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► **To cite this version:**

Olivier Maisonneuve, Stéphane Pagano, Pierre Alart, Frédéric Lebon. Evolution of phases in a shape memory alloy by local and global minimisations of a non convex potentials. IUTAM Symposium on Variations of Domain and Free-Boundary Problems in Solid Mechanics, 1999, Paris, France. pp.9-16, 10.1007/978-94-011-4738-5_2 . hal-01832737

HAL Id: hal-01832737

<https://hal.science/hal-01832737>

Submitted on 8 Jul 2018

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EVOLUTION OF PHASES IN A SHAPE MEMORY ALLOY BY LOCAL AND GLOBAL MINIMISATIONS OF A NON CONVEX POTENTIALS

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1. Introduction

A Shape Memory Alloy (SMA) is a mixture of martensite and austenite or only martensite or austenite. Austenite-martensite phase transformation leads to variations of composition. This transformation can appear by mechanical or thermal action. The characteristic pseudo-elastic behaviour appears from this modification in the material over certain conditions for which observe an hysteresis loop on the stress-strain relationship. This hysteresis can be influenced by several factors : thermal effect, dissipation, structural effect, existence of geometrical defect, etc..

Here, we use a model taking the temperature, the deformation and the volumic proportions of austenite and martensite as state variables. We adopt, here, Fremond's modelling in the non dissipative case which gives a non monotonic stress-strain relationship. Some experiments (Chrysochoos *et al.*, 1995) show that during room temperature test, dissipative effects are strongly dominated by effects resulting from temperature variations of material associated to the latent heat. In our case, after elimination of the volumic proportions of martensite, the bulk energy density is a non convex function.

For a given problem, it is classical to look for the mechanical equilibrium by a global minimization of the "total" energy (potential energy). Moreover, the energy associated at each problem is not quasiconvex. Existence of absolute minima is not guaranteed in all the case. It is possible to pose displacement boundary-value problems for which the total energy has no minimizer and then no absolute minimum ; the minimizing sequences are produced by displacements with fine-scale irregularities. Consequently, we

introduce two relaxation procedures (convexification and quasiconvexification) for which existence of minimizer is guaranteed in order to compare in the three cases, displacement solutions and evolutions of phases. The algorithm to find global minimum is based on an augmented Lagrangian method (decomposition-coordination method).

From a mechanical point of view, there is no reason to exclude local minima as possible equilibrium states. So, the evolution of phases may be different from the loading process to the unloading one. In order to find local minima, we write the non convex potential as a difference of two convex functions (D.C.). Then we can formulate a problem of two variational inequalities in term of displacements and stresses. In the finite dimensional case, this problem is equivalent to search solutions which locally minimize the "total" energy. By applying partial convex duality, an inf-inf problem can be formulated with respect to an appropriately defined Lagrangian function.

We present a theoretical and numerical comparison between these two points of view in focusing out the evolution of phases.

2. Constitutive law

Here, we adopt the Fremond modelling (Fremond, 1987) with only two variants of martensite, and we denote by β_1 and β_2 their volumic proportions. We assume that the volumic free energies of the phases (respectively the austenitic one and the two martensitic ones) have the following form involving the small strain tensor \mathbf{e} ,

$$\begin{aligned} W_0(\mathbf{e}, T) &= \frac{1}{2} \mathbf{e} \mathbf{K} \mathbf{e} - c(T) - C_0 T \log T \\ W_-(\mathbf{e}, T) &= W_0(\mathbf{e}, T) + \alpha(T) \boldsymbol{\tau} : \mathbf{e} + c(T) \\ W_+(\mathbf{e}, T) &= W_0(\mathbf{e}, T) - \alpha(T) \boldsymbol{\tau} : \mathbf{e} + c(T) \end{aligned}$$

$$\text{with } \alpha(T) = \begin{cases} -a(T - T_c) & \text{if } T \leq T_c \\ 0 & \text{otherwise} \end{cases} \quad \text{and } c(T) = \frac{L}{T_0} (T - T_0)$$

The phases are assumed to have the same elastic tensor \mathbf{K} , and the same heat capacity C . The austenite-martensite phase transformation is associated with a residual stress tensor $\alpha \boldsymbol{\tau}$ which is chosen identically for the two variants. L is the latent heat of phase transformation. Fremond writes the total volumic free energy Ψ as a convex combination of the three energies: the volumic proportions are constrained to stay in the simplex \mathbf{C} via the addition of the indicator function of this simplex :

$$\begin{aligned} \Psi(\mathbf{e}, T, \beta_1, \beta_2) &= \beta_1 W_-(\mathbf{e}, T) + \beta_2 W_+(\mathbf{e}, T) \\ &+ (1 - \beta_1 - \beta_2) W_0(\mathbf{e}, T) + T I_{\mathbf{C}}(\beta_1, \beta_2) \end{aligned}$$

where $I_{\mathbf{C}}(\beta_1, \beta_2)$ is the indicator function of the convex set :

$$C = \{(\gamma_1, \gamma_2) \mid 0 \leq \gamma_i \leq 1 \ ; \ \gamma_1 + \gamma_2 \leq 1\}.$$

We introduce the formalism of generalized standard materials and we neglect dissipation (Chrysochoos *et al.*, 1995): we can eliminate the internal variables (β_1, β_2) . Then, a new potential can be defined as the minimum of three convex functions. Note that this potential is not convex:

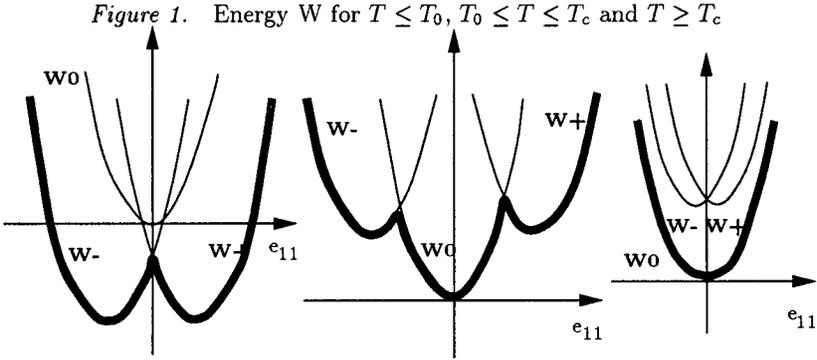
$$\begin{aligned} W(\mathbf{e}, T) &:= \min\{\Psi(\mathbf{e}, T, \beta_1, \beta_2), (\beta_1, \beta_2) \in C\} \\ &= \min\{W_0(\mathbf{e}, T), W_-(\mathbf{e}, T), W_+(\mathbf{e}, T)\} \end{aligned}$$

With the three-well energy W , which does not depend on β_1, β_2 , the material constitutive law is now written :

$$\sigma \in \bar{\partial}_{\mathbf{e}} W(\mathbf{e}(\mathbf{u}), T) \quad (1)$$

where $\bar{\partial}$ denotes the subdifferential operator of Clarke.

We consider an extension test and we represent the energy W at different temperatures in Figure 2 : low temperature $T \leq T_0$, intermediate temperature $T_0 \leq T \leq T_c$ and high temperature $T \geq T_c$.



With the constitutive law (1), we establish a classical formulation of the mechanical problem.

3. Mechanical problem at fixed temperature

Consider a boundary problem on a domain Ω of boundary Γ . Let \mathbf{f} denote the density of body force applied on Ω , \mathbf{F} the density of surfacic force applied on the part Γ_0 of Γ , and \mathbf{U} a displacement given on the complementary part Γ_1 .

The mechanical problem at fixed temperature consists in finding the displacement field \mathbf{u} and the stress field σ verifying the following equations

:

$$\begin{aligned}
\operatorname{div} \sigma + \mathbf{f} &= 0 & \text{in } \Omega \\
\mathbf{e}(\mathbf{u}) &= \nabla_s \mathbf{u} & \text{in } \Omega \\
\text{Constitutive law : } \sigma &\in \bar{\partial}_e W(\mathbf{e}(\mathbf{u})) & \text{in } \Omega \\
\mathbf{u} &= \mathbf{U} & \text{on } \Gamma_0 \\
\sigma \cdot \mathbf{n} &= \mathbf{F} & \text{on } \Gamma_1
\end{aligned}$$

In the following, the set of kinematically admissible displacement fields with finite energy of the structure will be defined by :

$$\mathbf{U}_{ad} = \left\{ \mathbf{v} \in [\mathbf{H}^1(\Omega)]^3, \mathbf{v} = \mathbf{U} \text{ on } \Gamma_0 \right\} \text{ and the stress spaces } \mathbf{H} = [\mathbf{L}^2(\Omega)]^6.$$

4. Global minimum

4.1. THE THREE-WELL ENERGY

At first, we search for a global minimum of the three-well potential energy. To solve this problem, we consider an augmented Lagrangian. It is a function of a multiplier μ and of two independent variables \mathbf{v}, \mathbf{q} corresponding to the displacement and strain fields.

$$L_r(\mathbf{v}, \mathbf{q}, \mu) = \int_{\Omega} W(\mathbf{q}) \, dx - l(\mathbf{v}) + \int_{\Omega} \mu : (\mathbf{e}(\mathbf{v}) - \mathbf{q}) \, dx + \frac{r}{2} \int_{\Omega} ((\mathbf{e}(\mathbf{v}) - \mathbf{q}))^2 \, dx$$

with $l(\mathbf{v}) = \int_{\Omega} \mathbf{f} \cdot \mathbf{v} \, d\Omega + \int_{\Gamma_1} \mathbf{F} \cdot \mathbf{v} \, d\Gamma$ and $r \geq 0$.

We extend this non-convex density energy, the classical strategy of searching for the saddle points of the augmented Lagrangian i.e. the $(\mathbf{u}, \mathbf{p}, \lambda)$ solutions of the problem :

$$L_r(\mathbf{u}, \mathbf{p}, \mu) \leq L_r(\mathbf{u}, \mathbf{p}, \lambda) \leq L_r(\mathbf{v}, \mathbf{q}, \lambda), \forall \mathbf{v} \in \mathbf{U}_{ad}, \forall \mathbf{q} \in \mathbf{H}, \forall \mu \in \mathbf{H}$$

To solve the initial problem, we use an algorithm inspired of by Uzawa method (LeTallec *et al.*, 1989) which involves a two-step iteration : a linear global problem and a non linear local problem.

4.2. THE "RELAXED" ENERGY

To profit by an existence theorem, we calculate the quasiconvexification QW of the previous potential by using the approach of Pipkin (Pipkin, 1990), and the convexification CW of W . To determine the quasiconvexification, we take a unit cube B , we use the definition of QW (Pipkin, 1990)

$$QW(\mathbf{e}) := \liminf_{\mathbf{u}_N \rightarrow 0 \text{ uniformly}} \int_B W(\mathbf{e} + \nabla_s \mathbf{u}_N) \, dx, \quad (2)$$

and consider a sequence of displacement fields \mathbf{u}_N for which the strain varies rapidly and periodically between two alternate constant values e_1 and e_2 . The details of the calculus are given in the paper (Pagano *et al.*, to appear). \mathbf{u}_N is a periodic function of the variable $\mathbf{n} \cdot \mathbf{x}$, of period $\frac{1}{N}$.

Pipkin defines this sequence on one period $[0, \frac{1}{N}]$ by

$$\mathbf{u}_N := \begin{cases} 2\theta(\mathbf{n} \cdot \mathbf{x})\mathbf{u} & \text{on } [0, \frac{1-\theta}{N}] \\ -2(1-\theta)(\mathbf{n} \cdot \mathbf{x} - \frac{1}{N})\mathbf{u} & \text{on } [\frac{1-\theta}{N}, \frac{1}{N}] \end{cases}$$

$$\text{and } \mathbf{e} + \nabla_s \mathbf{u}_N = \begin{cases} e_1 = e + \theta(\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}) \\ e_2 = e + (1-\theta)(\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}) \end{cases}$$

where \mathbf{u} and \mathbf{n} are two constant vectors and $0 < \theta < 1$. We can prove that the density energy QW is :

$$QW(\mathbf{e}) = \min_{\mathbf{u}, \mathbf{n}, 0 \leq \theta \leq 1} [(1-\theta)W(\mathbf{e}_1) + \theta W(\mathbf{e}_2)]. \quad (3)$$

This minimization can be performed by discrimination of all the possible cases for $W(\mathbf{e}_1)$ and $W(\mathbf{e}_2)$. We obtain a similar form, noted RW , for the convexification and the quasiconvexification of the density energy W . for $c + \frac{\mathcal{G}}{2} \geq 0$:

$$RW(\mathbf{e}) = \begin{cases} W_-(\mathbf{e}) & \text{if } \alpha\tau : \mathbf{e} \leq -c + \frac{\mathcal{G}}{2} \\ W_0(\mathbf{e}) + \frac{1}{2\mathcal{G}}(\alpha\tau : \mathbf{e} + c + \frac{\mathcal{G}}{2})^2 & \text{if } -c + \frac{\mathcal{G}}{2} \leq \alpha\tau : \mathbf{e} \leq -c - \frac{\mathcal{G}}{2} \\ W_0(\mathbf{e}) & \text{if } |\alpha\tau : \mathbf{e}| \leq c + \frac{\mathcal{G}}{2} \\ W_0(\mathbf{e}) + \frac{1}{2\mathcal{G}}(\alpha\tau : \mathbf{e} - c - \frac{\mathcal{G}}{2})^2 & \text{if } c + \frac{\mathcal{G}}{2} \leq \alpha\tau : \mathbf{e} \leq c - \frac{\mathcal{G}}{2} \\ W_+(\mathbf{e}) & \text{if } \alpha\tau : \mathbf{e} \geq c - \frac{\mathcal{G}}{2} \end{cases} \quad (4)$$

The functional RW is equal to the convexification of W if $\mathcal{G} = \mathcal{G}_c$ and to the quasiconvexification for $\mathcal{G} = \mathcal{G}_q$ with :

$$\mathcal{G}_c = 2 \left[\min_{\mathbf{E} \in M_s^{3 \times 3}} W_-(\mathbf{E}) - c \right] = -\alpha^2 \tau : \mathbf{K}^{-1} \tau$$

$$\text{and } \mathcal{G}_q = 2 \left[\min_{\mathbf{u}, \mathbf{n}} W_-(\mathbf{u} \otimes \mathbf{n} + \mathbf{n} \otimes \mathbf{u}) - c \right]$$

In particular, $\mathcal{G}_q = \mathcal{G}_c$ if τ has the form $\mathbf{a} \otimes \mathbf{b} + \mathbf{b} \otimes \mathbf{a}$ where \mathbf{a} and \mathbf{b} are two vectors. If we restrict our attention to the case of isotropic Hooke's law with Lamé coefficients λ and μ , and if we suppose that $\tau = \mathbf{I}$, we can calculate the coefficients \mathcal{G}_q and \mathcal{G}_c to obtain the following results :

$$\mathcal{G}_c = \frac{-\alpha^2}{2\lambda + \mu} \quad \text{and} \quad \mathcal{G}_q = \frac{-\alpha^2}{\lambda + 2\mu}$$

The optimal values of θ which minimize (3), noted θ_- and θ_+ may be interpreted as two internal variables which represent the "proportions of

martensite” of the mixture. These values are the following :

$$(\theta_-, \theta_+) = \begin{cases} (1, 0) & \text{if } \alpha\tau : \mathbf{e} \leq -c + \frac{g}{2} \\ \left(\frac{\alpha\tau : \mathbf{e} + c + \frac{g}{2}}{g}, 0 \right) & \text{if } -c + \frac{g}{2} \leq \alpha\tau : \mathbf{e} \leq -c - \frac{g}{2} \\ (0, 0) & \text{if } \alpha|\tau : \mathbf{e}| \leq c + \frac{g}{2} \\ \left(0, \frac{-\alpha\tau : \mathbf{e} + c + \frac{g}{2}}{g} \right) & \text{if } c + \frac{g}{2} \leq \alpha\tau : \mathbf{e} \leq c - \frac{g}{2} \\ (0, 1) & \text{if } \alpha\tau : \mathbf{e} \geq c - \frac{g}{2} \end{cases} \quad (5)$$

For the case $c + \frac{g}{2} \leq 0$ we obtain, also, similar expressions for QW and CW (analogous to the Pipkin’s result for a two-well energy). We see that QW and CW are piecewise quadratic and C^1 . From a well known result of Dacorogna, any solution of this relaxed problem is a limit of a minimizing sequence of the potential associated to the initial problem (Dacorogna, 1985). To solve the relaxed problem, we use the same method as for the initial problem.

5. Local minimum

The potential W , at fixed temperature, can appear as the difference of two convex functions (d.c.) (Pagano *et al.*, to appear) φ_1 and φ_2 :

$$\varphi_1(\mathbf{e}) = W_0(\mathbf{e}) \quad \text{and} \quad \varphi_2(\mathbf{e}) = \max(\alpha|\text{tre}| - c)$$

Based on this decomposition, we formulate the mechanical problem as two variational inequalities. In the finite dimensional case, this problem is equivalent to finding local minima of the potential energy. The decomposition leads to the introduction of a Lagrangian L_{Π} , in the terminology of Auchmuty (1989). It depends on the displacement field corresponding to a stress field, and it is function of the energy Φ_1 and the Fenchel convex conjugate function Φ_2^* . This Lagrangian is separately convex in each of the dual variables, but the convexity of L_{Π} is not guaranteed in general. An algorithm is derived to reach ∂ -critical points of the Lagrangians L_{Π} . These points are defined as follows :

$(\mathbf{u}, \sigma_2) \in \mathbf{U}_{ad} \times \mathbf{H}$ is a ∂ -critical point of L_{Π} if :

$$\begin{aligned} L_{\Pi}(\mathbf{u}, \sigma_2) &\leq L_{\Pi}(\mathbf{v}, \sigma_2), \quad \forall \mathbf{v} \in \mathbf{U}_{ad} \\ L_{\Pi}(\mathbf{u}, \sigma_2) &\leq L_{\Pi}(\mathbf{u}, \tau), \quad \forall \tau \in \mathbf{H} \end{aligned}$$

The relationship between critical points of the potential energy and those of L_{Π} is somewhat more delicate. If $(\mathbf{u}, \sigma_2) \in \mathbf{U}_{ad} \times \mathbf{H}$ is a ∂ -critical point of the Lagrangian then \mathbf{u} is a critical point of the potential energy.

This convex difference algorithm constructs minimizing sequence of L_{II} . It permits us to characterize a ∂ -critical point of L_{II} . In practice, it determines local minima of the Lagrangian. It is also split into two steps, (global and local steps).

We remark that the "relaxed" energy can, also, be split into the difference of two convex functions φ_1 and $R\varphi_2$. The same numerical method can be applied to the resolution of the relaxed problem.

$$(R\varphi_2) = \begin{cases} -\alpha\tau : \mathbf{e} - c & \text{if } \alpha\tau : \mathbf{e} \leq -c + \frac{g}{2} \\ \frac{-1}{2g}(\alpha\tau : \mathbf{e} + c + \frac{g}{2})^2 & \text{if } -c + \frac{g}{2} \leq \alpha\tau : \mathbf{e} \leq -c - \frac{g}{2} \\ 0 & \text{if } |\alpha\tau : \mathbf{e}| \leq c + \frac{g}{2} \\ \frac{-1}{2g}(\alpha\tau : \mathbf{e} - c - \frac{g}{2})^2 & \text{if } c + \frac{g}{2} \leq \alpha\tau : \mathbf{e} \leq c - \frac{g}{2} \\ \alpha\tau : \mathbf{e} - c & \text{if } \alpha\tau : \mathbf{e} \geq c - \frac{g}{2} \end{cases} \quad (6)$$

6. Numerical simulations at fixed temperature

In this part, we compare the three points of view. We assume that $\tau = \mathbf{I}$ and we consider a flat sample with a geometrical defect submitted to a strain controlled loading-unloading process. For symmetry reasons, only a quarter of the sample is represented [Figure 3].

Figure 2. Flat sample



The incremental process is performed using loading steps. At each step the algorithm is initialised to the state at the end of the previous step.

With the initial energy W and the D.C. approaches, we notice that a local non monotone strain-stress law (figure 1) leads to a monotone displacement-force diagram. Moreover a hysteresis behaviour is shown. For a given displacement value loading or unloading process, the phase transformation in the flat is not the same. The first picture in figure 4 represents the binary phases distribution in the flat. According to the chosen modelling, the proportions are either zero or one almost everywhere. Roughly speaking the phase transition is locally instantaneous.

With the global minimization, (quasiconvexified or not), the hysteresis vanishes. The distribution of phases, issuing from the minimisation of the quasiconvexification, appears as the "homogenization" of the phase distribution obtained for the non convex potential W . Some differences are obtained about the spatial repartition of phases for the quasiconvexification (figure 4-2) and the convexification (figure 4-3). With CW, the zone

where the volumic proportion of martensite lies between zero and one is more important than for relaxed energy QW.

Acknowledgement : We thank Doctor Licht for his very interesting and helpful comments.

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Figure 3. Results with energies W(4-1), CW(4-2) and QW(4-3)

