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Duality, inverse problems and nonlinear problems in solid mechanics

On temperature in thermoelastoplasticity

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Abstract

Nowadays, the determination of temperature needs often to be treated in the framework of thermoplasticity or thermoviscoplasticity, for example, during metal forming, crashes, …

There are still many great difficulties. Some concern the numerical integration of the equations involved; we can say that they are solved reasonably well. Others are more fundamental, and concern the basic constitutive equations and the writing of the thermodynamical equations; they still belong to unsolved problems.

Recently, many papers have been published in this area (for ex. [P. Germain, E.H. Lee, in: A. Sawczuk (Ed.), Problems of Plasticity, Noorthoff Int. Publ., 1974. [14]] and [D. Rittel, Z.G. Wang, M. Merzer, Adiabatic shear failure and dynamic stored energy of cold work, Phys. Rev. Lett. 96 (7) (2006) 075502. [18]]); we have thought that it would be useful to discuss our old paper that appeared, in French, in the Journal Archives of Mechanics 26 (4) (1974) 701–715, and to underline what our contributions were at that time:

(i) on a possible definition of the homogenized temperature of an aggregate (polycrystals or composites);
(ii) on a possible interpretation of the occurrence of 'adiabatic bands' by considering only the influence of temperature, for ex. [A. Baltov, T. Vinh, C. R. Acad. Sci. Paris Sér. A 291 (1972) 275. [13]] and [D. Rittel, Z.G. Wang, M. Merzer, Adiabatic shear failure and dynamic stored energy of cold work, Phys. Rev. Lett. 96 (7) (2006) 075502. [18]].

For this, with the help of a physical microscopical model, we have explained where some energy could be stored in the aggregate, and we have shown that only in the case of elastic and thermal isotropy, were we able to defined its temperature T, as the mean of the local temperature θ, of its constituents.

Then we wrote the thermodynamical equations (assuming small perturbations) for various hypotheses: isothermic, adiabatic or general heat condition.

Finally, we analyzed a simple rod that is subjected to a quasi-static loading at a constant strain rate and then, when the rod is dynamically loaded as during the Taylor test i.e. during the impact of the rod on a rigid wall. We have shown that there is a non-constant ratio between the plastic power and the stored power and that there was no concentration (adiabatic band), while taking into account the influence of the temperature in the equations. ***To cite this article: W.K. Nowacki, J. Zarka, C. R. Mecanique 336 (2008).***

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Résumé

Sur la température en thermoélastoplasticité. Actuellement, il est souvent nécéssaire de déterminer le champ de la température dans une structure comme c'est le cas dans la mise en forme des métaux, le crash, etc.

On est alors confronté à de grandes difficultés : si les problèmes concernant la résolution numérique des équations peuvent être traités d'une manière raisonnable, d'autres, plus fondamentaux concernent les relations de comportement des matériaux dans le cadre de la thermoplasticité ou la thermoviscoplasticité ainsi que les équations de la thermodynamique, ne sont pas encore résolus.

Comme, il y a eu récemment de nombreuses publications dans ce domaine (par ex. [P. Germain, E.H. Lee, in: A. Sawczuk (Ed.), Problems of Plasticity, Noorthoff Int. Publ., 1974. [14]] et [D. Rittel, Z.G. Wang, M. Merzer, Adiabatic shear failure and dynamic stored energy of cold work, Phys. Rev. Lett. 96 (7) (2006) 075502. [18]]), nous souhaitons revenir sur notre ancien travail qui avait été publié en français dans le Journal Archives of Mechanics 26 (4) (1974) 701–715 et de souligner quelle avait été alors notre contribution :

(i) sur la définition possible de la température globale homogène d'un agrégat (un polycristal ou un matériau composite) ;
(ii) sur l'explication qui avait été donnée sur la formation des « bandes adiabatiques » en considérant seulement l'influence de la température, par ex. [A. Baltov, T. Vinh, C. R. Acad. Sci. Paris Sér. A 291 (1972) 275. [13]] et [D. Rittel, Z.G. Wang, M. Merzer, Adiabatic shear failure and dynamic stored energy of cold work, Phys. Rev. Lett. 96 (7) (2006) 075502. [18]].

Pour cela, à l'aide d'un modèle physique construit par une analyse microscopique, nous avons explicité comment l'énergie pouvait être emmagasinée dans un agrégat et nous avons montré que, seulement dans le cas de l'isotropie élastique et l'isotropie thermique, nous étions capables de définir sa température T comme la moyenne de la température locale θ, de ses composants.

En utilisant cette définition de la température, nous avions pu écrire les équations thermodynamiques (supposant les petites perturbations) en prenant successivement l'hypothèse isotherme ou adiabatique ou de conductivité générale.

Enfin, nous avions analysé le cas d'une barre simple soumise à un chargement quasistatique à vitesse de déformation constante, puis le cas d'une barre était chargée dynamiquement comme dans le test de Taylor, c'est-à-dire lors de l'impact d'une barre sur un mur rigide. Nous avions démontré qu'il n'y avait pas un rapport constant entre l'énergie plastique et l'énergie emmagasinée et qu'il n'y avait pas de concentration sous la forme de bande adiabatique malgré la prise en compte de la température dans les équations.

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Keywords: Thermoelastoplasticity; Stored energy; Shear bands

Mots-clés : Thermoelastoplasticité ; Énergie emmagasinée ; Bande adiabatique

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1. Introduction

It is a classical procedure to perform numerical simulations in thermoplasticity or thermoviscoplasticity. The temperature is just taken as it is and some assumptions are usually made:

1. When there is a great input of the external heat: it is considered that there is a decoupling between the temperature field and the deformation of the structure; indeed the transient or stationary heat equations are solved and then the (known) temperature maps at different times are dumped to the plastic/viscoplastic equations. In any point of the structure, the material properties are just taken as function of the actual temperature;
2. When there is no great input of external heat, the contribution of the external heat is 'weak':
   a. It is considered that the internal dissipation is insignificant and the transformation is isothermic (this implies that the equations of the thermodynamics are deleted).
   b. Or, if this dissipation has to be taken into account, in any point of the structure, the transformation is adiabatic (conduction/radiation is neglected) while considering that it occurs during a dynamic or a very fast loading and that a 'part' of this dissipation is kept in a stored energy, with a constant ratio between these two energies. Many authors have explained the outbreak of 'adiabatic' bands by this coupling between temperature increase and material properties.

The objectives of this article are double:

1. We shall write the thermodynamic equations and the constitutive relations for an aggregate and we shall underline some difficulties, especially in the definition of temperature and where some energy could be stored;
2. We shall show their applications to the particular example of a rod that is subjected to quasi-static and dynamical loadings when making the successive assumptions on the temperature exchanges.

2. Energies in an aggregate/polycrystal

2.1. Stored energy in the single crystal

General accounts of the thermomechanics of elastic/plastic materials can be found in the books by J. Mandel [1], J. Lubliner [2] and the review article by P. Germain et al. [3].

For a particular well-defined Representative Volume Element (RVE) of the single crystal, we have shown (cf. J. Zarka, [4]) that for an adiabatic transformation, the thermodynamic equation could be written as:

$$\sigma_{ij}\dot{\varepsilon}^p_{ij} = \rho\frac{\partial U_2}{\partial y}\dot{y} + \alpha_{ij}\theta\dot{\sigma}_{ij} + \rho c\dot{\theta} \tag{1}$$

where

$\boldsymbol{\sigma}, \sigma_{ij}$	–	stress tensor,
$\dot{\boldsymbol{\varepsilon}}^p, \dot{\varepsilon}^p_{ij}$	–	plastic strain tensor rate,
ρ	–	specific mass,
$U_2(\theta, \{y\})$	–	specific internal energy stored in the internal defects represented by $\{y\}$,
θ	–	absolute temperature of the single crystal,
α_{ij}	–	thermal dilatation tensor,
c	–	specific heat.

This equation was deduced through some assumptions on the thermoelastic strain rate $\dot{\boldsymbol{\varepsilon}}^{e+\theta}$ and plastic strain rate $\dot{\boldsymbol{\varepsilon}}^p$, and on the thermodynamic functions' internal energy, U and entropy $\mathcal{S}$:

(i) $$\dot{\boldsymbol{\varepsilon}}^{e+\theta} \equiv \Lambda_{ijkl}(\boldsymbol{\sigma}, \theta)\dot{\sigma}_{kl} + \alpha_{ij}(\boldsymbol{\sigma}, \theta)\dot{\theta} \tag{2}$$

with $\boldsymbol{\Lambda}$ and $\boldsymbol{\alpha}$ independent of $\{y\}$ and satisfying the integrability conditions:

$$\frac{\partial}{\partial\theta}\Lambda_{ijkl} = \frac{\partial\alpha_{ij}}{\partial\sigma_{kl}} \tag{3}$$

(ii) $$\begin{cases} \dot{\varepsilon}^p_{ij} \equiv \dot{\varepsilon}^p_{ij}(\boldsymbol{\sigma}, \theta, \{y\}) \\ \dot{y} \equiv \dot{y}(\boldsymbol{\sigma}, \theta, \{y\}) \end{cases} \tag{4}$$

The rates of the stress and the temperature do not take part in these equations (viscoplasticity)

(iii) $$\begin{cases} U \equiv U(\boldsymbol{\sigma}, \theta, \{y\}) \\ \mathcal{S} \equiv \mathcal{S}(\boldsymbol{\sigma}, \theta, \{y\}) \end{cases}$$

The application of the second principle of the thermodynamic (an always non-negative production of entropy) leads to:

(i) the separation

$$U \equiv U_1(\boldsymbol{\sigma}, \theta) + U_2\big(\theta, \{y\}\big), \qquad \mathcal{S} \equiv \mathcal{S}_1(\boldsymbol{\sigma}, \theta) + \mathcal{S}_2\big(\theta, \{y\}\big) \tag{5}$$

with

$$\sigma_{ij}\Lambda_{ijkl} = \rho\left(\frac{\partial U_1}{\partial\sigma_{kl}} - \theta\frac{\partial\mathcal{S}_1}{\partial\sigma_{kl}}\right), \qquad \sigma_{ij}\alpha_{ij} = \rho\left(\frac{\partial U_1}{\partial\theta} - \theta\frac{\partial\mathcal{S}_1}{\partial\theta}\right) \tag{6}$$

and

$$\frac{\partial U_2}{\partial\theta} = \theta\frac{\partial\mathcal{S}_2}{\partial\theta} \tag{7}$$

(ii) when assuming local adiabaticity, it remains only to satisfy

$$\frac{\sigma_{ij}\dot{\varepsilon}_{ij}}{\rho} \geqslant \left(\frac{\partial U_2}{\partial y} - \theta \frac{\partial \mathcal{S}_2}{\partial y}\right)\dot{y} \tag{8}$$

Eq. (6), while taking into account (3), imply

$$\frac{\partial \mathcal{S}_1}{\partial \sigma_{kl}} = \alpha_{kl} \tag{9}$$

The first principle gives locally:

$$\rho \dot{U} = \sigma_{ij}\dot{\varepsilon}_{ij} = \sigma_{ij}(\dot{\varepsilon}_{ij}^{e+\theta} + \dot{\varepsilon}_{ij}^{p}) \tag{10}$$

where, by definition, $\sigma_{ij}\dot{\varepsilon}_{ij} = \sigma_{ij}(\dot{\varepsilon}_{ij}^{e+\theta} + \dot{\varepsilon}_{ij}^{p})$ is the power of deformation and

$$c = \theta \frac{\partial \mathcal{S}}{\partial \theta} \tag{11}$$

Eq. (1) is thus deduced.

Indeed in our paper, J. Zarka [4], we characterized the exact physical meaning of the internal parameters $\{y\}$ and we gave the explicit form of all the functions: $\dot{\varepsilon}_{ij}^{p} \equiv \dot{\varepsilon}_{ij}^{p}(\boldsymbol{\sigma}, \theta, \{y\})$, $\dot{y} \equiv \dot{y}(\boldsymbol{\sigma}, \theta, \{y\})$, $U_2(\theta, \{y\})$.

The $\{y\}$ define the distribution of the crystalline defects essentially the dislocations and $U_2(\theta, \{y\})$ *is energy stored in the free energies of the dislocations*; *the interaction energies are negligible within the representative volume element*.

2.2. *Stored energies in the aggregate/polycrystal*

In metals, as well as rocks, at the global (macroscopic) scale the Representative Volume Element (RVE) is an aggregate of single crystals, or grains, separated by joint boundaries at the local (microscopic) scale.

Composite materials may be also be considered as an aggregate of fibres and matrices.

In principle, it may be possible (using powerful computers and fast algorithms) to integrate the local equations at the level of the single crystal, defects, ... But this is not very realistic.

Homogenisation is preferred, with some simplifying hypotheses: the Representative Volume Element contains many crystals and macroscopic quantities which are defined based on the corresponding microscopic ones (cf. the recent general book by S. Nemat-Nasser [5]).

2.2.1. *Isotherm transformation*

For such a transformation, and when some conditions of macro-homogeneity are satisfied, many authors, for example, J. Mandel [6], R. Hill [7], H.D. Bui [8], J. Rice [9], have shown for any statically admissible stress field and any cinematically admissible strain field, that it is possible to define:

(i) the macroscopic stress tensor by

$$\boldsymbol{\Sigma} \cong \frac{1}{V} \int_V \boldsymbol{\sigma} \, \mathrm{d}V \tag{12}$$

(ii) the macroscopic strain tensor by

$$\boldsymbol{E} \cong \frac{1}{V} \int_V \boldsymbol{\varepsilon} \, \mathrm{d}V \tag{13}$$

(iii) the macroscopic work of transformation by

$$\boldsymbol{\Sigma E} = \Sigma_{ij} E_{ij} \cong \frac{1}{V} \int_V (\boldsymbol{\sigma \varepsilon}) \, \mathrm{d}V = \frac{1}{V} \int \sigma_{ij} \varepsilon_{ij} \, \mathrm{d}V \tag{14}$$

These macroscopic fundamental quantities are the direct mean on the RVE.

2.2.1.1. Elastic behaviour. Firstly, let as consider that the RVE is purely elastic. By applying the global stress $\boldsymbol{\Sigma}^*$, and by solving the exact elastic boundary value problem, we get, in any point, the local microscopic stress:

$$\sigma^* = A\boldsymbol{\Sigma}^*, \qquad \sigma^*_{ij} = A_{ijkl}\Sigma^*_{kl} \tag{15}$$

where $\boldsymbol{A}$, the elastic stress localization factor is linked to the geometries, positions and the elastic coefficient matrices of the crystals/grains.

Moreover, the local microscopic strain tensor is given by:

$$\boldsymbol{\varepsilon}^* = \boldsymbol{\Lambda}\boldsymbol{\sigma}^* = \boldsymbol{\Lambda}\boldsymbol{A}\boldsymbol{\Sigma}^*$$

thus with (13)

$$\boldsymbol{E}^* = \frac{1}{V}\int_V \boldsymbol{\varepsilon}^*\,\mathrm{d}V = \frac{1}{V}\int_V \boldsymbol{\Lambda}\boldsymbol{A}\boldsymbol{\Sigma}^*\,\mathrm{d}V = \left(\frac{1}{V}\int_V \boldsymbol{\Lambda}\boldsymbol{A}\,\mathrm{d}V\right)\boldsymbol{\Sigma}^*$$

and thus, a global macroscopic elastic coefficient matrix $\boldsymbol{\Lambda}^\circ$ is defined by:

$$\boldsymbol{\Lambda}^\circ = \frac{1}{V}\int_V \boldsymbol{\Lambda}\boldsymbol{A}\,\mathrm{d}V \tag{16}$$

2.2.1.2. Elastoplastic behaviour. At the local scale we may separate the elastic and plastic parts of the strains:

$$\begin{array}{ll} \dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^e + \dot{\boldsymbol{\varepsilon}}^p & \text{with } \dot{\boldsymbol{\varepsilon}}^e = \boldsymbol{\Lambda}\dot{\boldsymbol{\sigma}} \\ \dot{\boldsymbol{E}} = \dot{\boldsymbol{E}}^e + \dot{\boldsymbol{E}}^p & \text{with } \dot{\boldsymbol{E}}^e \equiv \boldsymbol{\Lambda}^\circ\dot{\boldsymbol{\Sigma}} \end{array} \tag{17}$$

But generally, $\dot{\boldsymbol{E}}^e$ and $\dot{\boldsymbol{E}}^p$ are not the direct means of $\dot{\boldsymbol{\varepsilon}}^e$ and $\dot{\boldsymbol{\varepsilon}}^p$

(i) the authors quoted have shown:

$$\begin{array}{ll} \dot{\boldsymbol{E}}^e = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{A}^T\dot{\boldsymbol{\varepsilon}}^e\,\mathrm{d}V, & \dot{E}^e_{ij} = \dfrac{1}{V}\displaystyle\int_V A_{klij}\dot{\varepsilon}^e_{kl}\,\mathrm{d}V \\ \dot{E}^p = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{A}^T\dot{\boldsymbol{\varepsilon}}^p\,\mathrm{d}V & \end{array} \tag{18}$$

where $\boldsymbol{A}^T$ is the transpose of $\boldsymbol{A}$,

(ii) they have also shown for $\boldsymbol{\Sigma}\dot{\boldsymbol{E}}^p$

$$\boldsymbol{\Sigma}\dot{\boldsymbol{E}}^p = \frac{1}{V}\int_V \boldsymbol{\sigma}^r\boldsymbol{\Lambda}\dot{\boldsymbol{\sigma}}^r\,\mathrm{d}V + \frac{1}{V}\int_V \boldsymbol{\sigma}\dot{\boldsymbol{\varepsilon}}^p\,\mathrm{d}V \tag{19}$$

where

$$\begin{array}{ll} \boldsymbol{\sigma}^r = \boldsymbol{\sigma} - \boldsymbol{A}\boldsymbol{\Sigma} & \text{is the residual stress} \\ \dot{\boldsymbol{\sigma}}^r = \dot{\boldsymbol{\sigma}} - \boldsymbol{A}\dot{\boldsymbol{\Sigma}} & \text{(there is no term in } \dot{\boldsymbol{A}}\boldsymbol{\Sigma}) \end{array} \tag{20}$$

Thus they underlined in Eq. (19) that there is a part of the energy, similar to the stored energy in the dislocations, that is stored with the elastic interactions between the grains.

However, as the transformation is assumed isothermic, this separation between energies brings nothing, the thermodynamic equation has no use.

2.2.2. Adiabatic transformation

Now, we consider that the transformation is locally adiabatic; we just apply stresses or strains on the aggregate RVE.

2.2.2.1. Thermoelastic behaviour. Eq. (1) is reduced to

$$\alpha_{kl}\theta\dot{\sigma}^*_{kl} + \rho c\dot{\theta}^* = 0 \tag{21}$$

from which we deduce

$$\dot{\theta}^* = -\frac{\alpha_{kl}\theta}{\rho c}\dot{\sigma}_{kl} \tag{22}$$

and thus

$$\dot{\varepsilon}^{*e+\theta}_{ij} = \left(\Lambda_{ijkl} - \frac{\alpha_{ij}\alpha_{kl}\theta}{\rho c}\right)\dot{\sigma}^*_{kl} \equiv \Lambda'_{ijkl}(\boldsymbol{\sigma},\theta)\dot{\sigma}^*_{kl} \tag{23}$$

By assuming that the temperature change due to the loading is not too high, we find the same problem as in Section 2.2.1.1, the matrix $\boldsymbol{\Lambda}$ just being replaced with another constant matrix $\boldsymbol{\Lambda}'$.

This implies:

$$\boldsymbol{\sigma}^* \equiv \boldsymbol{A}'\boldsymbol{\Sigma}^* \tag{24}$$

where $\boldsymbol{A}'$ is the new elastic stress localization factor and

$$\boldsymbol{\Lambda}'^{\circ} \equiv \frac{1}{V}\int_V \boldsymbol{\Lambda}'\boldsymbol{A}'\,\mathrm{d}V$$

2.2.2.2. Thermoelastoviscoplastic behaviour. At the microscopical scale we write:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}^{e+\theta} + \dot{\boldsymbol{\varepsilon}}^{p}$$

$$\dot{\varepsilon}_{ij} = \dot{\varepsilon}^{e+\theta}_{ij} + \dot{\varepsilon}^{p}_{ij} = \Lambda_{ijkl}\dot{\sigma}_{kl} + \alpha_{ij}\dot{\theta} + \dot{\varepsilon}^{p}_{ij}$$

and we split the temperature change, $\dot{\theta}$:

$$\dot{\theta} = \dot{\theta}_1 + \dot{\theta}_2 \tag{25}$$

where $\dot{\theta}_1$ is given by (22).

We thus get:

$$\begin{aligned} &\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}'^{e} + \dot{\boldsymbol{\varepsilon}}'^{p}, \qquad \dot{\varepsilon}_{ij} = \Lambda'_{ijkl}\dot{\sigma}_{kl} + \alpha_{ij}\dot{\theta}_2 + \dot{\varepsilon}^{p}_{ij} \equiv \dot{\varepsilon}'^{e}_{ij} + \dot{\varepsilon}'^{p}_{ij} \\ &\dot{\boldsymbol{\varepsilon}}'^{e} = \boldsymbol{\Lambda}'\dot{\boldsymbol{\sigma}}, \qquad \dot{\boldsymbol{\varepsilon}}'^{p} = \boldsymbol{\alpha}\dot{\theta}_2 + \dot{\boldsymbol{\varepsilon}}^{p} \end{aligned} \tag{26}$$

as we have assumed an adiabatic transformation, $\dot{\boldsymbol{\varepsilon}}'^{p}$ is the true irreversible plastic strain.

The thermodynamic equation (1) is reduced to:

$$\sigma_{ij}\dot{\varepsilon}^{p}_{ij} = \rho\frac{\partial U_2}{\partial y}\dot{y} + \rho c\dot{\theta}_2 \tag{27}$$

At the global macroscopic scale, by following the same reasoning that leads to Eqs. (18) and (19), we get:

$$\dot{\boldsymbol{E}} = \dot{\boldsymbol{E}}'^{e} + \dot{\boldsymbol{E}}'^{p} \quad \text{and} \quad \dot{\boldsymbol{E}}'^{e} = \boldsymbol{\Lambda}'\dot{\boldsymbol{\Sigma}} \tag{28}$$

$$\text{(i)} \qquad \begin{cases} \dot{\boldsymbol{E}}'^{e} = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{A}'^{\top}\dot{\boldsymbol{\varepsilon}}'^{e}\,\mathrm{d}V \\ \dot{\boldsymbol{E}}'^{p} = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{A}'^{\top}\dot{\boldsymbol{\varepsilon}}'^{p}A'^{p}\,\mathrm{d}V \end{cases} \tag{29}$$

$$\text{(ii)} \qquad \begin{cases} \boldsymbol{\Sigma}\dot{\boldsymbol{E}}'^{p} = \dfrac{1}{V}\displaystyle\int_V \boldsymbol{\sigma}\dot{\boldsymbol{\varepsilon}}'^{p}\,\mathrm{d}V + \dfrac{1}{V}\displaystyle\int_V \boldsymbol{\sigma}'^{r}\boldsymbol{\Lambda}'\dot{\boldsymbol{\sigma}}'^{r}\,\mathrm{d}V \\ \boldsymbol{\sigma}'^{r} = \boldsymbol{\sigma} - \boldsymbol{A}'\boldsymbol{\Sigma}, \qquad \dot{\boldsymbol{\sigma}}'^{r} = \dot{\boldsymbol{\sigma}} - \boldsymbol{A}'\dot{\boldsymbol{\Sigma}} \end{cases} \tag{30}$$

$$\boldsymbol{\Sigma}\dot{\boldsymbol{E}}'^{p} = \frac{1}{V}\int_V \boldsymbol{\sigma}\dot{\boldsymbol{\varepsilon}}^{p}\,\mathrm{d}V + \frac{1}{V}\int_V \boldsymbol{\sigma}'^{r}\boldsymbol{\Lambda}'\dot{\boldsymbol{\sigma}}'^{r}\,\mathrm{d}V + \frac{1}{V}\int_V \boldsymbol{\sigma}\boldsymbol{\alpha}\dot{\theta}_2\,\mathrm{d}V \tag{31}$$

We can see easily how the macroscopic plastic dissipation is split during an adiabatic transformation. The stored energies are in three parts:

1. The first one corresponds to the stored energy in the crystalline defects (dislocations) in the grains.
2. The second one is linked to the elastic interactions between the grains.
3. The last one is due to the irreversible temperature θ_2.

We can also see that it is difficult to define the temperature and the thermodynamic functions of the macroscopic RVE.

It is impossible to assume that the macroscopic internal energy is the sum of the internal energies of its constituents (grains/crystals), as we need to consider their interaction energies. E. Kröner [10] expressed that for such a medium, the principle of local action is not satisfied; indeed we are in a non-local description of the modelling.

However, some new simplifying hypotheses may be proposed:

1. The macroscopic temperature, T, of the aggregate is the direct mean of the microscopic temperature, θ, of the grains/crystals.
2. Globally, we define for the macroscopic RVE, the functions $\mathcal{U}$ and $\mathcal{S}$ as dependent a priori on $\boldsymbol{\Sigma}$, T and $\{Y\}$, where $\{Y\}$ represent the entire local $\{y\}$, the local residual stresses, and the local temperatures.
   In this framework, if, moreover, we assume:
3. The grains/crystals are thermally and elastically isotropic.
4. The thermal and elastic coefficients and the specific heat are constant for all the grains/crystals (the temperature change always being small).

We get the elementary splitting:

$$\dot{\boldsymbol{E}} = \dot{\boldsymbol{E}}^e + \dot{\boldsymbol{E}}^T + \dot{\boldsymbol{E}}^p \tag{32}$$

$$\begin{aligned} \dot{\boldsymbol{E}}^e &= \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}^e \,\mathrm{d}V = \frac{1}{V}\int_V \boldsymbol{\Lambda}^\circ \dot{\boldsymbol{\sigma}} \,\mathrm{d}V = \boldsymbol{\Lambda}^\circ \dot{\boldsymbol{\Sigma}} \\ \dot{\boldsymbol{E}}^T &= \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}^\theta \,\mathrm{d}V = \frac{1}{V}\int_V \alpha\boldsymbol{\delta}\dot{\theta} \,\mathrm{d}V = \alpha\boldsymbol{\delta}\dot{T} \\ \dot{\boldsymbol{E}}^p &= \frac{1}{V}\int_V \dot{\boldsymbol{\varepsilon}}^p \,\mathrm{d}V \end{aligned} \tag{33}$$

($\boldsymbol{\alpha} = \alpha\boldsymbol{\delta}$, δ_{ij}—Kronecker symbol).

Eq. (31) is thus reduced to:

$$\boldsymbol{\Sigma}\dot{\boldsymbol{E}}^p = \frac{1}{V}\int_V \boldsymbol{\sigma}\dot{\boldsymbol{\varepsilon}}^p \,\mathrm{d}V \tag{34}$$

that implies that the interaction energies between the crystals are null (do not confuse $\dot{\boldsymbol{E}}'^p$ with $\dot{\boldsymbol{E}}^p$) and that the global thermodynamic equation may be written:

$$\boldsymbol{\Sigma}\dot{\boldsymbol{E}}^p \approx \rho\frac{\partial\mathcal{U}_2}{\partial Y}\dot{Y} + \alpha T\boldsymbol{\delta}\dot{\boldsymbol{\Sigma}} + \rho c\dot{T} \tag{35}$$

This last equation is obtained by taking the direct mean of Eq. (1).

We present these views on the stored energy to underline its characteristics and to show that it is difficult to assume that it might be equal to a constant ratio of the plastic dissipation ($\boldsymbol{\Sigma}\dot{\boldsymbol{E}}^p/R$ with $R \approx 10$), as assumed by some famous researchers (Taylor [19]).

Indeed, in the following section, we shall see an explicit model and a quantitative discussion of this ratio.

3. Temperature field obtained in an elastoplastic rod

Here, (Σ, E, T, Y) refer to a macroscopic (aggregate) Representative Volume Element.

3.1. Quasi-static loading

3.1.1. Modelling

In J. Zarka ([11] or [12]), we have proposed an one-dimensional model for the viscoplastic behaviour of the polycrystal.
We assumed that:

1. There is one parameter, X, to represent the internal state and that is linked to the mean distribution of the crystalline defects (X being selected as without any dimension).
2. The limit elastic thresholds are proportional to X.
3. The viscoplastic strain rate is a function of Σ, T, X.
4. The stored energy is proportional to X^2.

From these conditions, we could write:

$$\begin{aligned} &\dot{E}^p = f(\Sigma, T, X) \\ &\dot{X} = g(\Sigma, T, X) \\ &U_2 = AX^2 \quad \text{with } A = \text{const} \end{aligned} \tag{36}$$

Since in this article, we are rather concerned by the high velocities/strain rates (where creep can be neglected), we consider here only a special form of (36), where creep and softening are neglected, by taking

$$\begin{aligned} &\dot{E}^p = \frac{|S|}{S} C_1(T)\big\langle |S| - X\big\rangle X \\ &\dot{X} = C_2(T)\big\langle |S| - X\big\rangle X^{-\nu+1} \\ &u_2 = \frac{U_2}{E_o} = aX^2 \end{aligned} \tag{37}$$

with $C_1(T)$ and $C_2(T)$ two constants function of the temperature[1]:

$$\begin{aligned} &C_1(T) \approx \frac{A_1}{kT} \exp\left\{-\frac{V}{kT}\right\} \\ &C_2(T) \approx \frac{A_2}{kT} \exp\left\{-\frac{V}{kT}\right\} \end{aligned} \tag{38}$$

- $|S|$ is the absolute value of $S = \Sigma/E_o$, where E_o is the Young modulus,
- $\langle S - X\rangle$ is the positive part of $S - X = \begin{cases} 0 & \text{if } S - X \leqslant 0 \\ S - X & \text{if } S - X \geqslant 0 \end{cases}$
- ν, a, A_1, A_2, V, k are physical constants, characteristic of the material.

3.1.2. Loading

We assume that the rod is loaded at a high constant strain rate C for which the hypothesis of adiabaticity may be taken.

We have thus to solve

$$\begin{aligned} &\dot{S} + \alpha\dot{T} + \frac{|S|}{S} C_1(T)\big\langle |S| - X\big\rangle X = C, \qquad \dot{E} = \dot{E}^e + \dot{E}^T + \dot{E}^p \\ &\dot{X} = C_2(T)\big\langle |S| - X\big\rangle X^{-\nu+1} \\ &|S| C_1(T)\big\langle |S| - X\big\rangle X = 2aX\dot{X} + \alpha T\dot{S} + \rho c\frac{\dot{T}}{E_o} \end{aligned} \tag{39}$$

with, for $t = 0$,

$$S(0) = 0, \qquad X(0) = X_0, \qquad T(0) = T_0 \tag{40}$$

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[1] The viscoplastic strain rates are linked to the motions of the defects which are thermally activated.

The ratio R between the plastic power dissipation and the stored power energy is given by:

$$R \equiv \frac{|S| C_1(T) X^{\alpha-1}}{2aC_2(T)} \tag{41}$$

Now, let us consider an aluminium rod at room temperature, $T \approx T_0 \approx 300\,^{\circ}\mathrm{C}$ for which, we may take the special values:

$$\begin{array}{lll} E_o = 72\,000\ \mathrm{MPa}, & X_0 = 5 \times 10^{-4}, & \nu \approx 4 \\ C_1(T_0) \approx 4.13 \times 10^{9}\ \mathrm{s}^{-1}, & C_2(T_0) \approx 3.444 \times 10^{-6}\ \mathrm{s}^{-1} & \\ \rho = 2700\ \mathrm{kg\,m}^{-3}, & c \approx 9 \times 10^{10}\ \mathrm{m}^2\,\mathrm{s}^{-2}\,\mathrm{C}^{-1} & \\ V \approx 8kT_0\ (\approx 0.2\ \mathrm{e.v.}), & a \approx 36, & \alpha = 25 \times 10^{-6} \end{array} \tag{42}$$

have made several computations to analyze the influence of the various hypotheses:

1. All the plastic power dissipation is in the temperature change (a is thus taken equal to 0) in the last equation in (39).
2. There is a stored energy with $a = 36$.
3. There is a constant ratio $R = 10$ and thus the last equation of (39) is changed into

$$0.9|S| C_1(T) \langle |S| - X \rangle X = \alpha T \dot{S} + \rho c \frac{\dot{T}}{E_o} \tag{43}$$

We have also considered that the constants $C_1(T)$ and $C_2(T)$ are not functions of the temperature to see if the responses were changed.

3.1.3. Responses

3.1.3.1. 'Static' response. As long that the strain rate is lower than s^{-1} but higher than $10^{-4}\ \mathrm{s}^{-1}$ (no creep), we get:

(i) the 'static' curve (as defined by J. Lubliner [2]) for which we consider that $\dot{E} \approx 0$

$$E \approx S + \frac{C_1(T_0)}{C_2(T_0)(1+\nu)} \langle |S|^{1+\nu} - X_0^{1+\nu} \rangle \tag{44}$$

(ii) and the ratio R for $\dot{E} \approx 0$ is

$$R \approx \frac{C_1(T_0)}{2aC_2(T_0)} |S|^{\alpha} \quad \text{as } |S| \approx X \tag{45}$$

3.1.3.2. Responses for $C \approx 50\ \mathrm{s}^{-1}$ and $C \approx 500\ \mathrm{s}^{-1}$. The equations were integrated with the Treanor algorithm with a variable step.

We can see only very slight differences between the various curves on Figs. 2 and 3.

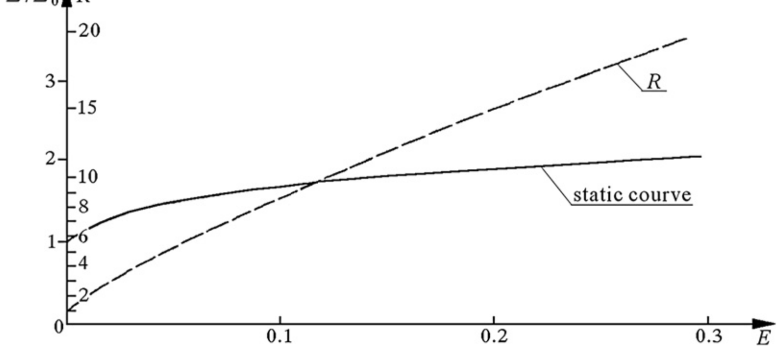

Fig. 1. Static curve and evolution of R with the deformation.

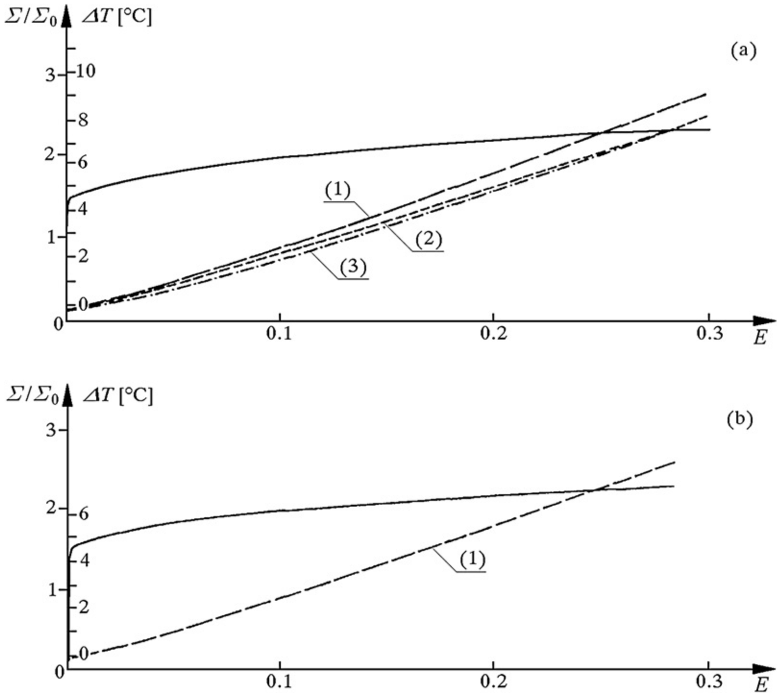

Fig. 2. Tensile curve and temperature change for $C = 50\,\mathrm{s}^{-1}$. Several hypothesis on C_1 and C_2 were successively taken: (a) independent of the temperature change, (b) linked to the temperature change, and: (1) no stored energy ($R = 0$) $\dot{U}_2 = 0$; (2) stored energy ($R = 10$) $\dot{U}_2 = 0.1\Sigma\dot{E}^p$; (3) stored energy according to Eq. (39) $\dot{U}_2 = aX\dot{X}$.

3.2. Dynamic loading

The behaviour of the material is still described by Eqs. (37), (38) and the values (42). But now, we are assuming that the loading is dynamic as during the impact on a rigid wall (Taylor's test). The rod has a length L and an initial velocity v_0, see for ex. [15], [16] or [17].

3.2.1. Equations

We have to solve the following system of differential equations:

(i) the dynamic equation

$$\frac{\partial\Sigma}{\partial x} = \rho\frac{\partial v}{\partial t} \tag{46}$$

(ii) the continuity equation

$$\frac{\partial E}{\partial t} = \frac{\partial v}{\partial x} \tag{47}$$

(iii) the constitutive equations

$$\begin{aligned} \frac{\partial E}{\partial t} &= \frac{1}{E_o}\frac{\partial\Sigma}{\partial t} + \alpha\frac{\partial T}{\partial t} + f(\Sigma, T, X) \\ \frac{\partial X}{\partial t} &= g(\Sigma, T, X) \end{aligned} \tag{48}$$

(iv) the thermodynamic equation

$$\Sigma f(\Sigma, T, X) = 2AX\frac{\partial X}{\partial t} + \alpha T\frac{\partial\Sigma}{\partial t} + \rho c\frac{\partial T}{\partial t} \tag{49}$$

where the unknown terms are Σ, v, E, X and T.

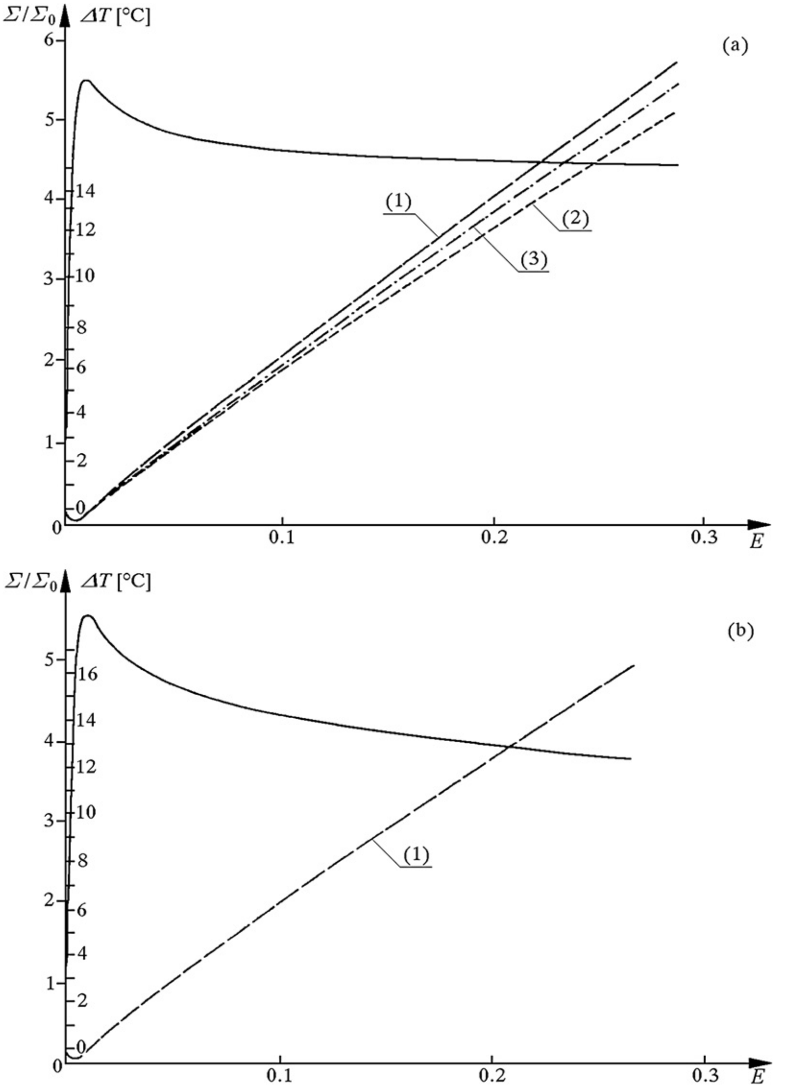

Fig. 3. Tensile curve and temperature change for $C = 500\,\mathrm{s}^{-1}$: (1) no stored energy ($R = 0$) $\dot{U}_2 = 0$; (2) stored energy ($R = 10$) $\dot{U}_2 = 0.1\Sigma\dot{E}^p$; (3) stored energy according to Eq. (39) $\dot{U}_2 = aX\dot{X}$.

The initial conditions for $t = 0^-$ are

$$\begin{aligned} &\Sigma(x,0) = 0, &&E(x,0) = 0\\ &X(x,0) = X_0, &&T(x,0) = T_0\\ &v(x,0) = v_0 \end{aligned} \tag{50}$$

and the boundary conditions are:

$$v(0,t) = 0 \text{ if } \Sigma(0,t) < 0 \quad \text{or} \quad \Sigma(0,t) = 0 \text{ for } x = 0 \quad \text{and} \quad \Sigma(L,t) = 0 \text{ for } x = L \tag{51}$$

To integrate numerically these equations, we used the nondimensional variables:

$$\begin{aligned} &\tilde{x} = \frac{x}{L}, &&\tilde{t} = \frac{a_0 t}{L}, &&\tilde{S} = \frac{S}{X_0}\\ &\tilde{X} = \frac{X}{X_0}, &&\tilde{T} = \alpha T, &&\tilde{V} = \frac{\rho a_0 v}{E_o X_0} \end{aligned} \tag{52}$$

where $a_0 = \sqrt{E_o/\rho}$ is the speed of the elastic waves.

We introduced the nondimensional parameters:

$$\begin{aligned} &\eta_1(T) = C_1(T) X_0^2 \frac{L}{a_0}, && \eta_2(T) = C_2(T) X_0^{1-\nu} \frac{L}{a_0} \\ &\eta_3 = 2a X_0^2, && B = \frac{\alpha X_0 E_o}{\rho c} \end{aligned} \tag{53}$$

The system of Eqs. (46) is hyperbolic; the characteristic lines are defined by:

$$\tilde{x} = \pm\tilde{t} + \text{const} \quad \text{and} \quad \tilde{x} = \text{const} \tag{54}$$

(i) We have along the characteristic lines $\tilde{x} = \pm\tilde{t} + \text{const}$ the relation

$$\mathrm{d}\tilde{S} \mp \mathrm{d}\tilde{V} + \eta_1(T) \frac{|\tilde{S}|}{\tilde{S}} \langle |\tilde{S}| - \tilde{X} \rangle \tilde{X} \, \mathrm{d}\tilde{t} = 0 \tag{55}$$

(ii) On the characteristic line $\tilde{x} = \text{const}$, we have:

$$\begin{aligned} &\mathrm{d}\tilde{X} = \eta_2(T) \langle |\tilde{S}| - \tilde{X} \rangle \tilde{X}^{1-\nu} \, \mathrm{d}\tilde{t} \\ &\tilde{T} \, \mathrm{d}\tilde{S} + \frac{\mathrm{d}\tilde{T}}{B} + \eta_3 \tilde{X} \, \mathrm{d}\tilde{X} = |\tilde{S}| \eta_1(T) \langle |\tilde{S}| - \tilde{X} \rangle \tilde{X} \, \mathrm{d}\tilde{t} \\ &\mathrm{d}E = \mathrm{d}\tilde{S} \, X_0 + \mathrm{d}\tilde{T} + \eta_1(T) + \frac{|\tilde{S}|}{\tilde{S}} \langle |\tilde{S}| - \tilde{X} \rangle \tilde{X} \, \mathrm{d}\tilde{t} \end{aligned} \tag{56}$$

The numerical resolution becomes easy. The integration with the Treanor's method is performed along the shock waves $\tilde{x} = \pm\tilde{t} + nL$.

3.2.2. Results

We considered the particular case of the rod with the length $L = 0.1$ m which reaches the wall at a velocity of 52 m s^{-1}.

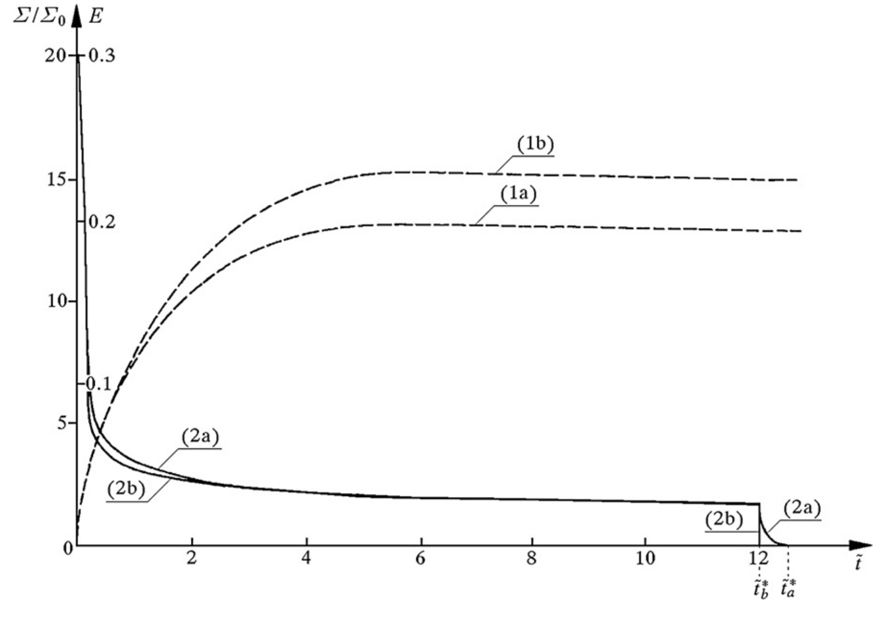

Fig. 4. Stress and strain on the first extremity: (1a) strain (1b) stress, no stored energy, the coefficients C_1 and C_2 are independent of the temperature change; (2a) strain (2b) stress: no stored energy, the coefficients C_1 and C_2 are function of the temperature change. $\tilde{t}_a$ is the contact time of the rod with the rigid wall.

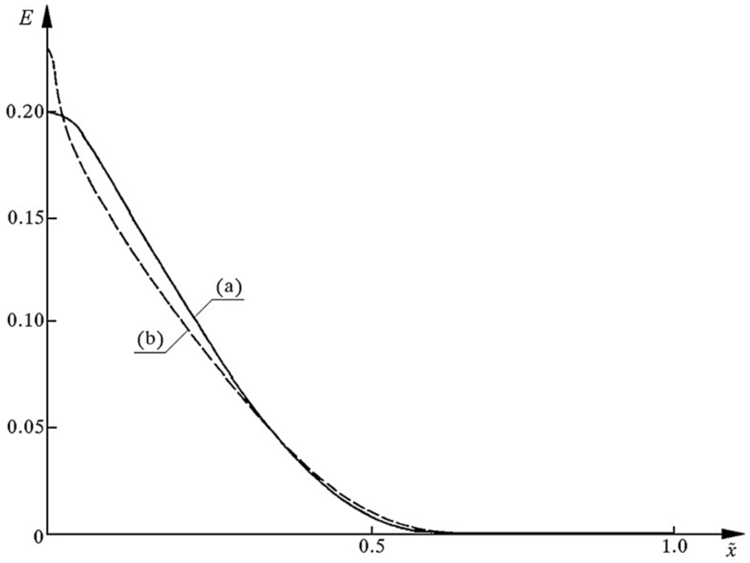

Fig. 5. Permanent strain along the rod; (a) the coefficients C_1 and C_2 are independent of the temperature change, (b) the coefficients C_1 and C_2 are function of the temperature change.

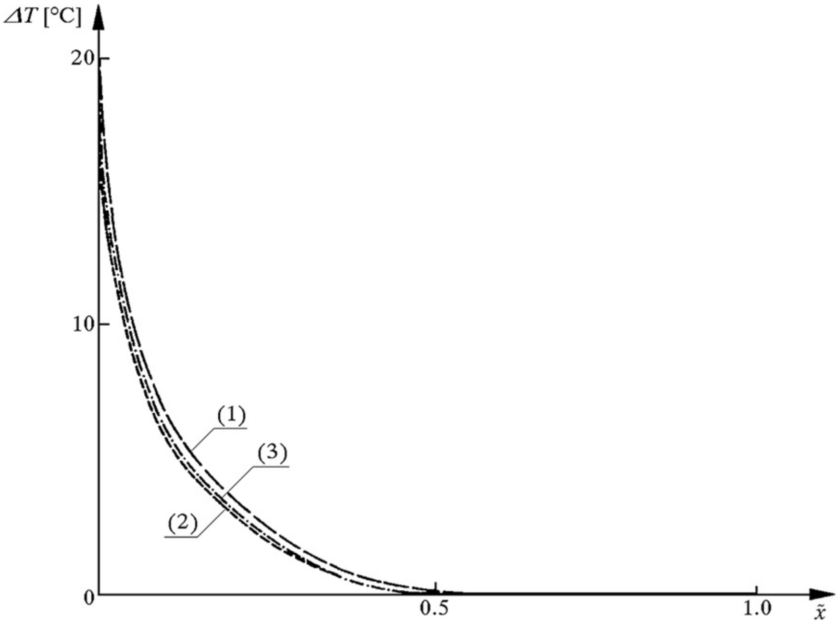

Fig. 6. Variation of the temperature along the rod the coefficients C_1 and C_2 are function of the temperature change; (1) no stored energy, (2) $\dot{U}_2 = 0.1\Sigma\dot{E}^p$, (3) $\dot{U}_2 = 2aX\dot{X}$.

In Figs. 4 to 6, we present the main results when

$$\begin{aligned} &\eta_1(T_0) = 0.02, \qquad &&\eta_2(T_0) = 0.5335 \\ &\eta_3 = 0.03, &&B = 3.704 \times 10^{-4} \end{aligned} \tag{57}$$

It is clear that we note only very slight differences according to the various hypotheses.

4. Conclusions

The results that are described in this article show clearly that:

- The definition of the temperature of an aggregate is not obvious.
- Considering several hypotheses on the constitutive modelling and the thermodynamic equation, only slight changes may be noticed. This implies that the influence of the temperature change is very weak.
- It is thus impossible to explain the instabilities (outbreak of the adiabatic bands and concentration of the strain in these bands) with only the coupling to the temperature.
- It is only useful to take into account the temperature change when there is an important external heat production (in the case of small transformations of course).

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