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SHAPE MEMORY ALLOY

A THERMOMECHANICAL MACROSCOPIC THEORY

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1. Introduction.

Shape memory alloys are mixtures of many martensites and of austenite. The composition of the mixture varies : the matensites and the austenite transform into one another. These phase changes can be produced either by thermal actions or by mechanical actions. The striking and well known properties of shape memory alloys results from these links between mechanical and thermal actions [4], [15], [26].

Shape memory alloys can be studied at the microscopic level by describing the microstructures of the constitutive crystals, [7], [17], [28]. They can also be studied by using statistical thermodynamics of a lattice of particles [3] [23].

Thermodynamics involving internal quantities is an other tool to study shape memory alloys at the macroscopic level, [1], [2], [5], [6], [9], [18], [19], [22] [25], [27], [29]. It is the one we have chosen [10], [11]. It gives a macroscopic theory which can be used for engineering purposes, for example to describe the evolution of structures made of shape memory alloys. The internal quantities we choose, the phase volume fractions, are submitted to constraints (for instance their actual value is between 0 and 1). We show that most of the properties of shape memory alloys result from a careful treatment of these constraints [10], [12].

The first paragraphs 1 to 8 describe the thermodynamical quantities, the free energy and the pseudo-potential of dissipation. They give also the basic tools for macroscopic modelling. The paragraph 9 is devoted to the macroscopic description of shape memory alloys.

Basic definitions and properties of convex analysis are given in the appendix 12.

2. Description of a material. The state quantities.

The state quantities are the basic quantities which describe the equilibrium and the evolution of a material. Their choice depends on the sophistication of the model we are searching for. Thus their choice depends on the scientist or the engineer concerned.

When the state quantities are constant with respect to the time, we say that the material is at an equilibrium. Thus the notion of equilibrium is subjective : it depends on the sophistication of the description.

The set of the state quantities is denoted by E. It usually contains quantities describing the deformations and the temperature. The other quantities of E are often called internal quantities.

3. Principle of Virtual Power without micoscopic velocities.

This is the classical situation. Let $\sqrt[7]{}$ be the linear space of the macroscopic virtual velocities, Ω be the domain of \mathbb{R}^3 occupied by the structure we consider at the time t. The principle of virtual power [14] is

(1),
$$\forall D \subset \Omega, \forall V \in \mathbb{V}, A(D, V) = P_i(D, V) + P_e(D, V),$$

where D is a subdomain of Ω . The virtual power of the acceleration forces is

$$A(D,\mathbf{V}) = \int_{D} \rho \gamma \mathbf{V} d\Omega,$$

where γ is the acceleration and ρ the density. The virtual power of the internal forces is

$$P_i(D,\mathbf{V}) = -\int_D \sigma: D(\mathbf{V}) d\Omega,$$

where $D(\mathbf{V}) = (D_{ij}(\mathbf{V}) = \frac{1}{6}(V_{i,j}+V_{j,i}))$ are the strain rates and $\sigma = (\sigma_{ij})$ the stresses. The virtual power of the external forces is the sum of the power of the at a distance forces.

$$\int_{D} \mathbf{f} \cdot \mathbf{V} d\Omega,$$

where **f** is the volumetric external force, and of the power of the contact forces

where **T** is the contact external force. The virtual power of the external forces is

$$P_e(D,\mathbf{V}) = \int_D \mathbf{f} \cdot \mathbf{V} d\Omega + \int_{\partial D} \mathbf{T} \cdot \mathbf{V} d\Gamma.$$

It is classical [14] to get the equations of the movement from the principle (1),

(2),
$$\rho\gamma = \operatorname{div}\sigma + \mathbf{f}$$
, in D ,

(3),
$$\sigma . N = T$$
, in ∂D ,

where N is the outwards normal unit vector to D.

4. <u>Principle of Virtual Power with microscopic velocities.</u> When the state quantities include internal quantities, the evolution of those quantities can result from microscopic movements. We think that the power of the microscopic movements can be taken into account in the power of the internal forces [13]. Let β be an internal quantity, for instance a volumetric proportion of austenite in a shape memory alloy, the volumetric proportion of a constituent in a mixture, the damage in a piece of concrete [13], the intensity of adhesion between two pieces [16], [32], the volume fraction of unfrozen water in a soil in winter... The only macroscopic quantity which is related to the micoscopic movements or velocities is $\frac{d\beta}{dt}$ which

describes their macroscopic effects i.e. the evolution of β . Thus we choose as actual power of the internal forces

$$P_i(D,\mathbf{U},\frac{\mathrm{d}\beta}{\mathrm{d}t}) = -\int_D \sigma: D(\mathbf{U})\mathrm{d}\Omega - \int_D \{B\frac{\mathrm{d}\beta}{\mathrm{d}t} + \mathbf{H}.\mathbf{grad}\frac{\mathrm{d}\beta}{\mathrm{d}t}\}\mathrm{d}\Omega,$$

and as virtual power of the internal forces,

$$\forall (\mathbf{V},\mathbf{c}) \in \mathbb{V} \times \mathbb{C}, \qquad P_i(D,\mathbf{V},\mathbf{c}) = -\int_D \sigma: D(\mathbf{V}) d\Omega - \int_D \{B\mathbf{c} + \mathbf{H}.\mathbf{gradc}\} d\Omega,$$

where C is the linear space of the virtual microscopic velocities. The elements (V,c) of $\mathbb{V}x\mathbb{C}$ are function of \mathbf{x} , $(\mathbf{V}(\mathbf{x}), \mathbf{c}(\mathbf{x}))$.

The gradient of the velocity of β takes into account the influence of the neighbourhood of a point onto this point. The two quantities B and H are new internal forces. The force B is a work and H is a work flux vector (if β is a volumetric proportion). Their physical meaning will be given by the equations of movement as the physical meaning of the stress tensor is given by (3). We will see that H like σ drescribes the effects of the neighbourhood of a point onto this point. The power of the internal forces has to satisfy the virtual power axiom [14]:

the power of the internal forces is zero for any rigid body movement.

A rigid body movement is such that the distance of two material points remains constant. It results that $D(\mathbf{U}) = 0$ for a rigid body movement with macroscopic velocity U. Because the distance of two points remains constant in a rigid body velocity there is no microscopic movement and the value of β remains constant. It results that $\frac{d\beta}{dt} = 0$ and $P_i(D, \mathbf{U}, \frac{d\beta}{dt}) = 0$. The virtual power is then satisfied by the power of the internal forces P_i .

It is natural to choose a new power of the external forces $P_e(D, U\frac{d\beta}{dt})$ depending on $\frac{d\beta}{dt}$. It is the sum of

$$\int_{D} \mathbf{f} \cdot \mathbf{U} \mathrm{d}\Omega + \int_{D} \mathbf{A} \frac{\mathrm{d}\beta}{\mathrm{d}t} \mathrm{d}\Omega,$$

the power of the at a distance external actions, and of the power of the external contact forces

$$\int \mathbf{T} \cdot \mathbf{U} d\Gamma + \int \mathbf{a} \frac{\mathrm{d}\beta}{\mathrm{d}t} \mathrm{d}\Gamma,$$

$$\partial D \qquad \partial D$$

where A is the volumic work provided from the exterior and a the surfacic work provided by contact to D. Thus the new power of the external forces we choose is

$$\forall (\mathbf{V}, \mathbf{c}) \in \mathbb{V} \times \mathbb{C}, P_{e}(D, \mathbf{V}, \mathbf{c}) = \int_{D} \mathbf{f} \cdot \mathbf{V} d\Omega + \int_{D} \mathbf{A} \mathbf{c} d\Omega + \int_{\partial D} \mathbf{T} \cdot \mathbf{V} d\Gamma + \int_{\partial D} \mathbf{a} \mathbf{c} d\Gamma.$$

We decide not to change the power of the acceleration forces. The principle of virtual power becomes [12],

(4),
$$\forall D \subset \Omega, \forall (\mathbf{V}, \mathbf{c}) \in \mathbb{V} \times \mathbb{C}, \quad A(D, \mathbf{V}, \mathbf{c}) = P_i(D, \mathbf{V}, \mathbf{c}) + P_e(D, \mathbf{V}, \mathbf{c}).$$

By letting c = 0 in (4), we get the classical equations of movement,

- (2), $\rho \gamma = \operatorname{div} \sigma + \mathbf{f}$, in *D*,
- (3), $\sigma N = T$, in ∂D .

By letting V = 0 in (4), an easy computation gives,

- (5), $0 = \text{div}\mathbf{H} \mathbf{B} + \mathbf{A}$, in *D*,
- (6), **H**.N = a , in ∂D .

The equation (6) gives the physical meaning of \mathbf{H} . It is a work flux vector : \mathbf{H} . \mathbf{N} is the amount of work provided to the body through the surface with normal \mathbf{N} (for an analoguous situation think of the heat flux vector).

When the power of the internal forces does not depend on $\mathbf{grad}\frac{d\beta}{dt}$ the principle of virtual power gives

(5 bis), 0 = -B + A, in D.

Of course this equation can be obtained by letting H = 0 in (5).

5. The energy balance.

The conservation of energy is for any subdomain D,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{D} \mathrm{edt} + \frac{\mathrm{d}K}{\mathrm{d}t} = P_e(D, \mathbf{U}, \frac{\mathrm{d}\beta}{\mathrm{d}t}) + \int_{\partial D} -\mathbf{q} \cdot \mathbf{N} \mathrm{d}\Gamma + \int_{D} \mathrm{rdt},$$

where e is the volumic internal energy, K the kinetic energy, q the heat flux vector and r the volumic rate of heat production. By using the kinetic energy theorem, i.e. the principle of virtual power with the actual velocities, we get for any D,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{D} \mathrm{edt} = -P_i(D, \mathbf{U}, \frac{\mathrm{d}\beta}{\mathrm{d}t}) + \int_{\partial D} -\mathbf{q} \cdot \mathbf{N} \mathrm{d}\Gamma + \int_{D} \mathrm{rdt}.$$

This equation gives,

(7),
$$\frac{d\mathbf{e}}{dt} + \mathrm{ediv}\mathbf{U} + \mathrm{div}\mathbf{q} = \mathbf{r} + \sigma: \mathbf{D}(\mathbf{U}) + \mathbf{B}\frac{d\beta}{dt} + \mathbf{H}.\mathbf{grad}\frac{d\beta}{dt}$$
, in Ω ,

(8),
$$-\mathbf{q} \cdot \mathbf{N} = \pi$$
, in $\partial \Omega$,

where π is the rate of heat provided to the stucture Ω by contact actions.

6. <u>The second principle of thermodynamics.</u> It is for any domain*D*,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{D} \mathrm{sdt} \geq \int_{D} \frac{-\mathbf{q} \cdot \mathbf{N}}{\mathrm{T}} \mathrm{d}\Gamma + \int_{D} \frac{\mathrm{r}}{\mathrm{T}} \mathrm{d}t,$$

where s is the volumic entropy and T the temperature. It gives,

(9),
$$\frac{\mathrm{ds}}{\mathrm{dt}} + \mathrm{sdiv}\mathbf{U} + \mathrm{div}\frac{\mathbf{q}}{\mathrm{T}} \ge \frac{\mathrm{r}}{\mathrm{T}}.$$

This equation is the second principle basic relation. It is to be satisfied like the balance equations by any actual evolution. The equation (9) multiplied by the temperature assumed to be positive and the energy balance equation give,

(10),
$$\frac{de}{dt} - T\frac{ds}{dt} + (e-Ts)divU \le \sigma:D(U) + B\frac{d\beta}{dt} + H.grad\frac{d\beta}{dt} + \frac{-q.gradT}{T}$$

by letting $\Psi = e^{-Ts}$ the volumic free energy, we get

(11),
$$\frac{d\Psi}{dt} + s\frac{dT}{dt} \le (\sigma - \Psi 1):D(U) + B\frac{d\beta}{dt} + H.grad\frac{d\beta}{dt} + \frac{-q.gradT}{T}$$
,

which is the Claudius-Duhem relation (1 is the identity tensor). This inequality is to be satisfied by any actual evolution.

7. Constitutive laws when there are no constraint on the internal quantities.

Let us assume that the internal quantity β can have any value : it is not submitted to any constraint.

From now on, for the sake of simplicity, we make the small perturbation assumption. The Clausius-Duhem inequality becomes

(11),
$$\frac{d\Psi}{dt} + s\frac{dT}{dt} \le \sigma: D(U) + B\frac{d\beta}{dt} + H.grad\frac{d\beta}{dt} + \frac{-q.gradT}{T}$$

because edivU, sdivU and Ψ divU are negligeable in the small perturbation theory. We assume that the state quantities are the small deformations ε , the internal quantity β , its gradient grad β and the temperature T: E = (ε , β ,grad β ,T). The free energy depends on E: Ψ (E). We assume it is differentiable and let

(12),
$$s = -\frac{\partial \Psi}{\partial T}$$
,

which is the Helmholtz relation, and define,

$$\sigma^{nd} = \frac{\partial \Psi}{\partial \varepsilon},$$

$$B^{nd} = \frac{\partial \Psi}{\partial \beta},$$

(13),
$$H^{nd} = \frac{\partial \Psi}{\partial (\mathbf{grad}\beta)},$$

The stress σ^{nd} is the non-dissipative stress, B^{nd} and H^{nd} are is the generalized non-dissipative forces. The Clausius-Duhem relation (11) gives

$$(\sigma - \sigma^{nd}): D(\mathbf{U}) + (\mathbf{B} - \mathbf{B}^{nd}) \frac{d\beta}{dt} + (\mathbf{H} - \mathbf{H}^{nd}) \cdot \mathbf{grad} \frac{d\beta}{dt} + T\mathbf{q} \cdot \mathbf{grad} \frac{1}{T} \ge 0,$$

for any actual evolution of the structure. To achieve the description of the constitutive laws, we assume that there exist four functions σ^d , B^d , H^d , Q^d depending on x, t, E, $\delta E = \{D(U), \frac{d\beta}{dt}, \operatorname{grad} \frac{d\beta}{dt}, \operatorname{grad} \frac{1}{T}\}$ and other quantities χ depending on the history of the material such that

$$\forall \mathbf{x}, \mathbf{t}, \forall \mathbf{E}, \forall \mathbf{W} = (\mathbf{f}, \mathbf{c}, \mathbf{g}, \mathbf{p}) \in \mathbf{S} \mathbf{x} \mathbf{R} \mathbf{x} \mathbf{R}^3 \mathbf{x} \mathbf{R}^3, \forall \chi,$$

 $(14), \quad \sigma^d(\mathbf{x}, t, E, W, \chi): \mathbf{f} + B^d(\mathbf{x}, t, E, W, \chi)\mathbf{c} + H^d(\mathbf{x}, t, E, W, \chi).\mathbf{g} + Q^d(\mathbf{x}, t, E, W, \chi).\mathbf{p} \ge 0,$

where S is the set of symetric tensors.

The quantity σ^d is the dissipative stress, B^d and H^d are the dissipative generalized forces and Q^d is a heat flux. The constitutive laws we choose are,

(15), $\sigma = \sigma^{nd}(E) + \sigma^{d}(\mathbf{x}, t, E, \delta E, \chi)$,

(16), $B = B^{nd}(E)+B^{d}(\mathbf{x},t,E,\delta E,\chi)$,

(17), $\mathbf{H} = \mathbf{H}^{nd}(\mathbf{E}) + \mathbf{H}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \boldsymbol{\chi}),$

(18), $Tq = Q^d(x,t,E,\delta E,\chi).$

It is very easy to prove that

<u>Theorem 1.</u> If the relation (14) are satisfied, the constitutive laws (15) to (18) are such that the Clausius-Duhem inequality is satisfied.

<u>Proof.</u> Write the relation (14) with actual velocities and use the constitutive laws.

Let us sum up the way we define a material : it is defined by

the state quantities E,

the linear spaces \mathbb{V} and \mathbb{C} ,

the power of the internal forces $P_i(D, V, c)$,

the free energy Ψ depending on E,

the functions σ^d , B^d , H^d , Q^d depending on E, δE and other quantities χ .

7.1. The pseudo-potential of dissipation.

A very general and powerful method to define the dissipative forces is to introduce a pseudo-potential of dissipation as defined by Moreau [21]. It is a function Φ of E, W and χ such that Φ is a positive function, convex with respect to W [20] and equal to 0 for W = 0. Let us prove,

<u>Theorem 2.</u> Let there be $\Phi(E,W,\chi)$ such that $\delta E \to \Phi(E,W,\chi)$ is convex, $\Phi(E,W,\chi)$ is positive and $\Phi(E,0,\chi) = 0$. Let for any W, $A \in \partial \Phi(E,W,\chi)$, then we have,

 $\mathbf{A}.\mathbf{W} \ge \mathbf{0},$

(A.W is the scalar product of A and W and $\partial \Phi(E,W,\chi)$ is the subdifferential set of Φ with respect to W).

Proof. Because $W \rightarrow \Phi((E, W, \chi))$ is convex we have for $A \in \partial \Phi((E, W, \chi))$,

 $\Phi(E,0,\chi) \ge \Phi(E,W,\chi) - A.W,$

which gives

 $A.W \ge \Phi(E,W,\chi) \ge 0$ and $A.W \ge 0$.

The dissipative forces σ^d , B^d, H^d, Q^d are defined by

 $(\sigma^{d}(x,t,E,\delta E,\chi), B^{d}(x,t,E,\delta E,\chi), H^{d}(x,t,E,\delta E,\chi), Q^{d}(x,t,E,\delta E,\chi)) \in \partial \Phi((E,\delta E,\chi).$

It results from the theorem 2 that the inequality (14) is satisfied. In the sequel we will always define the dissipative forces with a pseudo-potential of dissipation.

8. Constitutive laws when there are constraints on the internal quantities.

Let us assume that β is a volume fraction or a damage quantity. Because in the following paragraphs the β 's will be volume fractions, we choose β to be a damage quantity [13]. The damaged quantity can be defined as the quotient of the Young modulus of the damaged material by the Young modulus of the undamaged material. Obviously the value of β is between 0 and 1:

(19), $0 \le \beta \le 1$,

when $\beta = 1$, the material we consider is undamaged and when $\beta = 0$, the material is completely damaged. The internal quantity β is submitted to the internal constraint (19). We think that this constraint is a material property. Thus it must be taken into account by the elements which define a material. Because it is a constraint on the state, it appears convenient to use the free energy. We do it in the following manner: we decide that the free energy is defined for any value of β , even for the values which are physically impossible. The value of the free energy is $+\infty$ for values of β which are physically impossible, i.e. for $\beta \notin [0,1]$; its value is the usual physical value $\Psi(E)$ when $\beta \in [0,1]$. Thus we have

 $\underline{\Psi}(\mathbf{E}) = \Psi(\mathbf{E}) + \mathbf{I}(\boldsymbol{\beta}),$

where $\underline{\Psi}$ is the extended free energy defined for any value of β , $\Psi(E)$ is the usual physical value and I is the indicator function of the segment [0,1], (I(x) = + ∞ if $x \notin [0,1]$ and I(x) = 0 if $x \in [0,1]$), (see the appendix).

<u>Note</u> The temperature T is submitted to the internal constraint $T \ge 0$. For the sake of simplicity, we assume it is always satisfied. If one does not want to make this assumption, it is convenient to add $I_+(T)$ to Ψ where I_+ is the indicator function of $[0,+\infty)$.

Before we go on, let us remark that the time derivatives cannot be assumed to be continuous due to the effects of the internal constraint (19). For instance $\frac{d\beta}{dt}$ is discontinuous when β decreases to the value 0 (figure 1).





The function $\beta(t)$ decreases to 0 and remains equal to 0. The derivative $\frac{d\beta}{dt}$ is not a continuous function.

Left and right derivative must be investigated. The right derivative

$$\lim \frac{\beta(t+\Delta t) - \beta(t)}{\Delta t} = \frac{d^{r}\beta}{dt}$$
$$\Delta t \to 0$$
$$\Delta t > 0$$

depends on the future evolution of the material but the left derivative

$$\lim \frac{\beta(t) - \beta(t - \Delta t)}{\Delta t} = \frac{d^{1}\beta}{dt}$$
$$\Delta t \to 0$$
$$\Delta t > 0$$

depends on its past evolution.

The constitutive laws we are looking for must be determinist, i.e. relations between the state quantities E and the history of the material or its past evolution. The left derivative appears as a compulsory choice for any derivative with respect to the time which appears in the constitutive laws. Thus in the sequel all the time derivatives we use are left derivative.

Let us come back at the extended free energy and give one of its properties:

<u>Theorem 3.</u> If the function $\Psi(\varepsilon,\beta,\mathbf{grad}\beta,T)$ is smooth, we have for any actual evolution, i.e. for any evolution such that $\beta(t) \in [0,1]$ at any time t,

(20),
$$\forall C \in \partial I(\beta)$$
, $\frac{d^{l}\Psi}{dt} = \frac{d^{l}\Psi}{dt} \le \frac{d^{l}\Psi}{dt} + C \frac{d^{l}\beta}{dt}$

where the derivatives in the formula (20), $\frac{d^l}{dt}$, are left derivatives.

<u>Proof</u> Because the evolution is an actual evolution, we have $I(\beta(t)) = 0$ at any time t. It results the first equality of (20) because $\underline{\Psi}$ is equal to Ψ at any time t. The function $\Psi(\varepsilon,\beta,\mathbf{grad}\beta,T)$ being smooth we have,

(21),
$$\Psi(t) - \Psi(t - \Delta t) = \frac{d^{1}\Psi}{dt}(t) \Delta t + o(\Delta t)$$

where the function $o(\Delta t)/\Delta t$ tends to 0 when Δt tends to 0. Because I is a convex function, we have

(22),
$$I(\beta(t)) - I(\beta(t-\Delta t)) \le C (\beta(t)-\beta(t-\Delta t))$$
, for any $C \in \partial I(\beta(t))$.

By dividing (21) and (22) by Δt positive and adding those relations, we get

$$\frac{\Psi(t)-\Psi(t-\Delta t)}{\Delta t} \le \frac{d^{1}\Psi}{dt}(t) + C \frac{\beta(t)-\beta(t-\Delta t)}{\Delta t} + \frac{o(\Delta t)}{\Delta t}.$$

By letting Δt tend towards 0, we have the inequality of (20).

Because the free energy Ψ is not differentiable whith respect to the time (it has only a left derivative), we decide that all the quantities that are to be derived with respect to the time have left derivatives. We assume also that they are smooth enough with respect to x for the calculations to be coherent. The Clausius-Duhem inequality

$$(23), \quad \frac{\mathrm{d}\Psi}{\mathrm{d}t} + \mathrm{s}\frac{\mathrm{d}T}{\mathrm{d}t} \leq \sigma \mathrm{:} \mathsf{D}(\mathsf{U}) + \mathsf{B}\frac{\mathrm{d}\beta}{\mathrm{d}t} + \mathsf{H}.\mathsf{grad}\frac{\mathrm{d}\beta}{\mathrm{d}t} + \frac{-\mathsf{q}.\mathsf{grad}T}{\mathsf{T}},$$

can be proved like in paragraph 7, the time derivatives beeing left derivatives. The choice of left derivative we make is in agreement with the necessity for the the basic inequality (9) or the equivalent Clausius-Duhem inequality to be satisfied by the past evolution of the material. We wish also to keep the role of the Clausius-Duhem inequality as a guide to define the constitutive laws which are relations depending on the past evolution. The left derivative are, as we have already mentionned, deterministic. On the contrary the right derivative are not deterministic.

We use the notations of the preeceding paragraphs. We have the Helmholtz relation

(24),
$$s(E) = -\frac{\partial \Psi}{\partial T}(E)$$
.

Let us define the non dissipative forces. We assume that there exist functions σ^{nd} , B^{nd} , H^{nd} of E and B^{ndr} of (E,x,t) which satisfy

(13),
$$\sigma^{nd}(E) = \frac{\partial \Psi}{\partial \varepsilon}(E)$$
,
(13), $B^{nd}(E) = \frac{\partial \Psi}{\partial \beta}(E)$,
(25), $B^{ndr}(E, \mathbf{x}, t) \in \partial I(\beta(\mathbf{x}, t))$,

(13),
$$\mathbf{H}^{nd}(\mathbf{E}) = \frac{\partial \Psi}{\partial (\mathbf{grad}\beta)}(\mathbf{E}).$$

With those definitions we can write the Clausius-Duhem inequality as in the previous paragraph

$$(\sigma - \sigma^{nd}): D(\mathbf{U}) + (\mathbf{B} - \mathbf{B}^{nd})\frac{d\beta}{dt} + (\mathbf{H} - \mathbf{H}^{nd}).\mathbf{grad}\frac{d\beta}{dt} + T\mathbf{q}.\mathbf{grad}\frac{1}{T} \ge 0.$$

The relations (13), (24) and (25) are the state laws. It results from the preceding formulae that the smooth part of the extented free energy is differentiable and that the non-smooth part is subdifferentiable, i.e. that the subdifferential set $\partial I(\beta)$ is not empty. Let us see how important is this assumption. The quantity $B^{ndr}(E,x,t)$ is the thermodynamical reaction to the internal constraint (19). It is related to β by the state law (25). This one implies that the subdifferential $\partial I(\beta)$ is not empty, thus that β is between 0 and 1 which means that the internal constraint (19) is satisfied. One can also say that relation (25) has two meanings, first that the internal constraint (19) is satisfied, second that there exists a reaction to the internal constraint which is zero for $0 < \beta < 1$, positive for $\beta = 1$ and negative for $\beta = 0$. Let us also note that the sum of the reaction B^{ndr} and of the reversible force B^{nd} , ($B^{ndr} + B^{nd}$) is a generalized derivative of the free energy Ψ with respect to β ; B^{nd} is the smooth part and B^{ndr} is the non-smooth part of the derivative. If the indicator function I is approximated by a smooth function, B^{ndr} is approximated by a classical derivative and there is no more difference between the smooth part B^{nd} and the non-smooth part B^{ndr} . In our point of view, the non-smooth mechanics point of view, the free energy is Ψ and the non-dissipative force associated to β is $B^{ndr} + B^{nd} \in \partial \Psi$.

Note If we do not assume that the temperature is positive, we replace the relation (24) by :

the entropy is a function of (E,x,t) which satisfies

$$s(E,x,t) \in -\frac{\partial \Psi}{\partial T}(E) + \partial I_{+}(T).$$

This relation implies that $\partial I_+(T)$ is not empty. It results that the temperature T is positive. It shows also that if the temperature is strictly positive the classical Helmholtz relation (24) is verified.

To complete the description of the constitutive laws, we assume the assumption (14) made in paragraph 5 is satisfied : there exist four functions of E and of $f \in S$, $c \in \mathbb{R}$, $g \in \mathbb{R}^3$, $p \in \mathbb{R}^3$ and other quantities χ depending on the history of the material: σ^d , B^d , H^d , and Q^d which satisfy

$$\forall \mathbf{x}, \mathbf{t}, \forall \mathbf{E}, \forall \mathbf{W} = (\mathbf{f}, \mathbf{c}, \mathbf{g}, \mathbf{p}) \in \mathbf{S} \mathbf{x} \mathbf{R} \mathbf{x} \mathbf{R}^3 \mathbf{x} \mathbf{R}^3, \forall \boldsymbol{\chi},$$

 $(14), \quad \sigma^d(\mathbf{x}, t, E, W, \chi): \mathbf{f} + \mathbf{B}^d(\mathbf{x}, t, E, W, \chi)\mathbf{c} + \mathbf{H}^d(\mathbf{x}, t, E, W, \chi). \mathbf{g} + \mathbf{Q}^d(\mathbf{x}, t, E, W, \chi). \mathbf{p} \ge 0.$

Then the constitutive laws are defined by the following relations

(15), $\sigma = \sigma^d(\mathbf{x}, t, E, \delta E, \chi) + \sigma^{nd}(E)$,

- (26), $B = B^{d}(x,t,E,\delta E,\chi) + B^{nd}(E) + B^{ndr}(E,x,t)$,
- (17), $\mathbf{H} = \mathbf{H}^{d}(\mathbf{x},t,E,\delta E,\chi) + \mathbf{H}^{nd}(E)$,
- (18), $T\mathbf{q} = \mathbf{Q}^{d}(\mathbf{x},t,E,\delta E,\chi)$,

where $E = (\varepsilon, \beta, grad\beta, T)$ et $\delta E = (\frac{d^{l}\varepsilon}{dt}, \frac{d^{l}\beta}{dt}, grad\frac{d^{l}\beta}{dt}, grad\frac{l}{T})$.

The functions σ^d , B^d , H^d and Q^d are the dissipative or irreversible forces. Let us note that the constitutive laws are obviously deterministic because the time derivatives are left derivatives. We must prove that our choice is such that the Clausius-Duhem inequality is satisfied. The following theorem shows that we have the expected properties.

<u>Theorem 4.</u> If the state laws (13), (24) and (25), the constitutive laws (15), (26), (17) and (18) and the inequality (14) are satisfied then,

- (i) the internal constraint (19) is satisfied;
- (ii) the Clausius-Duhem rellation (23) is satisfied.

<u>Proof</u> We have already seen that the state law (25) implies that the internal constraint (19) is satisfied because the subdifferential set $\partial I(\beta)$ is not empty. Let us replace W by $\delta E = (\frac{d^{1}\varepsilon d^{1}\beta}{dt}, \frac{d^{1}\beta}{dt}, \frac{d^{1}\beta}{dt}, \frac{d^{1}\beta}{dt})$ in the inequality (14). Let us replace also the dissipative forces by their expression given by the constitutive laws (15), (26), (17) and (18). We get

$$\begin{split} (\sigma - \sigma^{nd}(E)) &: \frac{d^{l}\epsilon}{dt} + (B - B^{nd}(E) - B^{ndr}(E, \mathbf{x}, t)) \frac{d^{l}\beta}{dt} + (H - H^{nd}(E)) \cdot \mathbf{grad} \frac{d^{l}\beta}{dt} \\ &+ T\mathbf{q} \cdot \mathbf{grad} \frac{1}{T} \ge 0. \end{split}$$

This relation gives with the state laws (13), (24) and (25),

(27),
$$\sigma: \frac{d^{l}\varepsilon}{dt} + B\frac{d^{l}\beta}{dt} + H.\mathbf{grad}\frac{d^{l}\beta}{dt} - \frac{d^{l}\Psi}{dt} - B^{ndr}(E,x,t)\frac{d^{l}\beta}{dt} + T\mathbf{q}.\mathbf{grad}\frac{1}{T} - s\frac{d^{l}T}{dt} \ge 0.$$

Because the assumptions of theorem 3 are satisfied, the relation (20) with $C = B^{ndr}(E, x, t)$ gives

$$-\frac{\mathrm{d}^{\mathbf{l}}\Psi}{\mathrm{d}t}-\mathrm{B}^{\mathrm{ndr}}(\mathrm{E},\mathbf{x},t)\frac{\mathrm{d}^{\mathbf{l}}\beta}{\mathrm{d}t}\leq-\frac{\mathrm{d}^{\mathbf{l}}\Psi}{\mathrm{d}t}.$$

This inequality and (27) give

$$\sigma: \frac{d^{l}\varepsilon}{dt} + B\frac{d^{l}\beta}{dt} + H.grad\frac{d^{l}\beta}{dt} + Tq.grad\frac{1}{T} - s\frac{d^{l}T}{dt} \ge \frac{d^{l}\Psi}{dt}$$

which is the Clausius-Duhem inequality (23) with left derivatives.

Let us sum up. In this theory, a material is defined by choosing

the state quantities E,

the linear spaces \mathbb{V} and \mathbb{C} ,

the power of the internal forces $P_i(D, V, c)$,

the quantities χ ,

the function $\underline{\Psi}$,

the functions σ^d , B^d , H^d and Q^d or the pseudo-potential of dissipation Φ .

8.1. Constitutive laws on discontinuity surfaces.

In this paragraph we do not make the small perturbation assumption. The state quantities or the velocities can be discontinuous on some surface. It is easy to prove that the equations of movement on those surfaces are,

 $m[U] = [\sigma.N],$

[H.N] = 0,

where m is the mass flux, N is a unit normal vector to the discontinuity line which divides the spaces into two parts denoted with the indices 1 and 2; $[Z] = Z_2 - Z_1$ denotes the discontinuity of the quantity Z. The energy balance is

 $\mathbf{m}[\mathbf{e}'] - \mathbf{\underline{T}} \cdot [\mathbf{U}] - \mathbf{h}[\mathbf{b}] = [-\mathbf{q} \cdot \mathbf{N}],$

where e' is the specific internal energy ($e = \rho e', \rho$ is the density)

h = H.N,
$$\underline{T} = \frac{1}{2}(T_1 + T_2), Q = -q.N.$$

Let us recall that b is the actual velocity of β , $b = \frac{d\beta}{dt}$. By using the mass balance, we get,

$$m([e'] - \underline{T}_N [\frac{l}{\rho}]) - \underline{T}_T \cdot [U_T] - h[b] - [Q] = 0,$$

where

 $\underline{T}_N = \underline{T}.N$, $\underline{T}_T = \underline{T} - \underline{T}_N N$ and $\underline{U}_T = \underline{U} - \underline{U}_N N$ is the tangential velocity.

The second principle of thermodynamics is

(28),
$$m[s'] - [\frac{Q}{T}] \ge 0$$
,

where s' is the specific entropy (s = ρ s') or

$$mT_{h}[s'] - T_{h}Q[\frac{1}{T}] - [Q] \ge 0,$$

where T_h is the harmonic average temperature $(\frac{1}{T_h} = \frac{1}{2}(\frac{1}{T_1} + \frac{1}{T_2}))$ and Q_m the average heat flux $(Q_m = \frac{1}{2}(Q_1+Q_2))$. It gives with the energy balance

$$([\mathbf{T}_h \mathbf{s}' - \mathbf{e}'] + \underline{\mathbf{T}}_N [\frac{1}{p}])\mathbf{m} - \mathbf{T}_h \mathbf{Q}_m [\frac{1}{T}] + \underline{\mathbf{T}}_T \cdot [\mathbf{U}_T] + \mathbf{h}[\mathbf{b}] \ge 0.$$

To describe the evolution of the discontinuity surface constitutive laws are needed. They are defined by assuming that there exist four functions of $\Delta E = (m, \frac{l}{T}], [U_T], [b])$ and of (\mathbf{x}, t) , $E = (E_1, E_2)$ and other quantities ξ depending on the history of the material : Y^d, Q^d, F^d, and h^d which satisfy

$$\forall \mathbf{x}, \mathbf{t}, \forall \mathbf{E}, \forall \mathbf{W} = (\mathbf{f}, \mathbf{g}, \mathbf{V}, \mathbf{c}) \in \mathbf{R} \times \mathbf{R} \times \mathbf{R}^2 \times \mathbf{R}, \forall \xi,$$

(29), $Y^{d}(x,t,E,W,\xi)f + Q^{d}(x,t,E,W,\xi)g + F^{d}(x,t,E,W,\xi)$. $V + h^{d}(x,t,E,W,\xi)c \ge 0$.

The constitutive laws are

$$\begin{split} & [T_h s' - e'] + \underline{T}_N \left[\frac{1}{\rho} \right] = Y^d(\mathbf{x}, t, E, \Delta E, \xi) \\ & -T_h Q_m = Q^d(\mathbf{x}, t, E, \Delta E, \xi), \\ & \underline{T}_T = \mathbf{F}^d(\mathbf{x}, t, E, \Delta E, \xi), \\ & h = h^d(\mathbf{x}, t, E, \Delta E, \xi). \end{split}$$

It is easy to prove that the preceeding constitutive laws are such that the second principle is satisfied:

<u>Theorem 5</u> If the inequality (29) is satisfied, the fondamental inequality (28) is satisfied in any actual evolution such that the temperature is strictly positive.

<u>Proof.</u> Write the inequality (29) with the actual velocities $W = \Delta E = (m, [\frac{1}{T}], [U_T], [b])$ and substract the energy balance to get the fondamental inequality multiplied by the harmonic average temperature.

Let us sum up again. In this theory, a material is defined by choosing

the state quantities E,

the linear spaces \mathbb{V} and \mathbb{C} ,

the power of the internal forces $P_i(D, V, c)$,

the quantities χ ,

the function Ψ ,

the functions σ^d , B^d , H^d and Q^d or the pseudo-potential of dissipation Φ ,

the quantities ξ ,

the functions Y^d , Q^d , F^d , and h^d or the pseudo-potential of dissipation on the discontinuity surface

8.1.1. Example of constitutive laws on discontinuity lines.

We choose pseudo-potential of dissipation $\Phi_s(\Delta E) = I_{0r}(\frac{1}{|T|})$ where I_{0r} is the indicator function of $\mathbf{R} \times \{0\} \times \mathbf{R}^2 \times \mathbf{R}$. It gives the constitutive laws,

 $Y^{d}(\Delta E) = 0, Q^{d}(\mathbf{x}, t, E, \Delta E) \in \partial I_{0r}([\frac{1}{T}]), \mathbf{F}^{d}(\Delta E) = 0 \text{ and } h^{d}(\Delta E) = 0.$

It results from the second constitutive law that the temperature is continuous. If we assume that the density is continuous, the first constitutive law gives

 $[Ts'-e'] = -[\Psi'] = 0.$

The two last laws show that there is no friction and no flux of damage work on the discontinuity surface. These constitutive laws are often chosen to describe phase changes occuring in solids.

9. Shape memory alloys. A macroscopic theory.

9.1. Introduction.

This chapter is devoted to the construction of models able to describe at the macroscopic level the evolution of a structure made of shape memory alloys. The internal constraints on the state quantites will play a major role and account for most of the striking properties of the shape memory alloys.

9.2. The state quantities.

As already mentionned we deal only with macroscopic phenomenons and macroscopic quantities. Thus to describe the deformations of the alloy, we choose the macroscopic deformation ε . For the sake of simplicity we assume this deformation to be small (a large deformation theory based on those ideas exists). Of course the temperature T is a thermodynamical quantity.

The properties of shape memory alloys results from martensite-austenite phase changes produced either by thermal actions (as it is usual) or by mechanical actions. At the macroscopic level we need quantities to describe those phase changes. For this purpose we choose as new thermodynamical quantities the volume fractions β_i of the martensite and austenite. We think that

this choice is the more simple we can make. Again to be very simple we assume that only two martensites exist together with the austenite. The volume fractions of the martensites are β_1 and β_2 . The volume fraction of austenite is β_3 . Those volume fractions are not independent: they satisfy constraints, said as usual internal constraints,

 $(30), \quad 0 \le \beta_i \le 1,$

because the β 's are volumetric proportions. We assume that no void can appear in the evolutions of the alloy, i. e. $\beta_1+\beta_2+\beta_3 \ge 1$ and that no interpenetration of the phases can occur, i. e. $\beta_1+\beta_2+\beta_3 \le 1$. Thus the β 's satisfy an other internal constraint,

(31),
$$\beta_1 + \beta_2 + \beta_3 = 1$$
.

We think those internal constraints are physical properties.

The thermodynamical macroscopic state quantities we have chosen are $E = (\varepsilon, \beta_1, \beta_2, \beta_3, T)$ or $E = (\varepsilon, \beta_1, \beta_2, \beta_3, grad\beta_1, grad\beta_2, grad\beta_3, T)$ depending on the sophistication we wish. The second set $(\varepsilon, \beta_1, \beta_2, \beta_3, grad\beta_1, grad\beta_2, grad\beta_3, T)$ is chosen if we think that the composition of the alloy at one point is influenced by its neighbourhood. We note β the vector (β_i) .

9.3. The free energy.

As already said, we consider a shape memory alloy as a mixture of the three martensite austenite phases with volume fractions β_i . The volumetric energy of the mixture we choose is

(32),
$$\Psi(E) = \sum_{i=1}^{3} \beta_i \Psi_i(E) + Th(\beta)$$

where the Ψ_i are the volumetric free energies of the i phases and Th is a free energy describing interactions between the different phases. We have said that internal constraints are physical properties. Being physical properties we decide to take them into account with the two functions we have to describe the material, i.e. the free energy Ψ and the pseudo-potential of dissipation Φ . The pseudo-potential describes the kinematic properties, i.e. properties which depend on the velocities. The free energy describes the state properties. Obviously the internal constraints (30) and (31) are not kinematic properties. Thus we take them into account with the free energy Ψ . For this purpose, we assume the Ψ_i to be defined over the whole linear space spanned by the ε , β_i and grad β_i and define the extended free energy by

$$\underline{\Psi}(E) = \Psi(E) + TI_0(\beta) = \Psi(E) + I_0(\beta) = \sum_{i=1}^3 \beta_i \Psi_i(E) + T\underline{h}(\beta),$$

where I_0 is the indicator function of the convex set

$$C = \{(\gamma_1, \gamma_2, \gamma_3) \in \mathbb{R}^3; 0 \le \gamma_i \le 1; \gamma_1 + \gamma_2 + \gamma_3 = 1\},\$$

and the extended interaction free energy is defined by

$$\underline{h}(\beta) = h(\beta) + I_0(\beta).$$

The more simple choice for $h(\beta)$ we can make is $h(\beta) = 0$. There is no interaction between the different phases in the mixture. The extended interaction free energy $\underline{h}(\beta) = I_0(\beta)$ is equal to 0 when the mixture is physically possible ($\beta \in C$) and to $+\infty$ when the mixture is physically impossible ($\beta \notin C$). Properties of the extended free energies are given in the theorem,

<u>Theorem 6.</u> If the function $\Psi(\varepsilon, \beta, \operatorname{grad}\beta, T)$ is smooth, we have for any actual evolution, i.e. for any evolution such that $\beta \in C$ at any time t,

(33),
$$\forall \mathbf{B} \in \partial \mathbf{I}_0(\beta)$$
, $\frac{d^{\mathbf{U}}\Psi}{dt} = \frac{d^{\mathbf{U}}\Psi}{dt} \le \frac{d^{\mathbf{U}}\Psi}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta}{dt} = \frac{d^{\mathbf{U}}\Psi}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_1}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_3}{dt} = \frac{d^{\mathbf{U}}\varphi}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_1}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_3}{dt} = \frac{d^{\mathbf{U}}\varphi}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_1}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_2}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_3}{dt} + \mathbf{B} \cdot \frac{d^{\mathbf{U}}\beta_3}{dt}$

where the derivatives in the formula (33), $\frac{dl}{dt}$, are left derivatives.

<u>Proof</u>. It is identical to the proof of theorem 3.

The vector **B** is the thermodynamical reaction to the internal constraints (30) and (31). The subdifferential of the indicator function I_0 is rather easily computed :

<u>Theorem 7.</u> The subdifferential ∂I_0 is

 $\partial I_0(\beta) = (c,c,c)$, if β is an internal point of C ($0 < \beta_i < 1$ for any i);

 $\partial I_0(0,\beta_2,\beta_3) = (-a^2 + c,c,c)$, if $0 < \beta_i < 1$ for i = 2,3;

 $\partial I_0(0,0,1) = (-a^2 + c, -b^2 + c, c);$

where a, b and c are real numbers.

<u>Proof.</u> Let I_i be the indicator function of the set $\{(\gamma_1, \gamma_2, \gamma_3) \in \mathbb{R}^3 ; 0 \le \gamma_i \le 1\}$ and I_4 the indicator function of the set $\{(\gamma_1, \gamma_2, \gamma_3) \in \mathbb{R}^3 ; \gamma_1 + \gamma_2 + \gamma_3 = 1\}$. We have $I_0(\beta) = I_1(\beta) + I_2(\beta) + I_3(\beta) + I_4(\beta)$. It results from a theorem of convex analysis (see for instance Moreau [20]) that

 $\partial I_0(\beta) = \partial I_1(\beta) + \partial I_2(\beta) + \partial I_3(\beta) + \partial I_4(\beta),$

(be careful, this result obvious for smooth functions is not always true for convex non-smooth functions).

When $0 < \beta_i < 1$ for any i, we have $\partial I_0(\beta) = \partial I_4(\beta) = (c,c,c)$.

When $\beta_1 = 0$, $0 < \beta_i < 1$ for i = 2, 3, we have $\partial I_0(\beta) = \partial I_1(\beta) + \partial L_1(\beta) = (-a^2, 0, 0) + (c, c, c)$.

When $\beta_1 = \beta_2 = 0$, we have $\partial I_0(\beta) = \partial I_1(\beta) + \partial I_2(\beta) + \partial I_4(\beta) = (-a^2, 0, 0) + (0, -b^2, 0) + (c, c, c)$.

Note. It is also possible to prove the theorem by using the fact that the thermodynamical

reaction **B** is a vector of \mathbf{R}^3 normal to the convex set C of \mathbf{R}^3 .

As for the volumic free energies we choose,

$$\begin{split} \Psi_1(E) &= \frac{1}{2} \varepsilon^T : K_1 \varepsilon + \sigma_1(T)^T : \varepsilon - C_1 T LogT, \\ \Psi_2(E) &= \frac{1}{2} \varepsilon^T : K_2 \varepsilon + \sigma_2^T(T) : \varepsilon - C_2 T LogT, \\ \Psi_3(E) &= \frac{1}{2} \varepsilon^T : K_3 \varepsilon - \frac{l_a}{T_0} (T - T_0) - C_3 T LogT, \end{split}$$

where K_i are the elastic tensors, C_i the heat capacities of the phases. The stresses σ_1 and σ_2 depend on the temperature T. The quantity la is roughthy the martensite-austenite phase change latent heat (see paragraph 9.8.3). We denote σ^{T} : $\epsilon = \sigma_{ij}\epsilon_{ij}$. For the interaction function we choose

$$T\underline{h}(E) = I_0(\beta) \text{ or } T\underline{h}(E) = I_0(\beta) + \frac{k}{2}(\mathbf{grad}\beta_1)^2 + \frac{k}{2}(\mathbf{grad}\beta_2)^2,$$

depending on the sophistication of the model.

Because we want to describe the main basic features of the shape memory alloys behaviour, we assume for the sake of simplicity that the elastic tensors K_i and the heat capacities C_i are the same for all the phases:

$$C_i = C$$
, $K_i = K$, for $i = 1, 2$ and 3.

Always for the sake of simplicity we assume that

$$\sigma_1(T) = -\sigma_2(T) = -\tau(T).$$

Concerning the stress $\tau(T)$, we know that at high temperature the behaviour of the alloy is a classical elastic behaviour. Thus we have $\tau(T) = 0$ at high temperature and choose the schematic simple expression (always for the sake of simplicity),

$$\begin{aligned} \tau(T) &= (T - T_c)\underline{\tau}, \text{ for } T \leq T_c, \\ \tau(T) &= 0, \text{ for } T \geq T_c, \end{aligned}$$

with $\underline{\tau}_{11} \leq 0$ and assume the temperature T_c to be greater than T₀. With those assumption we get

$$\Psi(\mathbf{E}) = \frac{1}{2} \boldsymbol{\varepsilon}^{\mathrm{T}} : \mathbf{K} \boldsymbol{\varepsilon} - (\beta_1 - \beta_2) \boldsymbol{\tau}(\mathrm{T})^{\mathrm{T}} : \boldsymbol{\varepsilon} - \beta_3 \frac{\mathbf{l}_a}{\mathbf{T}_0} (\mathrm{T} - \mathrm{T}_0) - \mathrm{CTLogT}.$$

We have the Helmholtz relation

$$s(E) = -\frac{\partial \Psi}{\partial T}(E) = (\beta_1 - \beta_2) \underline{r}^T \cdot \varepsilon + \beta_3 \frac{l_a}{T_0} + C(1 + LogT), \text{ for } T \le T_c,$$

$$(24), \quad s(E) = -\frac{\partial \Psi}{\partial T}(E) = \beta_3 \frac{l_a}{T_0} + C(1 + LogT), \text{ for } T \ge T_c,$$

which gives the volumic internal energy,

$$e(E) = \Psi(E) + Ts(T) = \frac{1}{2} \varepsilon^T : K\varepsilon + (\beta_1 - \beta_2) T_c \underline{\tau}^T : \varepsilon + \beta_3 l_a + CT, \text{ for } T \le T_c,$$
$$e(E) = \Psi(E) + Ts(T) = \frac{1}{2} \varepsilon^T : K\varepsilon + \beta_3 l_a + CT, \text{ for } T \ge T_c.$$

<u>Note</u> When $T = T_c$, the energy can be discontinuous. On the discontinuity surface the equations of paragraph 8.1 apply. If one wants to avoid using them, the free energy function Ψ can be smoothed for the value $T = T_c$ to have the entropy continuous.

The non dissipative forces are defined by assuming that there exist functions σ^{nd} , B^{nd} , H^{nd} of E and B^{ndr} of (E,x,t) which satisfy

(13),
$$\sigma^{nd}(E) = \frac{\partial \Psi}{\partial \varepsilon}(E) = K\varepsilon - (\beta_1 - \beta_2)\tau(T),$$

(13),
$$\mathbf{B}^{nd}(\mathbf{E}) = \frac{\partial \Psi}{\partial \beta}(\mathbf{E}) = \begin{bmatrix} -\tau(\mathbf{T})^{\mathsf{T}:\mathbf{E}} \\ \tau(\mathbf{T})^{\mathsf{T}:\mathbf{E}} \\ \frac{\mathbf{l}_a}{\mathbf{T}_0}(\mathbf{T}-\mathbf{T}_0) \end{bmatrix}$$
,

(25),
$$\mathbf{B}^{ndr}(\mathbf{E},\mathbf{x},t) \in \partial I(\beta(\mathbf{x},t))$$
,

(13),
$$\mathbf{H}^{\mathrm{nd}}(\mathbf{E}) = \frac{\partial \Psi}{\partial (\mathbf{grad}\beta)}(\mathbf{E}) = \begin{vmatrix} \mathbf{k} \mathbf{grad}\beta_1 \\ \mathbf{k} \mathbf{grad}\beta_2 \\ \mathbf{0} \end{vmatrix}$$
.

To complete the description of the constitutive laws, we assume the assumption (14) made in paragraph 7 is satisfied: there exist four functions of E and of x,t, $f \in S$, $c \in \mathbb{R}^3$, $g \in \mathbb{R}^{3\times 3}$ and $p \in \mathbb{R}^3$ and other quantities χ depending on the history of the material : σ^d , \mathbb{B}^d , \mathbb{H}^d , and \mathbb{Q}^d which satisfy,

 $\forall \mathbf{x}, \mathbf{t} \forall \mathbf{E}, \forall \mathbf{W} = (\mathbf{f}, \mathbf{c}, \mathbf{g}, \mathbf{p}) \in \mathbf{Sx} \mathbf{R}^3 \mathbf{x} \mathbf{R}^3 \mathbf{x} \mathbf{R}^3, \forall \chi,$

 $(14), \quad \sigma^d(\mathbf{x}, t, E, W, \chi): \mathbf{f} + \mathbf{B}^d(\mathbf{x}, t, E, W, \chi)\mathbf{c} + \mathbf{H}^d(\mathbf{x}, t, E, W, \chi).\mathbf{g} + \mathbf{Q}^d(\mathbf{x}, t, E, W, \chi).\mathbf{p} \ge 0.$

Then the constitutive laws are defined by the following relations,

- (15), $\sigma = \sigma^{d}(\mathbf{x},t,E,\delta E,\chi) + \sigma^{nd}(E)$,
- (26), $\mathbf{B} = \mathbf{B}^{d}(\mathbf{x},t,E,\delta E,\chi) + \mathbf{B}^{nd}(E) + \mathbf{B}^{ndr}(E,\mathbf{x},t),$
- (17), $\mathbf{H} = \mathbf{H}^{d}(\mathbf{x}, t, E, \delta E, \chi) + \mathbf{H}^{nd}(E)$,
- (18), $Tq = Q^d(x,t,E,\delta E,\chi)$,

where $E = (\varepsilon, \beta, grad\beta, T)$ and $\delta E = (\frac{d^{l}\varepsilon}{dt}, \frac{d^{l}\beta}{dt}, grad\frac{d^{l}\beta}{dt}, grad\frac{l}{T})$.

9.4. The non-dissipative constitutive laws.

We assume that there is no mechanical dissipation (the functions σ^d , \mathbf{B}^d and \mathbf{H}^d are equal to 0) or that the non-thermal part of the pseudo-potential of dissipation is equal to 0. We know that this is not very realistic but it is a step towards the complete understanting of the constitutive laws. The results from this non-dissipative theory will be schematic. The constitutive laws are given by

(34),
$$\sigma = \sigma^{nd}(E) = \frac{\partial \Psi}{\partial \varepsilon}(E)$$
,

(35),
$$\mathbf{B} = \mathbf{B}^{nd}(\mathbf{E}) = \frac{\partial \Psi}{\partial \beta}(\mathbf{E}) + \mathbf{B}^{ndr}(\mathbf{E}, \mathbf{x}, t),$$

(36),
$$\mathbf{B}^{ndr}(\mathbf{E},\mathbf{x},t) \in \partial I_0(\beta(\mathbf{x},t))$$
,

(37),
$$\mathbf{H} = \mathbf{H}^{\mathrm{nd}}(\mathbf{E}) = \frac{\partial \Psi}{\partial (\mathbf{grad}\beta)}(\mathbf{E}),$$

(38),
$$T\mathbf{q} = \mathbf{Q}^{d}(\mathbf{E},\delta\mathbf{E},\boldsymbol{\chi}),$$

The last constitutive law gives the classical Fourier's law

$$\mathbf{q} = -\lambda \mathbf{grad} \mathbf{T},$$

where λ is the thermal conductivity, by choosing $Q^{d}(E, \delta E, \chi) = \lambda T^{3} \operatorname{grad}_{T}^{I}$.

9.5. Transformation of the equations. Elimination of $\beta_{3.}$

Because of the relation (31), we can select one of the β 's, for instance $\beta_3 = (1-\beta_1-\beta_2)$ and rewrite all the equations with the dissymetric set of state quantities $E_r = (\epsilon, \beta_1, \beta_2, T)$ or $E_r = (\epsilon, \beta_1, \beta_2, grad\beta_1, grad\beta_2, T)$.

Let us define

$$\beta_r = (\beta_1, \beta_2),$$

and the convex set C_r of \mathbb{R}^2 by

 $C_r = \{(\gamma_1, \gamma_2,) \in \mathbb{R}^2; 0 \le \gamma_1 \le 1; \gamma_1 + \gamma_2 \le 1\},\$

and note that $\gamma \in C$ is equivalent to $\gamma_r = (\gamma_1, \gamma_2) \in C_r$ and $\gamma_3 = 1 - \gamma_1 - \gamma_2$ or to $I_0(\gamma) = I_r(\gamma_r) = 0$, and $\gamma_3 = 1 - \gamma_1 - \gamma_2$ where I_r is the indicator function of C_r . Let us remark that $\mathbf{B}^{ndr} \in \partial I_0(\beta)$ is equivalent to

(39), $\beta \in C$ and $\forall \gamma \in C, 0 \ge B^{ndr}(\gamma - \beta) = B_1^{ndr}(\gamma_1 - \beta_1) + B_2^{ndr}(\gamma_2 - \beta_2) + B_3^{ndr}(\gamma_3 - \beta_3)$.

Thus the relation (39) is equivalent to

$$\beta_r = (\beta_1, \beta_2) \in C_r, \forall \gamma \in C_r, 0 \ge (B_1 - B_3)\gamma_1 + (B_2 - B_3)\gamma_2$$

or to

$$\mathbf{B}_{r}^{ndr} \in \partial \mathbf{I}_{r}(\beta_{r}) \text{ with } \mathbf{B}_{r}^{ndr} = \left| \begin{array}{c} \mathbf{B}_{1}^{ndr} - \mathbf{B}_{3}^{ndr} \\ \mathbf{B}_{2}^{ndr} - \mathbf{B}_{3}^{ndr} \end{array} \right|,$$

where I_r is the indicator function of the convex set C_r . Thus the equation (36) is equivalent to

(40),
$$\mathbf{B}_r^{ndr} \in \partial \mathbf{I}_r(\beta_r)$$
.

The power of the internal forces

$$P_{i}(D, \mathbf{U}, \frac{d\beta_{1}}{dt}, \frac{d\beta_{2}}{dt}, \frac{d\beta_{3}}{dt}, \mathbf{grad}, \frac{d\beta_{1}}{dt}, \mathbf{grad}, \frac{d\beta_{2}}{dt}, \mathbf{grad}, \mathbf{grad}, \frac{d\beta_{3}}{dt}) = -\int_{D} \sigma: D(\mathbf{U}) d\Omega$$
$$-\int_{D} \{B_{1}\frac{d\beta_{1}}{dt} + B_{2}\frac{d\beta_{2}}{dt} + B_{3}\frac{d\beta_{3}}{dt} + H_{1}.\mathbf{grad}, \frac{d\beta_{1}}{dt} + H_{2}.\mathbf{grad}, \frac{d\beta_{2}}{dt} + H_{3}.\mathbf{grad}, \frac{d\beta_{3}}{dt}\} d\Omega$$

becomes

$$P_{i}(D, \mathbf{U}, \frac{d\beta_{1}}{dt}, \frac{d\beta_{2}}{dt}, \mathbf{grad}\frac{d\beta_{1}}{dt}, \mathbf{grad}\frac{d\beta_{2}}{dt}) = -\int_{D} \sigma: D(\mathbf{U}) d\Omega$$
$$-\int_{D} \{(\mathbf{B}_{1} - \mathbf{B}_{3})\frac{d\beta_{1}}{dt} + (\mathbf{B}_{2} - \mathbf{B}_{3})\frac{d\beta_{2}}{dt} + (\mathbf{H}_{1} - \mathbf{H}_{3}).\mathbf{grad}\frac{d\beta_{1}}{dt} + (\mathbf{H}_{2} - \mathbf{H}_{3}).\mathbf{grad}\frac{d\beta_{2}}{dt}\} d\Omega$$
$$= -\int_{D} \sigma: D(\mathbf{U}) d\Omega - \int_{D} \{\mathbf{B}_{r}.\frac{d\beta_{r}}{dt} + \mathbf{H}_{r}.\mathbf{grad}\frac{d\beta_{r}}{dt}\} d\Omega,$$

with

$$\mathbf{B}_{\mathbf{r}} = \left| \begin{array}{c} \mathbf{B}_1 - \mathbf{B}_3 \\ \mathbf{B}_2 - \mathbf{B}_3 \end{array} \right| \text{ and } \mathbf{H}_{\mathbf{r}} = \left| \begin{array}{c} \mathbf{H}_1 - \mathbf{H}_3 \\ \mathbf{H}_2 - \mathbf{H}_3 \end{array} \right|.$$

The power of the external forces

$$P_{e}(D, \mathbf{U}, \frac{d\beta_{1}}{dt}, \frac{d\beta_{2}}{dt}, \frac{d\beta_{3}}{dt}) = \int_{D} \mathbf{f} \cdot \mathbf{U} d\Omega$$

+
$$\int_{D} \{A_{1} \frac{d\beta_{1}}{dt} + A_{2} \frac{d\beta_{2}}{dt} + A_{3} \frac{d\beta_{3}}{dt}\} d\Omega + \int_{\partial D} \mathbf{T} \cdot \mathbf{U} d\Gamma + \int_{\partial D} \{a_{1} \frac{d\beta_{1}}{dt} + a_{2} \frac{d\beta_{2}}{dt} + a_{3} \frac{d\beta_{3}}{dt}\} d\Gamma,$$

becomes

$$P_{e}(D, \mathbf{U}, \frac{d\beta_{1}}{dt}, \frac{d\beta_{2}}{dt}) = \int_{D} \mathbf{f} \cdot \mathbf{U} d\Omega$$

+ $\int_{D} \{(A_{1} - A_{3}) \frac{d\beta_{1}}{dt} + (A_{2} - A_{3}) \frac{d\beta_{2}}{dt}\} d\Omega + \int_{\partial D} \mathbf{T} \cdot \mathbf{U} d\Gamma + \int_{\partial D} \{(a_{1} - a_{3}) \frac{d\beta_{1}}{dt} + (a_{2} - a_{3}) \frac{d\beta_{2}}{dt}\} d\Gamma.$
= $\int_{D} \mathbf{f} \cdot \mathbf{U} d\Omega + \int_{D} \mathbf{A}_{r} \cdot \frac{d\beta_{r}}{dt} d\Omega + \int_{\partial D} \mathbf{T} \cdot \mathbf{U} d\Gamma + \int_{\partial D} \mathbf{a}_{r} \cdot \frac{d\beta_{r}}{dt} d\Gamma,$

with

$$\mathbf{A}_{\mathbf{r}} = \left| \begin{array}{c} \mathbf{A}_1 - \mathbf{A}_3 \\ \mathbf{A}_2 - \mathbf{A}_3 \end{array} \right|, \ \mathbf{a}_{\mathbf{r}} = \left| \begin{array}{c} \mathbf{a}_1 - \mathbf{a}_3 \\ \mathbf{a}_2 - \mathbf{a}_3 \end{array} \right|.$$

We define also

$$\begin{split} h_{r}(E_{r}) &= h(E), \ \Psi_{ir}(E_{r}) = \Psi_{i}(E), \ \text{with} \ \beta_{3} = (1-\beta_{1}-\beta_{2}), \\ \Psi_{r}(E_{r}) &= \beta_{1}\Psi_{1r}(E_{r}) + \beta_{2}\Psi_{2r}(E_{r}) + (1-\beta_{1}-\beta_{2})\Psi_{3r}(E_{r}) + Th_{r}(E_{r}), \\ \Psi_{r}(E_{r}) &= \Psi_{r}(E_{r}) + I_{r}(\beta_{r}) = \beta_{1}\Psi_{1r}(E_{r}) + \beta_{2}\Psi_{2r}(E_{r}) + (1-\beta_{1}-\beta_{2})\Psi_{3r}(E_{r}) + T\underline{h}_{r}(E_{r}), \end{split}$$

with

 $T\underline{h}_r(E_r) = Th_r(E_r) + I_r(\beta_r).$

The expressions of the different powers show that equations of the movement,

- (5), $0 = \operatorname{div} \mathbf{H} \mathbf{B} + \mathbf{A}$, in D,
- (6), $\mathbf{H}.\mathbf{N} = \mathbf{a}$, in ∂D ,

become,

 $(5ter),0 = div H_r - B_r + A_r$, in D,

(6ter), $\mathbf{H}_{r} \cdot \mathbf{N} = \mathbf{a}_{r}$, in ∂D .

In the case where the power of the internal forces does depend on the gradients the equation (5bis) becomes $% \left(\frac{1}{2} \right) = 0$

 $(5quatro), 0 = -\mathbf{B}_{r} + \mathbf{A}_{r}, \text{ in } D.$

The non dissipative internal forces are

$$\sigma_r^{nd}(E_r) = \frac{\partial \Psi_r}{\partial \varepsilon}(E_r) = \sigma^{nd}(E) = \frac{\partial \Psi}{\partial \varepsilon}(E), \text{ with } \beta_3 = (1 - \beta_1 - \beta_2).$$

$$\mathbf{B}_{\mathbf{r}}^{\mathsf{nd}}(\mathbf{E}_{\mathbf{r}}) = \frac{\partial \Psi_{\mathbf{r}}}{\partial \beta_{\mathbf{r}}} (\mathbf{E}_{\mathbf{r}}) = \mathbf{Y}_{\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) = \begin{vmatrix} \Psi_{1\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) - \Psi_{3\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) \\ \Psi_{2\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) - \Psi_{3\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) \end{vmatrix} = \begin{vmatrix} -\tau(\mathbf{T})^{\mathsf{T}} : \varepsilon - \frac{\mathbf{l}_{3}}{T_{0}}(\mathbf{T} - T_{0}) \\ \tau(\mathbf{T})^{\mathsf{T}} : \varepsilon - \frac{\mathbf{l}_{3}}{T_{0}}(\mathbf{T} - T_{0}) \end{vmatrix}$$

(40), $\mathbf{B}_{\mathbf{r}}^{nd\mathbf{r}}(\mathbf{E}_{\mathbf{r}},\mathbf{x},t) \in \partial \mathbf{I}_{\mathbf{r}}(\beta_{\mathbf{r}},(\mathbf{x},t))$,

$$\mathbf{H}_{r}^{nd}(\mathbf{E}_{r}) = \frac{\partial \Psi_{r}}{\partial (\mathbf{grad}\beta_{r})} (\mathbf{E}_{r}) = \begin{vmatrix} \mathbf{k} \mathbf{grad}\beta_{1} \\ \mathbf{k} \mathbf{grad}\beta_{2} \end{vmatrix}$$

The constitutive laws (34) to (38) give the constitutive laws for σ , \mathbf{q} and for \mathbf{B}_r , \mathbf{H}_r , depending on x,t, \mathbf{E}_r and $\delta \mathbf{E}_r = (\frac{d\varepsilon}{dt}, \frac{d\beta_1}{dt}, \frac{d\beta_2}{dt}, \mathbf{grad}, \frac{d\beta_2}{dt}, \mathbf{grad}, \frac{d\beta_2}{dt}, \mathbf{grad}, \mathbf{f})$ if there is dissipation,

(41), $\sigma = \sigma_r^{d}(\mathbf{x}, t, E_r, \delta E_r, \chi) + \sigma_r^{nd}(E_r),$

(42),
$$\mathbf{B}_r = \mathbf{B}_r^{d}(\mathbf{x}, t, E_r, \delta E_r, \chi) + \mathbf{B}_r^{nd}(E_r) + \mathbf{B}_r^{ndr}(E_r, \mathbf{x}, t)$$

(43),
$$\mathbf{H}_r = \mathbf{H}_r^d(\mathbf{x},t,E_r,\delta E_r,\chi) + \mathbf{H}_r^{nd}(E_r)$$
,

(44),
$$T\mathbf{q} = \mathbf{Q}_{\mathbf{r}}^{d}(\mathbf{x}, \mathbf{t}, \mathbf{E}_{\mathbf{r}}, \delta \mathbf{E}_{\mathbf{r}}, \chi),$$

and

(45),
$$\beta_3 = (1 - \beta_1 - \beta_2)$$
.

The dissipative forces σ_r^d , B_r^d , H_r^d and Q_r^d can be defined with the functions σ^d , B^d , H^d and Q^d , with

$$\begin{aligned} \mathbf{H}_{r}^{d}(\mathbf{x}, t, \mathbf{E}_{r}, \delta \mathbf{E}_{r}, \chi) &= \begin{vmatrix} \mathbf{H}_{1}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) - \mathbf{H}_{3}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) \\ \mathbf{H}_{2}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) - \mathbf{H}_{3}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) \end{vmatrix}, \\ \mathbf{B}_{r}^{d}(\mathbf{x}, t, \mathbf{E}_{r}, \delta \mathbf{E}_{r}, \chi) &= \begin{vmatrix} \mathbf{B}_{1}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) - \mathbf{B}_{3}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) \\ \mathbf{B}_{2}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) - \mathbf{B}_{3}^{d}(\mathbf{x}, t, \mathbf{E}, \delta \mathbf{E}, \chi) \end{vmatrix}, \text{ with } \beta_{3} = (1 - \beta_{1} - \beta_{2}), \end{aligned}$$

and

$$\sigma_r^d(\mathbf{x}, t, E_r, \delta E_r, \chi) = \sigma^d(\mathbf{x}, t, E, \delta E, \chi) \text{ and } \mathbf{Q}_r^d(\mathbf{x}, t, E_r, \delta E_r, \chi) = \mathbf{Q}^d(\mathbf{x}, t, E, \delta E, \chi),$$

with $\beta_3 = (1 - \beta_1 - \beta_2)$,

or directly with functions $\sigma_r^d(\mathbf{x},t,E_r,\delta E_r,\chi)$, $\mathbf{B}_r^d(\mathbf{x},t,E_r,\delta E_r,\chi)$, $\mathbf{H}_r^d(\mathbf{x},t,E_r,\delta E_r,\chi)$ and $\mathbf{Q}_r^d(\mathbf{x},t,E_r,\delta E_r,\chi)$ which satisfy the inequality,

$$\forall \mathbf{x}, \mathbf{t}, \forall \mathbf{E}_{\mathbf{r}}, \forall \mathbf{W}_{\mathbf{r}} = (\mathbf{f}, \mathbf{c}_{\mathbf{r}}, \mathbf{g}_{\mathbf{r}}, \mathbf{p}) \in \mathbf{S} \mathbf{x} \mathbf{R}^{2} \mathbf{x} \mathbf{R}^{2} \mathbf{x} \mathbf{R}^{3}, \forall \boldsymbol{\chi},$$

(14bis), $\sigma_r^d(\mathbf{x}, t, E_r, W_r, \boldsymbol{\gamma}): \mathbf{f} + \mathbf{B}_r^d(\mathbf{x}, t, E_r, W_r, \boldsymbol{\gamma})\mathbf{c}_r + \mathbf{H}_r^d(\mathbf{x}, t, E_r, W_r, \boldsymbol{\gamma}), \mathbf{g}_r + \mathbf{O}_r^d(\mathbf{x}, t, E_r, W_r, \boldsymbol{\gamma}), \mathbf{p} \ge 0$.

The constitutive laws we have are (40) to (44). Let us one more time emphasis that the internal constraints (30) and (31) are part of the constitutive laws.

9.6. <u>The first non-dissipative model.</u> A model is a set of partial differential equations able to describe the evolution of a structure i.e. able to compute the state E(x, t) knowing the initial situation at the initial time t = 0 and the external actions applied to the structure. In the case of a non dissipative model where $grad\beta$ is not a state quantity, $E = (\varepsilon, \beta_1, \beta_2, \beta_3, T)$ or $E_r = (\varepsilon, \beta_1, \beta_2, T)$ and $T\underline{h} = I$ or $T\underline{h}_r = I_r$. In fact we want to compute $(\mathbf{u}(\mathbf{x}, t), \beta_1(\mathbf{x}, t), \beta_2(\mathbf{x}, t), T(\mathbf{x}, t))$ where **u** is the small displacement. The equations are

- (2), $\rho\gamma = \text{div}\sigma + \mathbf{f}$, in Ω ,
- (3). σ .N = T, in $\partial \Omega$.

 $(5 \text{ quatro}), 0 = -\mathbf{B}_r + \mathbf{A}_r, \text{ in } \Omega,$

where Ω is the domain occupied by the structure. In the sequel we assume the external action A_r to be equal to 0;

(7bis),
$$\frac{\mathrm{d}\mathbf{e}_{\mathbf{r}}}{\mathrm{d}\mathbf{t}} + \mathrm{div}\mathbf{q} = \mathbf{r} + \sigma: \mathbf{D}(\mathbf{U}) + \mathbf{B}_{\mathbf{r}} \cdot \frac{\mathrm{d}\beta_{\mathbf{r}}}{\mathrm{d}\mathbf{t}}, \text{ in } \Omega,$$

(8),
$$-\mathbf{q} \cdot \mathbf{N} = \pi$$
, in $\partial \Omega$;

$$\sigma = \sigma^{nd}(E_r) = \frac{\partial \Psi_r}{\partial \varepsilon} (E_r),$$

$$B_r^{nd}(E_r) = \frac{\partial \Psi_r}{\partial \beta_r} (E_r) = Y_r(E_r) = \begin{vmatrix} \Psi_{1r}(E_r) - \Psi_{3r}(E_r) \\ \Psi_{2r}(E_r) - \Psi_{3r}(E_r) \end{vmatrix},$$

(40), $\mathbf{B}_{r}^{ndr}(\mathbf{E}_{r},\mathbf{x},t) \in \partial \mathbf{I}_{r}(\beta_{r},(\mathbf{x},t)),$

(46),
$$\mathbf{B}_{\mathbf{r}}^{\mathrm{nd}}(\mathbf{E}_{\mathbf{r}}) + \mathbf{B}_{\mathbf{r}}^{\mathrm{ndr}}(\mathbf{E}_{\mathbf{r}}, \mathbf{x}, t) = \mathbf{B}_{\mathbf{r}} = \mathbf{A}_{\mathbf{r}} = 0$$
,

$$\mathbf{q} = -\lambda \mathbf{grad}\mathbf{T},$$

and

(45), $\beta_3 = (1 - \beta_1 - \beta_2);$

$$e_r = \Psi_r - Ts_r$$

This long list of equation gives a set of partial differential equations for the unknowns $(\mathbf{u},\beta_1,\beta_2,T)$. It is completed with boundary conditions and initial conditions for the equations (2) and (7bis). This set of partial differential equations can be investigated with mathematics and numerical methods [8], [30], [31], [24], [33]. This model will be the basic model we study in the sequel.

9.7. <u>The second non-dissipative model.</u> It is the previous model with a new interaction function,

$$T\underline{h}_{r}(E_{r}) = \frac{k}{2}(\mathbf{grad}\beta_{1})^{2} + \frac{k}{2}(\mathbf{grad}\beta_{2})^{2} + I_{r}(\beta_{r}),$$

The equations which are new or different from those of the previous paragrah are:

the equations of movement,

 $(5ter),0 = div H_r - B_r + A_r$, in Ω ,

(6ter), $\mathbf{H}_{\mathbf{r}} \cdot \mathbf{N} = \mathbf{a}_{\mathbf{r}}$, in $\partial \Omega$;

the energy balance equation,

(7ter),
$$\frac{d\mathbf{e}_r}{dt} + di\mathbf{v}\mathbf{q} = \mathbf{r} + \sigma: \mathbf{D}(\mathbf{U}) + \mathbf{B}_r \cdot \frac{d\beta_r}{dt} + \mathbf{H}_r \cdot \mathbf{grad} \frac{d\beta_r}{dt}$$
, in Ω ,

and the new constitutive law

(47),
$$\mathbf{H}_{r} = \mathbf{H}_{r}^{nd}(\mathbf{E}_{r}) = \frac{\partial \Psi_{r}}{\partial (\mathbf{grad}\beta_{r})} (\mathbf{E}_{r}).$$

The list of equation is a long one! The partial differential equations are (2), (3), (5ter), (6ter) and (7ter), (8). The constitutive laws are (40), (41) with $\sigma_r^d = 0$, (42) with $\mathbf{B}_r^d = 0$, (43) with $\mathbf{H}_r^d = 0$, (44), (45) and (47).

9.8. An example of non-dissipative evolution.

Let us consider a unidimendional experiment and assume ε_{11} to be the only non zero deformation. Let us also assume that $grad\beta_i = 0$ in the second model for the results to apply to both the two non-dissipative models. Let us focus on the stress σ_{11} as a function of ε_{11} when the temperature is fixed. From relation (40) we have

(48), $\sigma_{11} = K_{1111} \epsilon_{11} + \tau_{11}(T)(\beta_2 - \beta_1)$,

from relations (41), (42) and (43) we get,

(49),
$$-Y_r(E_r) \in \partial I_r(\beta_r)$$
,

with

$$\mathbf{Y}_{\mathbf{r}}(\mathbf{E}_{\mathbf{r}}) = \begin{bmatrix} -\tau_{11}(T)\varepsilon_{11} + \frac{l_a}{T_0}(T-T_0) \\ \tau_{11}(T)\varepsilon_{11} + \frac{l_a}{T_0}(T-T_0) \end{bmatrix}.$$

The relation (49) means that the vector $-\mathbf{Y}_r(\mathbf{E}_r)$ is normal to the triangle C_r at the point β_r (figure 2).



Figure 2 The vector $-\mathbf{Y}_r(\mathbf{E}_r)$ is normal to the triangle C_r .

9.8.1. Low temperature behaviour $(T < T_0)$.

The temperature is fixed and low, $T < T_0$. We look for $\sigma_{11} = \sigma$, β_1 and β_2 as functions of $\epsilon_{11} = \epsilon$. The two components of $\mathbf{Y}_r(\mathbf{E}_r)$ $\mathbf{Y}_{r1}(\mathbf{E}_r) = -\tau_{11}(T)\epsilon + \frac{l_a}{T_0}(T-T_0)$ and $\mathbf{Y}_{r2}(\mathbf{E}_r) = \tau_{11}(T)\epsilon + \frac{l_a}{T_0}(T-T_0)$, are shown on figure 3.



Figure 3 The components of $Y_r(E_r)$ versus $\varepsilon = \varepsilon_{11}$ at low temperature.

When $\varepsilon = 0$, the two component of the vector $-\mathbf{Y}_r(\mathbf{E}_r)$ are equal and positive. This vector can be normal to the triangle C_r only on the side AB (figure 4). Thus $\beta_3 = 0$ and we have a mixture of the two martensites. The stress σ can take any value of the segment $[\tau_{11}(T), -\tau_{11}(T)]$ (we have $\tau_{11}(T) = (T-T_c)\underline{r}_{11} > 0$ because we have assumed $\underline{r}_{11} < 0$).

When $\varepsilon > 0$, we have $-Y_{r1}(E_r) > 0$ and $-Y_{r1}(E_r) > -Y_{r2}(E_r)$. The only point where $-Y_r(E_r)$ can be normal to the triangle C_r is the vertex A (figure 4).



Figure 4 The vector $-\mathbf{Y}_r(\mathbf{E}_r)$ for different deformations $\boldsymbol{\epsilon}$ at low temperature.

Thus $\beta_1 = 1$: there is only the martensite number one and $\sigma = K\epsilon - \tau_{11}(T)$ (figure 5), (we let $K = K_{1111}$).

When $\varepsilon < 0$, we have $-Y_{r2}(E_r) > 0$ and $-Y_{r2}(E_r) > -Y_{r1}(E_r)$. The vector $-Y(E_r)$ is normal to the triangle C_r at the vertex B (figure 4). Thus $\beta_2 = 1$: there is only the martensite number two and $\sigma = K\varepsilon + \tau_{11}(T)$, (figure 5).



Figure 5 The non-dissipative constitutive low at low temperature.

We get some of the properties of shape memory alloys : at low temperature there is no austensite but mixtures of martensites ; there is a softening of the behaviour when going from compression to tension. Of course the behaviour at the origin is not the actual one but it has some of its properties.

9.8.2. <u>Medium temperature behaviour $(T_0 < T < T_c)$ </u>. The temperature is fixed and satisfies $T_0 \le T \le T_c$. The two components of the vector $\mathbf{Y}_r(\mathbf{E}_r)$ are shown on figure 6.



When $\varepsilon = 0$ the two components of $Y_r(E_r)$ are equal and negative. The vector $Y_r(E_r)$ can be normal to the triangle C_r only at the vertex 0 (figure 7).



Figure 7 The vector $-\mathbf{Y}_r(\mathbf{E}_r)$ for different deformations $\boldsymbol{\epsilon}$ at medium temperature.

Thus $\beta_3 = 1$ and $\beta_1 = \beta_2 = 0$, there is only austenite. Relation (27) gives $\sigma = 0$ for $\varepsilon = 0$. When $\varepsilon \neq 0$, the vector $Y_{r1}(E_r)$ is normal to C_r at vertex 0 if its two components are negative i.e. for

$$-\frac{l_{a}(T-T_{0})}{T_{0}\tau_{11}(T)} \le \varepsilon \le \frac{l_{a}(T-T_{0})}{T_{0}\tau_{11}(T)} = \varepsilon_{1}.$$

Thus for $\varepsilon \in]-\varepsilon_1, \varepsilon_1[$, there is only austenite, $\beta_3 = 1$, and from (48), $\sigma = K\varepsilon$ (figure 8).



Figure 8 The constitutive low at medium temperature.

For $\varepsilon = \varepsilon_1$, we have $Y_{r1}(E_r) = 0$. The vector $-Y_r(E_r)$ is normal to the triangle C_r on the side OA (figure 7) and $\beta_1 + \beta_3 = 1$: we have a mixture of austenite and martensite number one. The stress σ can take any value of the segment [K ε_1 , K $\varepsilon_1 - \tau_{11}(T)$] (figure 8).

For $\varepsilon > \varepsilon_1$, we have $-Y_{r1}(E_r) > 0$ and $-Y_{r2}(E_r) < 0$. The vector $-Y_r(E_r)$ is normal to the triangle C_r at the vertex A (figure 7) and $\beta_1 = 1$, there is only the martensite number one and the stress is $\sigma = K\varepsilon - \tau_{11}(T)$.

The increase of deformation produces the martensite-austenite phase change. We have the same result when decreasing the deformation: phase change from austenite to martensite number two occurs at $\varepsilon = -\varepsilon_1$. When $\varepsilon < -\varepsilon_1$ there is only martensite number two, $\beta_2 = 1$, and the stress is $\sigma = K\varepsilon + \tau_{11}(T)$, (figure 8).

9.8.3. <u>Austenite martensite phase change latent heat</u>. Let us compute

$$\begin{split} Tds &= -Td(\frac{\partial\Psi}{\partial T}) = CdT + l_a \frac{T}{T_0} d\beta_3 - \underline{\tau}^T : \epsilon(d\beta_2 - d\beta_1) - (\beta_2 - \beta_1) \underline{\tau}^T : d\epsilon \\ &= Tds_r = CdT - (\underline{\tau}^T : \epsilon + l_a \frac{T}{T_0}) d\beta_2 + (\underline{\tau}^T : \epsilon - l_a \frac{T}{T_0}) d\beta_1 - (\beta_2 - \beta_1) \underline{\tau}^T : d\epsilon. \end{split}$$

When phase-change occurs at fixed medium temperature from austenite to martensite number one, at the deformation $\varepsilon = \varepsilon_1$, i.e when going from ε slightly lower than ε_1 to ε slightly greater than ε_1 the reversible heat received by the material is

$$\Delta Q = -l_a \frac{T}{T_0} + \underline{\tau}_{11} \varepsilon_1,$$

because $\Delta T = 0$, $\Delta \beta_3 = -1$, $\Delta \beta_2 = 0$, $\Delta \beta_1 = 1$. We have assumed $\underline{\tau}_{11} < 0$. Thus $\Delta Q < 0$. The austenite-martensite phase change is exothermic at medium temperature: when the material is deformed heat is produced. This result is in accordance with experiments [15], [26]. Let us note that the quantity l_a is the martensite austenite volumetric phase change latent heat at temperature T_0 of the undeformed material ($\varepsilon_1 = 0$ when $T = T_0$).

9.8.4. <u>High temperature behaviour $(T > T_c)$ </u>.

The temperature is fixed and satisfies $T > T_c$. We have $\tau_{11}(T) = 0$. Thus the two components of $-Y_r(E_r)$ are negative, equal and do not depend on ε . The vector $-Y_r(E_r)$ is normal to the triangle C_r at the vertex 0. Thus $\beta_3 = 1$: there is only austenite. The stress is given by (48), $\sigma = K\varepsilon$ (figure 26). We have the classical elastic behaviour at high temperature in accordance with experiments.

Let us conclude that even without dissipation we get some of the important features of the behaviour of shape memory alloys : the relatonships (σ , ε) at different temperatures looks like the actual ones; loading is exothermic at medium temperature, unloading is endothermic [15].

Even if it is not reasonable to expect a good description of evolutions with this non dissipative constitutive law, let us consider a deformed unloaded material at low temperature ($\varepsilon = \tau_{11}(T)$)

 $\varepsilon_2 = \frac{\tau_{11}(T)}{K}$, $\sigma = 0$, figure 5) and heat it to high temperature : the material goes back to the

undeformed state ($\varepsilon = 0$, $\sigma = 0$). This is one kind of shape memory!

The results will be much more better with an educated alloy.

9.9. The dissipation. The pseudo-potential of dissipation.

From experiments it is known that the behaviour of shape memory alloys depends on time, i.e the behaviour is dissipative. It results that the mechanical part of the pseudo-potential of dissipation Φ is not zero.

Again to deal only with the main features of the behaviour, we assume there is only dissipation with respect to the $\frac{\partial \beta_i}{\partial t}$. Because relation (45) implies

$$\frac{\partial \beta_3}{\partial t} = -\frac{\partial \beta_1}{\partial t} - \frac{\partial \beta_2}{\partial t},$$

we can eliminate the velocity $\frac{\partial \beta_3}{\partial t}$ in the constitutive laws. As we have already mentionned, we can also define directly the dissipative internal forces. We choose this way and define a pseudo-potential of dissipation,

(50),
$$\Phi_{r}(T, \frac{\partial \beta_{1}}{\partial t}, \frac{\partial \beta_{2}}{\partial t}, \operatorname{grad}_{\overline{T}}^{1}) = c \sqrt{\left\{ (\frac{\partial \beta_{1}}{\partial t})^{2} + (\frac{\partial \beta_{2}}{\partial t})^{2} \right\} + k\left\{ (\frac{\partial \beta_{1}}{\partial t})^{2} + (\frac{\partial \beta_{2}}{\partial t})^{2} \right\} + \frac{\lambda T^{3}}{2} (\operatorname{grad}_{\overline{T}}^{1})^{2}},$$

with $c \ge 0$ and $k \ge 0$. Of course this expression is induced by experimental results: the first term is related to the permanent deformations exhibited by experiments; the second term is related to the viscous aspect. It has a smoothing effect. We have also

$$\Phi_{r}(T,\frac{\partial\beta_{1}}{\partial t},\frac{\partial\beta_{2}}{\partial t},\mathbf{grad}_{\overline{T}}^{1}) = c \left\| \frac{\partial\beta_{r}}{\partial t} \right\| + k\left(\left\| \frac{\partial\beta_{r}}{\partial t} \right\| \right)^{2} + \frac{\lambda T^{3}}{2} (\mathbf{grad}_{\overline{T}}^{1})^{2},$$

where the euclidian norm is

$$\left\|\frac{\partial \beta_{t}}{\partial t}\right\| = \sqrt{\left\{(\frac{\partial \beta_{1}}{\partial t})^{2} + (\frac{\partial \beta_{2}}{\partial t})^{2}\right\}}.$$

9.10. <u>The dissipative constitutive laws.</u> Following paragraph 9.5 and assuming there is no quantity, we define the dissipative forces.

$$\sigma_{r}^{d}(\mathbf{x},t,\mathbf{E}_{r},\delta\mathbf{E}_{r}) = 0,$$
$$\mathbf{H}_{r}^{d}(\mathbf{x},t,\mathbf{E}_{r},\delta\mathbf{E}_{r}) = 0,$$
$$\partial \mathbf{G}_{r},\partial \mathbf{G}_{r},\partial \mathbf{G}_{r}$$

$$\mathbf{B}_{r}^{d}(\delta \mathbf{E}_{r}) \in \partial \Phi_{r}(\frac{\partial \mathbf{p}_{1}}{\partial t}, \frac{\partial \mathbf{p}_{2}}{\partial t}),$$

where the subdifferential of the non-smooth function Φ_r is

$$\begin{split} \partial \Phi_{\mathrm{r}}(\mathbf{x}, t, \frac{\partial \beta_{1}}{\partial t}, \frac{\partial \beta_{2}}{\partial t}) &= \mathbf{c} \cdot \frac{\frac{\partial \beta_{\mathrm{r}}}{\partial t}}{\left|\left|\frac{\partial \beta_{\mathrm{r}}}{\partial t}\right|\right|} + \mathbf{k} \frac{\partial \beta_{\mathrm{r}}}{\partial t}, \text{ if } \left|\left|\frac{\partial \beta_{\mathrm{r}}}{\partial t}\right|\right| \neq 0, \\ \partial \Phi_{\mathrm{r}}(\mathbf{x}, t, 0, 0) &\in S \text{ , if } \left|\left|\frac{\partial \beta_{\mathrm{r}}}{\partial t}\right|\right| = 0, \text{ with } S = \{S \in \mathbf{R}^{2}; \|S\| \leq c\}. \end{split}$$

The constitutive laws are then

(51),
$$\sigma = \sigma_r^{nd}(E_r)$$
,
(41), $\mathbf{B}_r^{nd}(E_r) = \frac{\partial \Psi_r}{\partial \beta_r}(E_r) = \mathbf{Y}_r(E_r) = \begin{vmatrix} \Psi_{1r}(E_r) - \Psi_{3r}(E_r) \\ \Psi_{2r}(E_r) - \Psi_{3r}(E_r) \end{vmatrix}$,
(42), $\mathbf{B}_r^{ndr}(E_r, \mathbf{x}, t) \in \partial I_r(\beta_r(\mathbf{x}, t))$,

$$(52), \quad \mathbf{B}_r = \mathbf{B}_r^{nd}(\mathbf{E}_r) + \mathbf{B}_r^{ndr}(\mathbf{E}_r, \mathbf{x}, t) + \mathbf{B}_r^{d}(\mathbf{x}, t, \frac{\partial \beta_1}{\partial t}, \frac{\partial \beta_2}{\partial t}),$$

(53),
$$\mathbf{H}_{r} = \mathbf{H}_{r}^{nd}(\mathbf{E}_{r})$$
,
(18), $T\mathbf{q} = \mathbf{Q}^{d}(\mathbf{E}_{r},\delta\mathbf{E}_{r}) = \lambda T^{3}\mathbf{grad}\frac{1}{T} \text{ or } \mathbf{q} = -\lambda \mathbf{grad}T$.

9.11. <u>The dissipative behaviour.</u> Although the dissipation is more interesting to describe evolutions of the material, let us briefly look for the equilibrium states, i.e find the (σ, ε) and β_r such that $\frac{\partial \beta_r}{\partial t} = 0$ in relations (52) and (5bis). We have already assumed that the external action A_r is equal to 0. For the sake of simplicity let us also assume that in the sequel grad $\beta_i = 0$. So the results apply at the two models taking or not taking into account the grad β_i . It results from our assumptions ($A_r = 0$ and grad $\beta_i =$ 0) and from the movement equations (5) or (5bis) that

(52bis),
$$0 = \mathbf{B}_{r}^{nd}(\mathbf{E}_{r}) + \mathbf{B}_{r}^{ndr}(\mathbf{E}, \mathbf{x}, t) + \mathbf{B}_{r}^{d}(\mathbf{x}, t, \frac{\partial \beta_{1}}{\partial t}, \frac{\partial \beta_{2}}{\partial t}).$$

9.11.1. Equilibrium at low temperature.

Because we have $\frac{\partial \beta_r}{\partial t} = 0$, $\mathbf{B}_r^d \in S$. The constitutive laws (41), (42) and the relation (52bis)

give

$$\mathbf{Y}_r + \mathbf{S}_r + \mathbf{R}_r = 0$$
, with $\mathbf{S}_r \in S$, $\mathbf{R}_r \in \partial \mathbf{I}_r(\beta_r)$.

This relation means that the vector $-(Y_r+S_r)$ is normal to the triangle C_r .



Figure 9 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle C_r .

Let $\varepsilon = 0$, the vectors $-(\mathbf{Y}_r + \mathbf{S}_r)$ (figure 9) have positive components (we have assumed $\frac{l_a}{T_0}(T_0 - T) > c$). Thus the only possibility for $-(\mathbf{Y}_r + \mathbf{S}_r)$ to be normal to the triangle is to be normal on the side AB. Thus $\beta_1 + \beta_2 = 1$: we have a mixture of the two martensites.

Let us increase ε , the vector $-\mathbf{Y}_r$ leans slightly on the side AB but because of \mathbf{S}_r it is still possible for the vector $-(\mathbf{Y}_r+\mathbf{S}_r)$ to be normal to the triangle C_r on the side AB. We still have a mixture of the two martensites: $\beta_1+\beta_2 = 1$. The stress is $\sigma \in K\varepsilon + [\tau_{11}(T), -\tau_{11}(T)]$, (figure 10).



Figure 10 The equilibrium position at low temperature .

When ε increases the vector $-\mathbf{Y}_r$ leans more and more on the side AB and for $\varepsilon > \frac{c}{\tau_{11}(T)} =$ ε_3 it is no more possible for $-(Y_r+S_r)$ to be normal to the side AB (figure 9). It is normal to the triangle at the vertex A: $\beta_1 = 1$, there is only the martensite number one. The stress is (figure 10), $\sigma = K\epsilon_3 - \tau_{11}(T).$

<u>Note</u>. We have assumed $\varepsilon_3 > \varepsilon_1$ or $cK = cK_{1111} > \tau_{11}^2(T)$. The results are slightly different when this assuption is not satisfied.

We have the symmetric result for ε negative (figure 10). The effect of dissipation is to increase the domain (σ , ε) where equilibrium is possible (figure 10).

9.11.2. Equilibrium at medium temperature. The effect of the set S is the same, it allows the vector $-(Y_r+S_r)$ to be normal to the triangle

 C_r on the side OA not only for $\varepsilon = \varepsilon_1$ but also for a small interval $[\varepsilon_4, \varepsilon_5]$ around ε_1 (figures 11 and 12).



Figure 11 The vector - $(Y_r + S_r)$ is normal to the triangle C_r .



Figure 12 The equilibrium position at medium temperature.

When ε is within this interval we have $\beta_1+\beta_3 = 1$: a mixture of austenite and martensite number one. Thus the stress is $\sigma \in K\epsilon + [-\tau_{11}(T), 0]$.

An analogous result is obtained for ε negative (figure 12).

9.11.3. Equilibrium at high temperature. The components of $-(Y_r+S_r)$ remain negative (we have assume $T > T_c$ and T large enough). Thus the vector $-(Y_r+S_r)$ is normal to the triangle C_r only at the vertex 0, (figure 13).



Figure 13 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ normal to the triangle C_r at high temperature.

We have only austenite, $\beta_3 = 1$, and $\sigma = K\epsilon$ (figure 26). The equilibrium position are not modified at high temperature by the dissipation.

9.12. Evolution of a shape memory alloy.

The dissipative terms of the constitutive law (52) or of the relation (52bis) involve derivatives with respect to the time. Thus they are differential equations. The natural problem to look at is the evolution of a material submitted to time dependant external actions. In this paragraph we study unidimensional experiments. We choose to apply the deformation $\varepsilon(t)$ because it is more easy to inverstigate the structure of the equations and exhibit the hysteretical properties of shape memory alloys.

To be specific we look at three experiments. The two first are at fixed low temperature, the last one at fixed high temperature.

In the first experiment, the deformation $\varepsilon(t)$ starting from 0 increases then decreases till the stress σ is zero (figure 14).



In the first experiment the applied deformation $\varepsilon(t)$ increases from 0 and decreases till the stress $\sigma(t)$ is zero. In the second experiment the applied deformation $\varepsilon(t)$ (dotted line) increases to a larger value, then decreases till the stress $\sigma(t)$ is zero.

In the second experiment, the deformation increases to a larger value then decreases again to a value such that the stress is zero (figure 14). In the last experiment, the deformation starting from 0 increases.

In all experiments the initial mixture is made of the two martensites with equal volume fractions $\beta_1(0) = \beta_2(0) = \frac{1}{2}$. The point which represents this mixture in the plane (β_1, β_2) is $\beta_r^0 = (\frac{1}{2}, \frac{1}{2})$.

9.12.1. First experiment at low temperature ($T < T_0$).

The point β_r^0 is an equilibrium position when $\varepsilon = 0$. The deformation $\varepsilon(t)$ increases from 0 as shown in figure 14. The vector $-\mathbf{Y}_r$ which at t = 0 is normal to the line AB leans progressively towards it (figure 15).



Figure 15 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle C_r .

When ε is not too large, $\varepsilon < \varepsilon_3 = \frac{c}{\tau_{11}(T)}$, it is possible to find $S_r \in S$ and $R_r \in \partial I_r(\beta_r)$ such that (52bis) is satisfied (figure 15). Thus we have $\frac{\partial \beta_r}{\partial t} = 0$. In the plane (σ, ε), (figure 17), this part of the evolution correspond to the line 1.

<u>Note</u>. The point $\beta_r(t)$ cannot go inside C_r because when $\beta_r(t)$ is inside $\mathbf{R}_r = 0$, $(\partial I_r(\beta_r) = \{0\})$. It would result from (52bis) that

 $-(Y_r+S_r) = 0$, which means that S_r and $\frac{\partial \beta_r}{\partial t}$ are directed outwards which is impossible because $\frac{\partial \beta_r}{\partial t}$ is directed inwards!

When $\varepsilon(t)$ goes beyong ε_3 it is no more possible to satisfy (52bis) with $\frac{\partial \beta_r}{\partial t} = 0$. Thus $\frac{\partial \beta_r}{\partial t}$ becomes non zero and is tangent to the triangle C_r (figure 15) with

$$\mathbf{S}_{\mathbf{r}} = \mathbf{c}\mathbf{t}_{\mathbf{r}} + \mathbf{k}\frac{\partial\beta_{\mathbf{r}}}{\partial t},$$

where t_r is the unit vector $\frac{AB}{|AB|}$. The volume fraction of the martensite number one increases while

the volume fraction of the martensite number two decreases. The stress σ is given by relation (48),

$$\sigma(t) = K\varepsilon(t) + \tau_{11}(T)(\beta_2(t) - \beta_1(t)).$$

The quantity $K\varepsilon(t)$ increases and the quantity $\tau_{11}(T)(\beta_2(t)-\beta_1(t))$ decreases. Assuming the first one to increase more than the second one decreases, the stress $\sigma(t)$ increases but more slowly than previously. It follows the line 2 in the (σ,ε) plane (figure 17).

Before $\beta_r(t)$ reaches the point A, we decrease the applied deformation (figure 14). The vector $-\mathbf{Y}_r$ begins to go back towards the normal vector to the line AB. Thus the modulus of the vector \mathbf{S}_r decreases. But it is still larger than c. The vector $\frac{\partial \beta_r}{\partial t}$ is not 0 but its modulus decreases.

The volume fraction $\beta_1(t)$ is still encreasing but more and more slowly. The stress $\sigma(t)$ decreases quickly because it is the sum of two decreasing quantities. It follows the line 3 in the (σ, ε) plane (figure 17).

When $\varepsilon(t)$ becomes lower than ε_3 , S_r is lower than c. Thus $\frac{\partial \beta_r}{\partial t} = 0$ and the composition of

the mixture β_r^1 remains constant. The value of the stress is

 $\sigma(t) = \mathrm{K}\varepsilon(t) + \tau_{11}(T)(\beta^1 2 - \beta^1 1).$

It is shown in figure 17 on the line 4. The stress is zero for (figure 17),

$$\varepsilon_0 = \frac{-\tau_{11}(T)(\beta_2 - \beta_1)}{K}.$$

The material remains in this position if no load is applied.

9.12.2. Second experiment at low temperature $(T < T_0)$.

The deformation applied at the beginning is the one applied in the first experiment. The deformation $\varepsilon(t)$ is increased till the point $\beta_r(t)$ reaches the vertex A. At this point $\partial I_r(A)$ is a larger set and is possible to find $\mathbf{R}_r \in \partial I_r(\beta_r) = \partial I_r(A)$ and $\mathbf{S}_r \in S$ such that the vector $-(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle (figure 16),

 $-(\mathbf{Y}_r + \mathbf{S}_r) = \mathbf{R}_r \in \partial \mathbf{I}_r(\beta_r).$



Figure 16 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle C_r at low temperature.

Thus we have $\frac{\partial \beta_r}{\partial t} = 0$. The stress σ versus the deformation ε before the point $\beta_r(t)$ reaches the vertex A is shown in figure 17 on the line 5.



Figure 17 The stress $\sigma(t)$ versus the deformation $\epsilon(t)$ in the first and second experiment.

When $\varepsilon(t)$ still increases the point $\beta_r(t)$ remains at the vertex A. The stress is

(54),
$$\sigma(t) = K\varepsilon(t) - \tau_{11}(T)$$
.

It is shown in figure 17 on the line 6. If we let $\varepsilon(t)$ decrease, we still have (52bis) with $S_r = 0$. Thus $\frac{\partial \beta_r}{\partial t} = 0$ and the stress is given by (54). It is zero for (figure 17), $\varepsilon = \varepsilon_2 = \frac{\tau_{11}(T)}{K}$.

The stress σ is shown on the line 7 of figure 17. The material remains in the position ($\beta_1 = 1$, $\beta_2 = \beta_3 = 0$, $\sigma = 0$, $\varepsilon = \varepsilon_2$) if no load is applied.

Note. It is clear that any point of the segment $[-\varepsilon_2, \varepsilon_2]$ can be reached. We have assumed that $\varepsilon_2 = \frac{\tau_{11}(T)}{K} < \frac{c}{\tau_{11}(T)}$ or $\tau_{11}^2(T) < cK$. When it is not true the results are slightly different.

An other evolution at medium temperature is shown in figure 18 exhibiting the classical features of hysteresis. The applied deformations starts from 0, increases and comes back to 0. The point ($\sigma(t)$, $\varepsilon(t)$) in figure 1! follows the path 1, 2, 3, 4, 5.



Figure 18 The stress $\sigma(t)$ versus the deformation $\epsilon(t)$ in an experiment at medium temperature.

9.12.3. Third experiment at high temperature $(T > T_c)$.

Let us repeat the first or second experiment at high temperature. The point β_r^0 is not an equilibrium point for $\beta_r(t)$. Thus the point $\beta_r(t)$ goes from β_r^0 to 0 on the segment [β_r^0 ,0] following the equation $\mathbf{Y}_r + \mathbf{S}_r = 0$ or

$$\begin{vmatrix} \frac{l_{a}}{T_{0}}(T-T_{0}) \\ \frac{l_{a}}{T_{0}}(T-T_{0}) \end{vmatrix} + \begin{vmatrix} -\frac{c}{\sqrt{2}} + k\frac{\partial\beta_{1}}{\partial t} \\ -\frac{c}{\sqrt{2}} + k\frac{\partial\beta_{1}}{\partial t} \end{vmatrix} = 0.$$

<u>Note</u>. We have assumed T large enough for $\frac{l_a}{T_0}(T-T_0) - \frac{c}{\sqrt{2}} > 0$.

When $\beta_r(t)$ reaches the origin, it remains at this point. During all the evolution, relation (48) shows that

 $\sigma(t) = K\epsilon(t).$

9.13. <u>The one shape memory effect.</u> Let us deform the alloy at low temperature, for instance let us make the first experiment. The alloy is deformed to the state ($\sigma = 0, \varepsilon = \varepsilon_0, \beta_r^{-1}$).

Let us heat it without applying any load ($\sigma(t) = 0$ during the process). The state ($\sigma = 0, \varepsilon =$ ϵ_0, β_r^1 is no more an equilibrium position for the alloy at high temperature thus it evolves towards the state ($\sigma = 0, \epsilon = 0, \beta_r = 0$).

The deformation is produced by thermal action: the alloys goes back to its reference shape. It remembers this reference shape.

Let us cool it. Nothing occurs! Because the situation ($\sigma = 0, \epsilon = 0, \beta_r = 0$) is an equilibrium position at low temperature.

9.14. The two shape memory effect.

The two shape memory effect can be obtained by a special thermomechanical treatment of the alloy which then can remember two shapes : one at low temperature an other one at high temperature. Depending on the temperature the shape goes from one to the other.

The thermomechanical treatment is called the education of the shape memory alloy. Its effect is to make one martensite to be dominant. It is much more present than the other one. In our point of view the effect of education is to replace the triangle C_r by the flattened triangle C_r^e (figure 19): the possible compositions of an educated shape memory alloy are within the triangle C_r^e (figure 19).



Figure 19 The educated shape memory triangle C_r^e . The possible compositions of the educated shape memory alloy are within the triangle C_r^e .

It is obvious that the martensite number one is much more present than the martensite number two. We assume that the point $\beta_r^0 = (\frac{1}{2}, \frac{1}{2})$ does not belong to C_r^e .

9.14.1. Equilibrium states at low temperature $(T < T_0)$. In the plane (σ, ε) the possible equilibrium positions are shown in figure 21.



Figure 20 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle C_r^e .



Figure 21 Equilibrium positions of an educated shape memory alloy at low temperature.

They result from equation (52bis) or

$$\mathbf{Y}_{\mathbf{r}} + \mathbf{S}_{\mathbf{r}} + \mathbf{R}_{\mathbf{r}} = \mathbf{0},$$

with $S_r \in S$ and $R_r \in \partial I_r^e(\beta_r)$, where I_r^e is the indicator function of the triangle C_r^e . Let us remind that equation (52bis) means that the vector $-(Y_r + S_r)$ is normal to the triangle C_r^e (figure 20).

When $\varepsilon = 0$, the two components of $-Y_r$ are positive and equal. Let us assume T » T₀ such that the components of $-(Y_r+S_r)$ are also positive. Thus the only possibility for the vector $-(Y_r+S_r)$ to be normal to the triangle C_r^e is to be normal on the side AB_e . Because the point $\beta_r^0 = (\frac{1}{2}, \frac{1}{2})$ does not belong to C_r^e , the stress $\sigma = K\varepsilon + \tau_{11}(T)(\beta_2 - \beta_1)$ cannot be equal to 0. Thus the point ($\varepsilon = 0$, $\sigma = 0$) cannot be an equilibrium state at low temperature.

The possible equilibrium states at low temperature are shown in figure 21. Depending on the values of T and c there are different possibilities for the equilibrium domain at low temperature (see figures 20, 21 and figures 22, 23). On figure 23, the deformation ϵ_4 is the smallest deformation for which there exists S_r for which $-(Y_r+S_r)$ is normal to AB_e and OB_e (figure 22). The deformation ϵ_5 is also the largest deformation for which $-(Y_r+S_r)$ can be normal to C_r^e on AB_e and OB_e (figure 22).



Figure 22 The vector - $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to the triangle C_r^e . It can be normal to the sides $\mathbf{B}_e \mathbf{A}$ and \mathbf{OB}_e for different vectors $\mathbf{S}_r \in S$.



Figure 23 Equilibrium positions of an educated shape memory alloy at low temperature.

9.14.2. Equilibrium states at medium temperature ($T_0 < T < T_c$).

They are shown in figure 24.



Figure 24 Equilibrium states of an educated shape memory alloy at medium temperature.

9.14.3. Equilibrium states at high temperature $(T > T_c)$. The components of $-Y_r$ are equal and negative. We assume $T \gg T_c$ such that the components of $-(Y_r+S_r)$ are also negative (figure 25).



Figure 25 The vector – $(\mathbf{Y}_r + \mathbf{S}_r)$ is normal to C_r^e at high temperature.

Thus the only possibility for this vector to be normal to C_r^e is to be normal at the point 0 ($\beta_r = 0$), (figure 25). The equilibrium states at high temperature satisfy (figure 26)

σ= Κε.



Figure 26 The constitutive law at high temperature.

9.14.4. Constitutive laws of a non-dissipative educated shape memory alloy They are obtained by letting c = 0 in the previous figures showing the equilibrium positions of the dissipative shape memory. The constitutive laws for the low and medium temperature are shown in the following figures 27 and 28. The constitutive law at high temperature is the one shown in the previous figure 26.



Figure 27 Constitutive law of a non-dissipative educated shape memory alloy at low temperature.



Figure 28 Constitutive law of a non-dissipative educated shape memory alloy at medium temperature.

9.14.5. The two shape memory effect.

Let us consider an unloaded ($\sigma = 0$) educated shape memory alloy at high temperature, T⁺. We have $\varepsilon = 0$. Let us cool it, the only unloaded ($\sigma = 0$) equilibrium state at low remperature, T⁻, is ($\sigma = 0, \varepsilon = \varepsilon_2$). If the temperature is again increased the alloys goes back to the state ($\sigma = 0, \varepsilon = 0$) and so on (figure 29). The alloys remembers two shapes: the state $E_r^+(\varepsilon = 0, \sigma = 0, \beta_3 = 1, T^+)$ and the state $E_r^-(\varepsilon = \varepsilon_2, \sigma = 0, \beta_1 = 1, T^-)$! One at high temperature and an other one at low temperature. The heat ΔQ which is received from the exterior during the phase change, for instance when going from E⁻ fo E⁺, is

$$\Delta Q = \Delta e_r = e_r^{+} - e_r^{-} = C\Delta T - \frac{1}{2} K(\epsilon_2)^2 - T_c \tau_{11} \epsilon_2 + l_a, (K = K_{1111})$$

with $\Delta T = T^{+} - T^{-}$ and $\epsilon_2 = \frac{\tau_{11}(T)}{K}$,
 $= C\Delta T + l_a - \{(T^{-})^2 - T_c^2\} \frac{\tau_{11}^2}{2K}$.

As we expect, it is positive because $T^- \leq T_c$.



Figure 29 The two shape memory effect. The state goes from $E_r^+(T^+, \varepsilon = 0, \sigma = 0, \beta_3 = 1)$ to $E_r^-(T^-, \varepsilon = \varepsilon_2, \sigma = 0, \beta_1 = 1)$ and from E_r^- to E_r^+ .

9.15. Smooth constitutive laws.

The equilibrium curves showing the stresses versus the deformations are non-smooth. They are angular. Experiments have shown that the pure martensite variants or mixtures, corresponding to the extreme points A and B in the triangle C_r . There is always a slight fraction of the second martensite at the point A (β_2 is very small but not zero). To take this property into account we replace the set of the possible mixture by a convex curvilinear triangle C_{rc} as shown in figure 30.



Figure 30 The curvilinear set of the possible mixtures of the martensites.

The effect of replacing the triangle C_r by the curvilinear C_{rc} on the extended free energy is to replace the indicator function I_r of C_r by the indicator function I_{rc} of C_{rc} . The effect on the constitutive laws is to replace the subdifferential ∂I_r by ∂I_{rc} . For instance the relations (40) is replaced by

(40bis),
$$\mathbf{B}_r^{ndr} \in \partial \mathbf{I}_{rc}(\beta_r)$$
,

which means that the reaction B_r^{ndr} is normal to the convex curvilinear triangle C_{rc} . The equation of movement (46) where we assume no dissipation,

(46),
$$\mathbf{B}_r^{nd}(\mathbf{E}_r) + \mathbf{B}_r^{ndr}(\mathbf{E}_r, \mathbf{x}, t) = \mathbf{B}_r = \mathbf{A}_r = 0$$
,

with

$$\mathbf{B}_{r}^{nd}(\mathbf{E}_{r}) = \frac{\partial \Psi_{r}}{\partial \beta_{r}} \left(\mathbf{E}_{r}\right) = \mathbf{Y}_{r}(\mathbf{E}_{r}) = \left| \begin{array}{c} \Psi_{1r}(\mathbf{E}_{r}) - \Psi_{3r}(\mathbf{E}_{r}) \\ \Psi_{2r}(\mathbf{E}_{r}) - \Psi_{3r}(\mathbf{E}_{r}) \end{array} \right|,$$

gives

 $-\mathbf{Y}_{r} \in \partial I_{rc}(\beta_{r}),$

which means that the vector $-\mathbf{Y}_r$ is normal to the convex curvilinear triangle C_{rc} (figure 30). The result is a smoothing effect as shown in the figure 31 on the constitutive law at low temperature.



figure 31 The smooth constitutive law at low temperature.

10. Evolutions of structures made of shape memory alloys.

The evolution of a structure made of shape memory alloys, i.e. the computation of $E_r(x,t) = (\varepsilon(x,t),\beta_1(x,t),\beta_2(x,t),T(x,t))$ depending on the point x of the domain occupied by the structure and on the time t can be performed by solving numerically the set of partial differential equations resulting from the movement equations (2), (3), (5ter), (6ter), (or (5bis)) and the energy balance (7ter), (or (7bis), (8), the constitutive laws (40), (41), (42), (43), (44), (45) and (47). completed by convenient initial and boundary conditions. Let us mention the numerical results given by Wörshing [33] where numerous practical and theoretical results can be found. The coherence in term of mathematics of the set of partial differential equations has been proved in theoretical mathematical papers[8], [30], [31].

11. Conclusion.

The models we have described are able to account for the different features of the shape memory alloys macroscopic mechanical and thermal properties. We have used schematic free energies and pseudo-potentials of dissipation. There are many possibilities to sophisticate the basic choices we have made to take into account the practical properties of the shape memory alloys. Let us for instance mention that the pseudo-potential of dissipation can be modified to describe more precisely the hysteretical properties of the shape meuory alloys. There is no difficulty to have more than two martensites, for instance to take care of the 24 possible martensites: 22 more β 's are to be introduced and the triangle C_r has to be replaced by the convex set C₂₄ = { $\beta \in \mathbb{R}^{24}$; $0 \le \beta_i \le 1$ for i =

1 to 24

Let us remark that the physical quantities to characterise an educated shape memory alloys are: K, C, l_a , T_a , T_c , $\underline{\tau}$, the two coordinates of \mathbf{B}_e for the tree energy and c, k for the pseudopotential of dissipation. It is not so many to have a complete multidimentional model which can be used for engineering purposes.

Let us also note the very important role of the internal constraints and of the reaction B^{ndr} to these internal constraints which are responsible for many properties. The way we have taken into account the internal constraints is general and can be developped in other circumstances [12], [13], [16], [32].

12. Appendix.

12.1. Convex function.

A convex function from **R** into $\mathbf{R} = \mathbf{R} \cup \{+\infty\}$; (figure 32), [20] is an application f whose value can be $+\infty$ at some point (the value $-\infty$ is forbidden) such that

 $\forall x, y \text{ and } \forall \theta \in]0,1[, f(\theta x + (1-\theta)y) \le \theta f(x) + (1-\theta)f(y).$

A convex function f from \mathbb{R}^2 into $\mathbb{R} = \mathbb{R} \cup \{+\infty\}$ is a function f such that

 $\forall \gamma \in \mathbf{R}^2, \forall \beta \in \mathbf{R}^2, \forall \theta \in]0,1[, f(\theta \gamma + (1-\theta)\beta) \le \theta f(\gamma) + (1-\theta)f(\beta).$



Figure 32

The convex function is not differentiable at point A. It has a generalized derivative: the slope of any line which passes through point A and is under the function f.

12.2. Subgradient and subdifferential of a convex function.

A convex function does not always have a derivative (for instance at the point A of figure 32) but it can have generalized derivatives, subgradients, which are the slopes of the lines which

pass through point A and are always under the function. The set of all the sub-gradients is the subdifferential denoted $\partial f(x_A)$. The subgradients have the following property

(55), $\forall p \in \partial f(x_A), \forall y, f(y) \ge f(x_A)+(y-x_A)p.$

Let us remark that the set $\partial f(x)$ is empty if $f(x) = +\infty$ (because f(y) which is finite for some y cannot be greater than $+\infty$). Thus the relation $p \in \partial f(x)$ has two meanings: first that f(x) is finite and second that relation (55) is satisfied.

A vector $Y \in \mathbb{R}^2$ is a subgradient of the convex function f from \mathbb{R}^2 into $\mathbb{R} = \mathbb{R} \cup \{+\infty\}$ at the point β if

(56), $\forall \gamma \in \mathbf{R}^2$, $f(\gamma) \ge f(\beta) + \mathbf{Y} \cdot (\gamma - \beta)$.

The set of all the subgradients of f at the point β is the subdifferential, $\partial f(\beta)$.

12.3. Indicator function of a set.

The indicator function I_C of a set C is defined by

 $I_C(\gamma)=0, \text{ if } \gamma {\in C},$

 $I_C(\gamma) = +\infty$, if $\gamma \notin C$.

If the set C is convex, the function I_C is convex. Let us recall that a set is convex iff

 $\forall \gamma \in \mathbb{C}, \forall \beta \in \mathbb{C}, \forall \theta \in]0,1[, \theta \gamma + (1-\theta)\beta \in \mathbb{C}.$

Let us give some useful examples.

12.4. Subdifferential of the indicator function I of the segment [0,1]. The convex set is C = [0,1]. Let Y be a subgradient, we have from (55), (figure 33),

 $\forall \gamma \in [0,1], 0 \ge I(\beta) + Y.(\gamma - \beta).$



Figure 33

A subgradient of the indicator function I of the segment [0,1] at the point $\beta = 1$ is the slope of a line passing through the point (1,0) and which is under the function I.

It results (figure 34),

 $\partial I(\beta) = \emptyset$, if $\beta \notin [0,1]$,

and

 $\partial I(\beta) = \{0\}, \text{ if } \beta \in]0,1[,$ $\partial I(1) = \mathbf{R}^+,$ $\partial I(0) = \mathbf{R}^-.$



Figure 34 The graph $\partial I(\beta)$.

12.5. Subdifferential of the indicator function I_{0r} of the origin of **R**. The convex set is C = {0}. Let Y be a subgradient, we have from (55),

 $0 \ge I_{or}(x)+Yx.$

It results that

$$\partial I_{or}(x) = \emptyset$$
, if $x \neq 0$,

 $\partial I_{or}(0) = \mathbf{R};$

because any subgradient at the origin x = 0 is such that $0 \ge Y0$, (figure 35).



Figure 35 Any subgradient of the indicator function of the origin is the slope of a linear function.

12.6. Subdifferential of the indicator function Ir of a triangle C.

Let \mathbf{Y} be a subgradient, we have from (56),

 $\forall \gamma \in \mathbb{C}, 0 \ge I_r(\beta) + Y_r(\gamma - \beta).$

It results that

 $\partial I_r(\beta) = \emptyset$, if $\beta \notin C$,

and that the vector Y is normal to the triangle C at the point β if $\beta \in C$ (figure 36).



Figure 36 The triangle C with vertices $\mathbf{O} = (0,0)$, $\mathbf{A} = (1,0)$ and $\mathbf{B} = (0,1)$. The vector \mathbf{Y} is normal to the triangle C at the point \mathbf{A} .

Thus we have

 $\partial I_r(\beta) = \{0,0\}$, if β is in the interior of the triangle,

 $\partial I_r(\beta) = \{(Y,Y); Y \ge 0\}, \text{ if } \beta \text{ is on the side AB };$

 $\partial I_r(\beta) = \{(0, Y); Y \le 0\}, \text{ if } \beta \text{ is on the side OA};$

 $\partial I_r(\beta) = \{(Y,0); Y \le 0\}, \text{ if } \beta \text{ is on the side OB };$

 $\partial I_{\mathbf{r}}(\mathbf{O}) = \{(Y_1, Y_2); Y_1 \le 0, Y_2 \le 0\};$

 $\partial I_r(\mathbf{A}) = \{(Y_1, V_2); Y_1 \ge 0, Y_2 \le Y_1\};$

$$\partial I_{\mathbf{r}}(\mathbf{B}) = \{(Y_1, Y_2) ; Y_2 \ge 0, Y_1 \le Y_2\}.$$

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