the Lie derivative influence the hyperbolicity conditions derived for the system of equations and the propagation of waves in the material. The differences between the results obtined for each description are very significant. Let us restrict their discussion for the case when the thermomechanical couplings are neglected. For the material description, the speed of the thermal wave depends on the quantities describing the thermal properties of the material such as relaxation time, specific heat and the coefficient of thermal conductivity. The speed of the mechanical wave depends on the material density and the constants describing the plastic properties of the material.

Application of the Lie derivative influences the speed of the mechanical as well as thermal wave. For the mechanical wave, we obtained the additional term which depends on the actual stress τ (see Eq. (4.8)). The wave is symetric. But the thermal wave, which has symmetry in the material description, is not symmetric in the Lie formulation. It has also the additional term which depends on the heat flux q.

The introduction of the Lie derivative generalizes the description of the thermomechanical process but we have to realize that it changes the structure of the equations, what gives finally different criteria for locatization.

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