

Zentrum für Technomathematik Fachbereich 3 – Mathematik und Informatik

A Note on Finite Thermoplasticity with Phase Changes

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Report 02-04

Berichte aus der Technomathematik

Report 02-04 Juli 2002

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1 Introduction

The common approach in most theories of plasticity is based on the concept of intermediate configurations. It postulates the existence of a so called unloaded placement (configuration) and the decomposition of deformations into elastic and plastic parts, cf. [Sed70], [Hau77], [Hil89], [HR99], [Hau00] e.g.. However there are disadvantages of such theories mentioned by some authors, such as: Rotations of such unloaded placements remain undetermined or arbitrary. Therefore some problems related to objectivity arise (see [Ber02], p.2 and the papers quoted there). Another approach, based on the concept of elastic ranges and material isomorphisms [Nol72], has been proposed in [Ber92], [Ber98], which does not use the concept of unloaded configurations and decomposition of deformations. This approach is free of the shortcomings mentioned before. To model thermoplasticity the notion of isomorphic thermoelastic ranges has been introduced by A. Bertram (see also [Nol72], p.48). A modified version of this theory can be found in [Ber02].

It is known that in some processes under certain thermal conditions there are additional deformations due to phase changes in the material under consideration. A typical situation is quenching of steel. Such phase changes occur not only in ferrous alloys but also in other materials. These changes and hence the deformations can be reversible as well as irreversible, but they have another nature as the usual elastic or plastic deformation. To deal with such processes the notion of Transformation-induced Plasticity (or TRIP for brevity) has been introduced, see [FST96] for definitions and discussions on this subject, we refer also to the book by W. Mitter [Mit87] for experimental data of phase changes and for some analytical considerations. There are a lot of micromechanical and phenomenological models (specially for martensitic phase transformations) which have been proposed in last decades by different authors, see e.g. [FS95], [Lev98], [CBL00] and papers quoted there. A

model of this phenomenon under elasto-plastic deformation based on the concept of intermediate configurations can be found in [WB01]. To model both plastic and phase-change induced deformations, in [WB01] two intermediate configurations have been introduced.

Following Bertram we are going to introduce a model of thermoplasticity allowing for TRIP. For this purpose we will introduce the notion of thermoelastic range with phase changes. We call it *thermo-phase-elastic range*.

2 Preliminaries and definitions

2.1 Dependent and independent variables

In this subsection we specify the primary variables. To be independent from the observer we will keep all considerations in Lagrangean coordinates. Hence all equations and variables are invariant under rigid motions of the material body. The reference placement is supposed to be (arbitrarily) chosen once. Thus our setting is reference-free.

We suppose that the process is governed by deformations. Hence we choose the right Cauchy-Green strain tensor $C = F^T F$ as independent variable. F is the deformation gradient. Recall that $C = F^T F$ characterizes the local deformations of material points and that it is symmetric by definition. Further independent variables are the temperature θ and $q := \nabla \theta$. Since we assume that phase changes might occur during the deformation, i.e. in a thermo-phase-kinematical process, we have to introduce some parameters describing phase changes. There are a lot of different parameters used in the literature for this purpose such as volume fractions of phases $\xi = \frac{V_{\xi}}{V}$, V_{ξ} is the volume of the product phase in a control volume V, (see e.g. [FST96]). Note that ξ may change even in case of a pure elastic deformation process if the elastic moduli are different in parent and product phases. Another possible parameter is the internal dimensionless time $\xi = \frac{|\varepsilon_t|}{|\varepsilon_t^{\text{max}}|} \in [0, 1]$, where ε_t is the TRIP deformation tensor (see e.g. [Lev98]). As it was proved by Levitas the standard thermodynamic approach cannot be applied because of the local stress fluctuations due to the phase changes, which should be filtered by the time averaging of the of the thermodynamic parameters responsible for the phase changes over the duration of the phase change. We prefer to use mass fractions, because they are invariant under pure elastic and plastic deformations. So we introduce the following variables

$$Y = (Y_1, ..., Y_m)$$
 with $\sum_{i=1}^m Y_i = 1, Y_i \ge 0, i = 1, ..., m.$

Y describes the mass fractions of the relevant components, such as austenite, pearlite or martensite in the case of steel. We refer to Y as internal variables. Note that Y is a collection of scalar parameters which is not to be treated as a vector. The evolution of the internal variables is supposed to satisfy an ordinary differential equation of first order.

$$Y^{\bullet} = \beta(C, \theta, g, Y), \tag{2.1}$$

where ($^{\bullet}$) denotes time derivative. β is a given function for a given material. Time t is always nonnegative and time dependent (deformation-, phase change- and other) processes are considered on finite time intervals.

Let $S = JF^{-1}TF^{-T}$ be the symmetric second Piola-Kirchhoff stress tensor, where J = det(F) and T is the Cauchy stress tensor. Let $q = JF^{-1}q_E$ be the material heat flux, where q_E is the corresponding heat flux in Eulerian coordinates. Let e and η be the internal free energy and entropy, resp.

At the end of a given thermo-phase-kinematical process, say at time t > 0, these quantities should be determined. Therefore they are considered as dependent variables. Summarizing this setting, we have the following constitutive equations

$$S(C, \theta, g, Y)(t) = F^{S}\{C, \theta, g, Y\}_{0}^{t},$$

$$q(C, \theta, g, Y)(t) = F^{q}\{C, \theta, g, Y\}_{0}^{t},$$

$$e(C, \theta, g, Y)(t) = F^{e}\{C, \theta, g, Y\}_{0}^{t},$$

$$\eta(C, \theta, g, Y)(t) = F^{\eta}\{C, \theta, g, Y\}_{0}^{t},$$
(2.2)

where F^S , F^q , F^e , F^η are (in general) functionals taking the history of the whole process into account.

The set of S, q, e, η is called a *caloro-dynamical state* of the process. All variables are supposed to be differentiable up to the order necessary for the following considerations.

2.2 Material isomorphisms and symmetries

The notion of material isomorphisms has been introduced by W. Noll, cf. [Nol58], §11 or [Nol72], §9. In our context it reads as follows: Let X_1 and X_2 be two material points of the same body and let functionals $\mathsf{F}^S_{X_1,X_2}$, $\mathsf{F}^q_{X_1,X_2}$, $\mathsf{F}^e_{X_1,X_2}$, describe the caloro-dynamical state of the body at the points X_1 and X_2 , respectively, as in (2.2).

Definition 2.1. If there exists a linear invertible mapping P and two real constants e_c , η_c such that

$$\begin{split} S_{X_2}(C,\theta,g,Y) &= \det(P^{-1})PS_{X_1}(P^TCP,\theta,P^Tg,Y)P^T, \\ q_{X_2}(C,\theta,g,Y) &= \det(P^{-1})Pq_{X_1}(P^TCP,\theta,P^Tg,Y), \\ e_{X_2}(C,\theta,g,Y) &= e_{X_1}(P^TCP,\theta,P^Tg,Y) + e_c, \\ \eta_{X_2}(C,\theta,g,Y) &= \eta_{X_1}(P^TCP,\theta,P^Tg,Y) + \eta_c, \end{split} \tag{2.3}$$

hold for all thermo-phase-kinematical states, then X_1 and X_2 are called isomorphic and P is called material isomorphism.

The purpose of this definition is to clarify what it means that two points X_1 and X_2 consist of the same material. In the sequel we assume that we deal with a material body whose points are materially isomorphic, i.e., the body is homogeneous.

Following Noll (see [Nol72], §10) we introduce the symmetry group of a material point X as follows: Choose $X_2 = X_1$ in Definition 2.1. Then P in (2.3) is called a material automorphism or a symmetry transformation at the point X. The equations (2.3) are obviously satisfied if we choose P as identity, i.e., P = I and $e_c = 0$, $\eta_c = 0$. It could be that not only the identity satisfies (2.3). The collection of all such symmetries is called the symmetry group of the material. In particular, a material point is called isotropic, if its symmetry group coincides with the group of all orthogonal transformations. We quote a theorem from [Ber92], which lists some relations between symmetries and material isomorphisms.

Theorem 2.1. (i) Let P be a material isomorphism between two material points and G_1 the symmetry group of the first point. Then PG_1P^{-1} is the symmetry group of the second one.

- (ii) If P is a material isomorphism between two material points with symmetry groups G_0 and G_p , respectively, then A_pPA_0 is a material isomorphism between these points for all $A_0 \in G_0$ and $A_p \in G_p$.
- (iii) Let P and \tilde{P} be material isomorphisms between two material points with symmetry groups G_0 and G_p , respectively, then $P\tilde{P}^{-1} \in G_p$ and $P^{-1}\tilde{P} \in G_0$.

2.3 Thermo-phase-elastic ranges and assumptions

Adapting an idea of Bertram (see for example [Ber98]), we introduce the concept of thermo-phase-elastic ranges.

Definition 2.2. A thermo-phase-elastic range consists of a quintuple $\{E_p, S_p, q_p, e_p, \eta_p\}$, such that

- (i) E_p is a path-connected subset of the space of all independent and internal variables (C, θ, g, Y) which is supposed to form a differentiable manifold with boundary $\partial \mathsf{E}_p$,
- (ii) there is a set of material functions F^S , F^q , F^e , F^η (see comment below), which is continuously differentiable on E_p and which can be extended onto the whole space of independent variables such that the extension is still continuously differentiable.

The boundary of E_p is called the yield limit or yield surface. We formulate the following

Assumption 2.1. (Existence of thermoelastic ranges) For any thermo-kinematical process with phase changes $\{C(t), \theta(t), g(t), Y(t)\}, t \in [0, T],$ there exists a thermo-phase-elastic range $\{\mathsf{E}_p, S_p, q_p, e_p, \eta_p\}$ such that

- (i) its final value $\{C(T), \theta(T), g(T), p(T)\}\$ is in E_p and
- (ii) for any continuation of this process which is entirely in E_p , the caloro-dynamical state at its end is determined by the elastic laws (corresponding to the elastic range E_p) F_p^S , F_p^q , F_p^e , F_p^q by its final value

$$S = \mathsf{F}_{p}^{S}(C, \theta, g, Y),$$

$$q = \mathsf{F}_{p}^{q}(C, \theta, g, Y),$$

$$e = \mathsf{F}_{p}^{e}(C, \theta, g, Y),$$

$$\eta = \mathsf{F}_{p}^{\eta}(C, \theta, g, Y).$$

$$(2.4)$$

It seems to be a common understanding that the vast majority of solid material has some elastic range which might be very small or not. Therefore this assumption is not very restrictive. The second one below is stronger. It assumes that mechanical properties of the material under consideration do not change under any inelastic deformations.

Assumption 2.2. (Isomorphy of thermo-phase-elastic ranges) Let $\{E_0, S_0, q_0, e_0, \eta_0\}$ and $\{E_p, S_p, q_p, e_p, \eta_p\}$ be two thermo-phase-elastic ranges of the same material point. Then the constitutive elastic functionals are isomorphic,

i.e., there exists a material isomorphism P such that

$$S(C, \theta, g, Y) = PF_0^S(P^TCP, \theta, P^Tg, Y)P^T,$$

$$q(C, \theta, g, Y) = PF_0^q(P^TCP, \theta, P^Tg, Y),$$

$$e(C, \theta, g, Y) = F_0^e(P^TCP, \theta, P^Tg, Y) + e_c,$$

$$\eta(C, \theta, g, Y) = F_0^\eta(P^TCP, \theta, P^Tg, Y) + \eta_c$$
(2.5)

hold for all thermo-phase-kinematical states $\{C, \theta, g, Y\}$. Note, that we have dropped any index referring to a material point.

Some comments: As long as the thermo-phase-kinematical process belongs to the current elastic range E_p , the set of elastic laws (2.4) are the one-to-one relations between dependent and independent variables (and hence functionals in (2.4) and (2.5) become functions). But as soon as the process leads to a penetration of the yield surface $\partial \mathsf{E}_p$, the functions describing the thermo-phase-elastic laws change. This change can be described by the time-dependent variable P. With its help we can reduce the whole lot of elastic laws in different elastic ranges to the set of initial elastic laws $\mathsf{F}_0^s, \mathsf{F}_0^q, \mathsf{F}_0^p, \mathsf{F}_0^n, \mathsf{F}_0^n$

3 Description of the model

3.1 Yield criterion

As usual, in order to describe the set E_p and its evolution during yielding we use an indicator function ϕ . ϕ is called the yield criterion. It assigns to each deformed state some real number being zero on the boundary $\partial \mathsf{E}_p$ of the elastic range E_p , negative in its interior and positive otherwise. It is supposed to be independent of the temperature gradient g. We collect all additional variables (which describe such features as hardening, e.g.) in a vector H and include H as a parameter in ϕ . H is supposed to belong to some finite dimensional linear space. The yield criterion

$$\phi = \phi(C, \theta, P, Y, H) \tag{3.1}$$

is assumed to be continuously differentiable with respect to all its arguments. We say that yielding occurs if and only if the deformation process does not only reach the yield limit but also penetrates it, i.e., if both

$$\phi(C, \theta, P, Y, H) = 0 \qquad \text{(yield condition)} \tag{3.2}$$

and

$$\frac{\partial \phi}{\partial C} C^{\bullet} + \frac{\partial \phi}{\partial \theta} \theta^{\bullet} + \frac{\partial \phi}{\partial Y} Y^{\bullet} > 0 \qquad \text{(loading condition)} \tag{3.3}$$

hold.

Note that loading does not necessarily mean the increase of stress, as it is defined in the space of deformations. In our context loading can also mean phase change or change of temperature. If both yielding and loading conditions simultaneously hold at some point X, then its elastic range changes. We assume that this change can be described by appropriate evolution equations for P and H:

$$P^{\bullet} = p(P, C, \theta, g, Y, H, C^{\bullet}, \theta^{\bullet}) \quad \text{flow rule}$$
 (3.4)

$$H^{\bullet} = h(P, C, \theta, g, Y, H, C^{\bullet}, \theta^{\bullet})$$
 hardening rule (3.5)

Note that P and H remain constant if the process remains in the same elastic range and that they change if yielding occurs, i.e., both (3.2) and (3.3) hold. For simplicity we consider only quasistatic processes, i.e. the functional description of the caloro-dynamical state is rate independent. In this case the functions p and h must be homogeneous of first degree in C^{\bullet} and θ^{\bullet} . Therefore the last two equations can be rewritten as

$$P^{\bullet} = \lambda P^{\circ} = \lambda p^{\circ}(P, C, \theta, g, Y, H, C^{\bullet}, \theta^{\bullet}), \tag{3.6}$$

$$H^{\bullet} = \lambda H^{\circ} = \lambda h^{\circ}(P, C, \theta, g, Y, H, C^{\bullet}, \theta^{\bullet}), \tag{3.7}$$

where $C^{\circ} = \frac{C^{\bullet}}{|C^{\bullet}|}$ and $\theta^{\circ} = \frac{\theta^{\bullet}}{|\theta^{\bullet}|}$ show the direction of the corresponding increments and p° , h° denote the restrictions of p and h, respectively, to the normalized increments of deformation and temperature.

The positive plastic parameter λ can be determined from the condition that the deformation state belongs to the yield surface during yielding:

$$0 = \phi^{\bullet}(C, \theta, Y, P, H)$$

$$= \frac{\partial \phi}{\partial C} \cdot C^{\bullet} + \frac{\partial \phi}{\partial \theta} \theta^{\bullet} + \frac{\partial \phi}{\partial Y} \cdot Y^{\bullet} + \frac{\partial \phi}{\partial P} \cdot P^{\bullet} + \frac{\partial \phi}{\partial H} \cdot H^{\bullet}$$

$$= \frac{\partial \phi}{\partial C} \cdot C^{\bullet} + \frac{\partial \phi}{\partial \theta} \theta^{\bullet} + \frac{\partial \phi}{\partial Y} \cdot Y^{\bullet} + \frac{\partial \phi}{\partial P} \cdot \lambda P^{\circ} + \frac{\partial \phi}{\partial H} \cdot \lambda H^{\circ} = k - \lambda \alpha,$$
(3.8)

where $\alpha = -\frac{\partial \phi}{\partial P} \cdot \lambda P^{\circ} - \frac{\partial \phi}{\partial H} \cdot \lambda H^{\circ}$.

3.2 Consequences from the second law of thermodynamics

In this section we derive some restrictions from the thermodynamic postulates. For this purpose we introduce the Helmholtz free energy by means of the Legendre transformation $\psi = e - \eta\theta$, for which we set

$$\psi_0(P^T C P, \theta, P^T g, Y) = e_0(P^T C P, \theta, P^T g, Y) - \theta \eta_0(P^T C P, \theta, P^T g, Y)$$
(3.9)

and

$$\psi_c(P, H) = e_c(P, H) \tag{3.10}$$

so that during yielding the following holds

$$\psi_p(C, \theta, g, Y) = \psi_0(P^T C P, \theta, P^T g, Y) + \psi_c(P, H) - \eta_c(P, H).$$
 (3.11)

From the second law of thermodynamics it follows that the dissipation inequality

$$\psi^{\bullet} + \eta \theta^{\bullet} + \frac{1}{\theta} q \nabla \theta - \frac{1}{2} \rho_0^{-1} S_p \cdot C^{\bullet} \le 0$$
 (3.12)

holds for all admissible thermodynamical processes. For the rate of the free energy we obtain

$$\begin{split} \boldsymbol{\psi}^{\bullet} &= \boldsymbol{\psi}_{0}^{\bullet}(P^{T}CP, \boldsymbol{\theta}, P^{T}g, Y) + \boldsymbol{\psi}_{c}^{\bullet}(P, H) - \boldsymbol{\theta}^{\bullet}\eta_{c}(P, H) - \boldsymbol{\theta}\,\eta_{c}^{\bullet}(P, H) \\ &= \frac{\partial \psi_{0}}{\partial C} \cdot (P^{T}CP)^{\bullet} + \frac{\partial \psi_{0}}{\partial \boldsymbol{\theta}}\,\boldsymbol{\theta}^{\bullet} + \frac{\partial \psi_{0}}{\partial g} \cdot (P^{T}g)^{\bullet} + \frac{\psi_{0}}{\partial Y} \cdot Y^{\bullet} + \frac{\partial \psi_{c}}{\partial P} \cdot P^{\bullet} \\ &+ \frac{\partial \psi_{c}}{\partial H} \cdot H^{\bullet} - \boldsymbol{\theta}^{\bullet}\eta_{c}(P, H) - \boldsymbol{\theta}\left(\frac{\partial \eta_{c}}{\partial P} \cdot P^{\bullet} + \frac{\partial \eta_{c}}{\partial H} \cdot H^{\bullet}\right) \\ &= P\frac{\partial \psi_{0}}{\partial C}P^{T} \cdot C^{\bullet} + \frac{\partial \psi_{0}}{\partial \boldsymbol{\theta}}\,\boldsymbol{\theta}^{\bullet} + P\frac{\partial \psi_{0}}{\partial g} \cdot g^{\bullet} + \frac{\partial \psi_{0}}{\partial Y} \cdot Y^{\bullet} - \boldsymbol{\theta}^{\bullet}\eta_{c}(P, H) \\ &+ \left(2CP\frac{\partial \psi_{0}}{\partial C} + g \otimes \frac{\partial \psi_{0}}{\partial g} + \frac{\partial \psi_{c}}{\partial P} - \boldsymbol{\theta}\frac{\partial \eta_{c}}{\partial P}\right) \cdot \lambda P^{\circ} + \left(\frac{\partial \psi_{c}}{\partial H} - \boldsymbol{\theta}\frac{\partial \eta_{c}}{\partial H}\right) \cdot \lambda H^{\circ} \end{split}$$

For the stress power we have the following expression

$$\frac{1}{2}\rho_0^{-1}S_p(C,\theta,g,Y)\cdot C^{\bullet} = \frac{1}{2}\rho_0^{-1}\det(P^{-1})PS_0(P^TCP,\theta,P^Tg,Y)P^T\cdot C^{\bullet}$$
(3.13)

Substituting these expressions into the dissipation inequality (3.12) we obtain

$$0 \geq -\frac{1}{2}\rho_{0}^{-1}S \cdot C^{\bullet} + q_{p}(C,\theta,g,Y) \cdot \frac{g}{\rho_{0}\theta} + \psi_{p}^{\bullet}(C,\theta,g,Y) + \eta_{p}(C,\theta,g,Y)\theta^{\bullet}$$

$$= -\frac{1}{2}\rho_{0}^{-1}\det(P^{-1})PS_{0}(P^{T}CP,\theta,P^{T}g,Y)P^{T} \cdot C^{\bullet} + P\frac{\partial\psi_{0}}{\partial C}P^{T} \cdot C^{\bullet}$$

$$+ \frac{g}{\rho_{0}\theta} \cdot \det(P^{-1})Pq_{0}(P^{T}CP,\theta,P^{T}g,Y) + \frac{\partial\psi_{0}}{\partial \theta}\theta^{\bullet} + P\frac{\partial\psi_{0}}{\partial g} \cdot g^{\bullet} \quad (3.14)$$

$$+ \eta_{0}(P^{T}CP,\theta,P^{T}g,Y)\theta^{\bullet} + \frac{\partial\psi_{0}}{\partial Y} \cdot Y^{\bullet}$$

$$+ \left(2CP\frac{\partial\psi_{0}}{\partial C} + g \otimes \frac{\partial\psi_{0}}{\partial g} + \frac{\partial\psi_{c}}{\partial P} - \theta\frac{\partial\eta_{c}}{\partial P}\right) \cdot \lambda P^{\circ} + \left(\frac{\partial\psi_{c}}{\partial H} - \theta\frac{\partial\eta_{c}}{\partial H}\right) \cdot \lambda H^{\circ}$$

This inequality holds for all C^{\bullet} , θ , θ^{\bullet} , g, g^{\bullet} , Y^{\bullet} . It follows that for any thermokinematical processes we have

Theorem 3.1. (i) The Helmholtz free energy does not depend on the temperature gradient g.

(ii) The Gibbs relations

$$S_0 = 2\rho_0 P \frac{\partial \psi_0}{\partial C} P^T, \tag{3.15}$$

$$\eta_0 = -\frac{\partial \psi_0}{\partial \theta}.\tag{3.16}$$

hold.

(iii) The heat-conduction inequality

$$q \cdot g \le 0. \tag{3.17}$$

holds.

(iv) For the thermodynamic forces $\phi_i = -\frac{\partial \psi_0}{\partial Y_i}$, $1 \leq i \leq m$, the following inequality

$$\sum_{i=1}^{m} \phi_i \cdot Y_i \ge 0, \tag{3.18}$$

holds, i.e the dissipation rate due to the thermodynamical forces is nonnegative.

(v) During yielding the following residual inequality must be also fulfilled:

$$- \rho_0^{-1} C S p^{-T} \cdot P^{\bullet} + \left(\frac{\partial \psi_c}{\partial P} (P, H) - \theta \frac{\partial \eta_c}{\partial P} (P, H) \right) \cdot P^{\bullet}$$

$$+ \left(\frac{\partial \psi_c}{\partial H} (P, H) - \theta \frac{\partial \eta_c}{\partial H} (P, H) \right) \cdot H^{\bullet} \le 0.$$
(3.19)

3.3 Constitutive functions

We conclude our considerations by summarizing the complete set of constituent functions for the thermo-elasto-plastic material with phase changes:

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the referential law for the heat flux q_0(C, \theta, g, Y) the rule for the phase changes \beta(C, \theta, g, Y) the free energies \psi_0(C, \theta) and \psi_c(P, H) - \theta \eta_c(P, H) the yield criterion \phi(C, \theta, P, H) the rule for the flow direction p^{\circ}(P, C\theta, g, H, C^{\circ}, \theta^{\circ}) the rule for the hardening direction h^{\circ}(P, C, \theta, g, H, C^{\circ}, \theta^{\circ})
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which should be known for a given material. This finishes the formulation of the model.

4 Conclusions

The phenomenological model described above is a generalization of the finite thermoplastisity theory of Bertram for the deformation processes with phase changes. Mass fractions of the phases were used to keep the objectivity of the model. Rate-independence has also been assumed. A generalization to the rate-dependent case can be done as in [Ber02], the relation of this approach to the classical theories based on the concept of the unloaded configuration can be found in [Ber98].

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Berichte aus der Technomathematik

ISSN 1435-7968

http://www.math.uni-bremen.de/zetem/berichte.html

— Vertrieb durch den Autor —

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