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Continuum Mechanics — *Melting and solidification of pure metals by a phase-field model*, by Michele Caputo, Michele Ciarletta, Mauro Fabrizio and Vincenzo Tibullo, communicated on February 10, 2017.

This paper is dedicated to the memory of Professor Giuseppe Grioli.

Abstract. — In this paper, we study melting and solidification for metallurgical processes related with phase transitions of pure metals, which during the solid phase show an evident ductility. So, the transition is between a viscous fluid and a viscoplastic state. In this work these particular phenomena can be well described by a phase field fractional model, whose evolution has to satisfy a Ginzburg–Landau equation. Then, we prove the compatibility with the Thermodynamic Laws.

Hence, for metallurgical phase transitions, we have considered a similar model by a new fractional derivative and compared the behavior of the first with this second model. Finally, a generalization to finite deformation for the same models is presented in the last section.

Key words: Phase field transform, fatigue and damage, thermodynamics

Mathematics Subject Classification: 74Nxx, 26A33

1. Introduction

The phase transitions are consequence of a change of the internal material structure with significant variations of the physical, mechanical and thermodynamic behavior of the bodies. So, in a phase transition the qualitative and phenomenological properties of a material change by varying some physical quantities, as pressure, magnetic field, temperature, etc. In this sense, it should be emphasized that in many transitions we observe a change of the molecular structure of the material. As for example the transitions consequence of temperature and pressure variations, among solid, liquid and gases, but also from an amorphous solid to a crystalline solid state with high symmetry.

In the mathematical-physical framework, fundamental results related to the formulation of models that represent the phase transitions were formalized by Landau in [12] and in his fundamental work on superconductivity with Ginzburg [10].

Recently, this theory was applied and extended to different transitions of interest in the technology by the use of fractional derivatives with variable coefficients, which help to better highlight the structural changes of materials.

In this the paper, we present a phase field model for the study of phase transitions related with melting and solidification of metals (see Fig. 1) by the

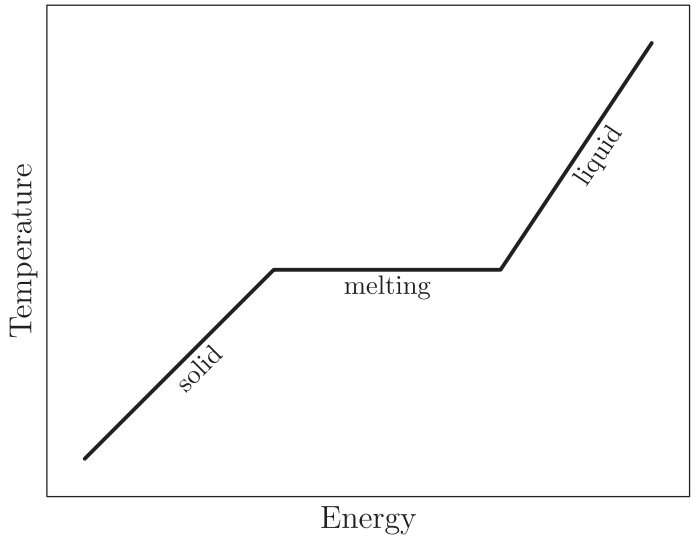

Figure 1. Phase diagram of solid-melting-liquid transition

use of two fractional models. In particular, we study pure metals, as aluminum, iron, copper, zinc, silver, etc., which show an evident ductility in solid phase. Then, during the phase transition, the material passes from a viscous fluid to a viscoplastic solid state. In the first part of the paper, we consider a constitutive equation related with Caputo fractional derivative and we suppose that along the transition, we have only small deformations, so that we can use the eulerian view point also when we study the viscoplastic solid phase. This transition will be described by a phase field $\alpha(x,t)$, which satisfies the Ginzburg–Landau equation and the restriction $\alpha \in [a,1]$, where $0 < a \ll 0.5$. For $\alpha = 1$ we obtain the liquid phase, while $\alpha = a$ describes the viscoplastic phase. Then, we prove the compatibility of the model with the First and Second Laws of Thermodynamics.

In the last part of the paper, by a suitable use of phase parameter α, we generalize the mechanical processes, in order to consider also finite deformations. So that we can consider and study general mechanical processes without to unify the Lagrangian and Eulerian view point.

2. Differential model

For our model, we denote with $\Omega \subset \mathbb{R}^3$ the domain of the body $\mathscr{B}$ and with $[0,T]$ the time interval in which we observe the transition. So that, $(x,t) \in \Omega \times [0,T]$. For the study of these materials, it appears convenient the use of the following constitutive equation

$$\boldsymbol{\sigma}(x,t) = -p_\alpha(\theta)\boldsymbol{I} + \boldsymbol{A}(x)\,{}^{C}D_t^{\alpha}\boldsymbol{\varepsilon}(x,t) \tag{2.1}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ denote stress and strain tensors, while $\boldsymbol{A}(x)$ is a positive defined four order tensor function of α and θ the absolute temperature. The operator ${}^{C}D_t^{\alpha}$ represents the Caputo fractional derivative (see [1], [2]) of order α defined by

$$ {}^{C}D_t^{\alpha}\varepsilon(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\boldsymbol{\varepsilon}'(x,\tau)}{(t-\tau)^{\alpha}}d\tau \tag{2.2} $$

where $\boldsymbol{\varepsilon}'(x,\tau) = \frac{d}{d\tau}\boldsymbol{\varepsilon}(x,\tau)$ and Γ is the Gamma function. Finally, we suppose the body incompressible in the liquid and solid phase, otherwise during the transition the pressure p is a function of α and θ. So that we have the restrictions

$$ p_{\alpha}(\theta) = \begin{cases} \text{not defined} & \text{for } \alpha = a \\ \gamma(\theta-\theta_T)+p_T, & \text{for } \alpha \in (a,1) \\ \text{undetermined} & \text{for } \alpha = 1 \end{cases} \tag{2.3} $$

where θ_T and p_T denote the absolute temperature and pressure of triple point related with phase diagram of the Fig. 2. While $\gamma > 0$ represents the inclination of solid-liquid line transition. Finally, when $\alpha = a$ the pressure is not defined because is embedded in the stress.

Therefore, by (2.1), (2.2) and (2.3), we obtain the stress-strain constitutive equation

$$ \boldsymbol{\sigma}(x,t) = -p_{\alpha}(\theta)\boldsymbol{I} + \frac{\boldsymbol{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^t \frac{\boldsymbol{\varepsilon}'(x,\tau)}{(t-\tau)^{\alpha(x,\tau)}}d\tau \tag{2.4} $$

In this framework, the model for $\alpha = 1$ describes a viscoelastic fluid, while the viscoplastic solid phase is represented by $\alpha = a$.

When we study phase transitions, the α-coefficient will be a function of (x,t). So that, the function $\alpha(x,t)$ is a new unknown able to describe the evolution of the transition, which will be controlled by the Ginzburg–Landau equation

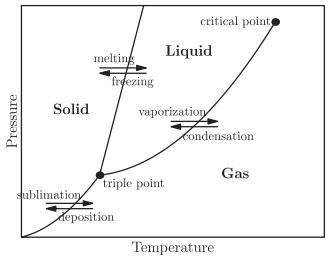

Figure 2. Melting and freezing phase transition

$$\lambda(x)\frac{\partial}{\partial t}\alpha(x,t) = \kappa(x)\nabla^2\alpha(x,t) - \theta_T F'(\alpha(x,t)) - \left(\theta - \frac{1}{\gamma}(p-p_T)\right)G'(\alpha(x,t)) - \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{(s)^{2+\alpha}}ds \tag{2.5}$$

where we have denoted $\boldsymbol{\varepsilon}^t(x,\tau) := \boldsymbol{\varepsilon}(x,t-\tau)$ the past history of the strain $\boldsymbol{\varepsilon}(x,t)$, while the potential $F(\alpha)$ and $G(\alpha)$ describe a transition of first order, which can be represented by the polynomials of forth order

$$F(\alpha) = \frac{(\alpha-a)^4}{4(1-a)} - \frac{(\alpha-a)^3}{3(1-a)}, \quad G(\alpha) = \frac{(\alpha-a)^4}{4(1-a)} - 2\frac{(\alpha-a)^3}{3(1-a)} + \frac{(\alpha-a)^2}{2(1-a)} \tag{2.6}$$

Moreover for fluid and solid phase, we suppose an incompressible condition, then the pressure will be well defined only during the phase transition.

Finally, we introduce the motion equation

$$\rho(x)\frac{\partial}{\partial t}\mathbf{v}(x,t) = -\nabla p(x,t) + \nabla\cdot\boldsymbol{\sigma}_E(x,t) + \rho(x)\mathbf{b}(x,t) \tag{2.7}$$

where the vector $\mathbf{v}$ denotes the velocity, $\mathbf{b}$ the body forces and the extra-stress $\boldsymbol{\sigma}_E$ is defined by

$$\boldsymbol{\sigma}_E(x,t) = \frac{\boldsymbol{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^t \frac{\boldsymbol{\varepsilon}'(x,\tau)}{(t-\tau)^{\alpha(x,\tau)}}d\tau = \frac{\boldsymbol{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^t \frac{\boldsymbol{\varepsilon}'(x,t-s)}{s^{\alpha(x,t-s)}}ds \tag{2.8}$$

The last equation connected with mechanical evolution is given by the continuity equation, which we write in the classical form

$$\dot{\rho}(x,t) = -\rho(x,t)\nabla\cdot\mathbf{v}(x,t)$$

It is important to remember that we have supposed the incompressibility of the liquid phase.

For this model, where the phase field α denotes a new variable which satisfies the balance law (2.5), it is suitable to introduce the Landau free energy by the functional

$$\psi_L(\theta,\alpha,\varepsilon^t,\nabla\alpha) = \frac{1}{2}\kappa(\nabla\alpha)^2 + \theta_T F(\alpha) + \left(\theta - \frac{1}{\gamma}(p-p_T)\right)G(\alpha) + \frac{1}{\Gamma(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds \tag{2.9}$$

So that, the equation (2.5) can be written as

$$\lambda(x)\frac{\partial}{\partial t}\alpha(x,t) = -\delta_\alpha \psi_L(\theta, \alpha, \nabla\alpha)$$

where δ_α denote the variational derivative on α (see [8]).

Finally, because the temperature plays a major role in the phase transition, we have to consider the heat balance equation

$$\rho(x)h(x,t) = -\nabla\cdot\mathbf{q}(x,t) + \rho(x)r(x,t) \tag{2.10}$$

where the scalar $h(x,t)$ denotes the *internal heat power*, the vector $\mathbf{q}$ the *heat flux* and the scalar r the *heat supply*. In the following the heat flux will be supposed function of $\nabla\theta$ such that

$$\mathbf{q}(x,t) = -k(x)\nabla\theta(x,t), \quad k(x) \geq 0 \tag{2.11}$$

3. Thermodynamic Laws

In this section, we introduce the First and Second Laws of Thermodynamics, then we obtain the heat equation and we prove the thermodynamic compatibility of our system.

Before, we need to introduce the internal mechanical and structural powers $\mathscr{P}_m^i$ and $\mathscr{P}_s^i$ respectively defined by

$$\begin{aligned}\mathscr{P}_m^i(t) &= \boldsymbol{\sigma}(x,t)\cdot\dot{\boldsymbol{\varepsilon}}(x,t) \\ &= \left(-p(\alpha,\theta)\boldsymbol{I} + \frac{\boldsymbol{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^t \frac{\boldsymbol{\varepsilon}'(\tau)}{(t-\tau)^{\alpha(x,\tau)}}d\tau\right)\cdot\dot{\boldsymbol{\varepsilon}}(x,t)\end{aligned} \tag{3.1}$$

$$\begin{aligned}\mathscr{P}_s^i(t) &= \frac{d}{dt}\left(\kappa\frac{(\nabla\alpha)^2}{2}\right) + \theta_T\dot{\boldsymbol{F}}(\alpha) + \left(\theta - \frac{1}{\gamma}(p-p_T)\right)\dot{\boldsymbol{G}}(\alpha) + \gamma\dot{\alpha}^2 \\ &\quad + \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\dot{\alpha}(x,t)\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds\end{aligned} \tag{3.2}$$

In the following we need to introduce the notion of *state s* and *process P*, which in this framework are defined by

$$\begin{aligned}s(x,t) &= (\theta(x,t), \varepsilon^t(x,s), \alpha(x,t), \nabla\alpha(x,t)), \\ P &= (\dot{\theta}(x,t), \nabla\mathbf{v}(x,t), \nabla\theta(x,t), \dot{\alpha}(x,t), \nabla\dot{\alpha}(x,t))\end{aligned}$$

Now, by the notion of state and process we consider

First law of thermodynamics
There exists a state function $e(s)$, called *internal energy*, such that

$$\rho\dot{e}(s) = \mathscr{P}_m^i(s,P) + \mathscr{P}_s^i(s,P) + \rho h(s,P) \tag{3.3}$$

where the internal heat power h is a function of the pair state-process (s,P).

Because the internal energy $e(s)$ is a state function, we suppose $e(s) = e(\theta,\alpha,\boldsymbol{\varepsilon}^t,\nabla\alpha)$.

Hence we have from (3.1)–(3.3) the equation

$$\begin{aligned}\rho h(s,P) = {} & \rho\dot{e}(\theta,\alpha,\boldsymbol{\varepsilon}^t,\nabla\alpha) - \boldsymbol{\sigma}(x,t)\cdot\dot{\boldsymbol{\varepsilon}}(x,t) - \frac{d}{dt}\left(\kappa\frac{(\nabla\alpha)^2}{2}\right)\\ & - \theta_T\dot{\boldsymbol{F}}(\alpha) - \left(\theta - \frac{1}{\gamma}(p-p_T)\right)\dot{\boldsymbol{G}}(\alpha) - \gamma\dot{\alpha}^2\\ & - \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\dot{\alpha}(x,t)\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\,ds\end{aligned} \tag{3.4}$$

Following [3] we have

$$\begin{aligned}&\boldsymbol{\sigma}_E(x,t)\cdot\dot{\boldsymbol{\varepsilon}}(x,t)\\ &\quad = \frac{\alpha\mathbf{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^\infty \frac{\varepsilon^t(x,s)-\varepsilon(x,t)}{s^{1+\alpha(x,t-s)}}\cdot\frac{d}{dt}(\varepsilon(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds\\ &\qquad + \frac{\alpha\mathbf{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^\infty \frac{\varepsilon^t(x,s)-\varepsilon(x,t)}{s^{1+\alpha(x,t-s)}}\cdot\frac{d}{ds}(\varepsilon(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds.\end{aligned} \tag{3.5}$$

So, the free mechanical energy $\Psi_E(\varepsilon^t(x,s))$ is defined by the functional

$$\Psi_E(\varepsilon^t(x,s)) = \frac{\alpha\mathbf{A}(x)}{2\Gamma(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{1+\alpha(x,t-s)}}\,ds. \tag{3.6}$$

whereby we have by (3.5)

$$\begin{aligned}&\dot{\Psi}_E(\varepsilon^t(x,s))\\ &\quad = \boldsymbol{\sigma}_E(x,t)\cdot\dot{\boldsymbol{\varepsilon}}(x,t) - \frac{\Gamma'(1-\alpha(x,t))}{2\Gamma^2(1-\alpha(x,t))}\dot{\alpha}(x,t)\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\,ds\\ &\qquad - \frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\tilde{\alpha}(x,t-s)\,ds\end{aligned} \tag{3.7}$$

where $\tilde{\alpha}(x,t-s) = \frac{d}{ds}\alpha(x,t-s)$. Finally, from definition (3.1)

$$\mathscr{P}_m^i(s,P) = p\frac{\dot\rho}{\rho} + \boldsymbol{\sigma}_E(x,t)\cdot\dot{\boldsymbol{\varepsilon}}(x,t) \tag{3.8}$$

$$= p\frac{\dot\rho}{\rho} + \dot\Psi_E(\varepsilon^t(x,s))$$

$$+ \frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\tilde\alpha(x,t-s)\,ds$$

$$+ \frac{\Gamma'(1-\alpha(x,t))}{2\Gamma^2(1-\alpha(x,t))}\dot\alpha(x,t)\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds$$

Now, we consider the function

$$e_r(\theta,\alpha) = e(\theta,\alpha,\boldsymbol{\varepsilon}^t,\nabla\alpha) - \Psi_E(\varepsilon^t(x,s)) - \kappa\frac{(\nabla\alpha)^2}{2} - \Big(\theta_T + \frac{1}{\gamma}p_T\Big)G(\alpha).$$

Then, the heat equation (2.10) assumes the form

$$\rho\dot e_r(\theta,\alpha) + p\frac{\dot\rho}{\rho} - \frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha}}\tilde\alpha(x,t-s)\,ds \tag{3.9}$$

$$- \Big(\theta - \frac{1}{\gamma}p\Big)\dot G(\alpha) - \gamma\dot\alpha^2 + \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\dot\alpha(x,t)$$

$$\times\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds$$

$$= -\nabla\cdot\mathbf{q}(x,t) + \rho(x)r(x,t)$$

Second law of thermodynamics
There exists a upper potential $\eta(s)$, called the *entropy* function, such that

$$\rho\dot\eta(s(x,t)) \geq \rho\frac{h(s(x,t),P(x,t))}{\theta(x,t)} - \frac{1}{\theta^2}\mathbf{q}(\nabla\theta(x,t))\cdot\nabla\theta(x,t) \tag{3.10}$$

From the inequality (3.10) and using (3.3) we have

$$\rho\theta\dot\eta \geq \rho h(s(x,t),P(x,t)) - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta \tag{3.11}$$

$$= \rho\dot e_r(\theta,\alpha) + p\frac{\dot\rho}{\rho} - \frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{(s)^{2+\alpha(x,t-s)}}\tilde\alpha(x,t-s)\,ds$$

$$- \Big(\theta - \frac{1}{\gamma}p\Big)\dot G(\alpha) + \gamma\dot\alpha^2 - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta$$

then by the free energy $\psi = e_r - \theta\eta$ and the Fourier law (2.11), we have

$$\rho\dot{\psi} + \rho\eta\dot{\theta} + p\frac{\dot{\rho}}{\rho} - \frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\tilde{\alpha}(x,t-s)\,ds$$
$$-\left(\theta - \frac{1}{\gamma}p\right)\dot{\boldsymbol{G}}(\alpha) - \left(\theta - \frac{1}{\gamma}p\right)\dot{\boldsymbol{G}}(\alpha) - \gamma\dot{\alpha}^2 + \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\dot{\alpha}(x,t)$$
$$\times\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}\tilde{\alpha}(x,t-s)\,ds - \frac{k}{\theta}(\nabla\theta)^2 \le 0 \tag{3.12}$$

Now, we suppose the free energy ψ and entropy η are function only of θ, α, $\nabla\alpha$. Hence upon substitution of $\mathscr{P}_m^i$ and $\mathscr{P}_s^i$ we obtain

$$\rho(\psi_\theta + \eta)\dot{\theta} - \rho\gamma\dot{\alpha}^2 - p\left(\frac{\dot{\rho}}{\rho} + \lambda\rho\dot{\boldsymbol{G}}(\alpha)\right) + \delta_{\varepsilon^t}\psi$$
$$+\rho\left[\psi_\alpha - \theta G' + \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds\right]\dot{\alpha}$$
$$-\frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds$$
$$+(\rho\psi_{\nabla\alpha} - \varkappa\nabla\alpha)\cdot\nabla\dot{\alpha} - \frac{k}{\theta}(\nabla\theta)^2 \le 0. \tag{3.13}$$

Then, from the Second Law in the form of inequality (3.13), we have by the arbitrariness and linearity of $\dot{\theta}$, $\dot{\alpha}$ and $\nabla\dot{\alpha}$ the identities

$$\eta(\theta,\alpha,\nabla\alpha) = -\psi_\theta(\theta,\alpha,\nabla\alpha), \quad \rho\psi_{\nabla\alpha}(\nabla\alpha) = \varkappa\nabla\alpha,$$
$$\psi_\alpha(\theta,\alpha) = \theta G'(\theta) + \frac{\Gamma'(1-\alpha(x,t))}{\Gamma^2(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds \tag{3.14}$$

Finally, as consequence of the incompressibility of the liquid and solid phase, the pressure p is undefined. Therefore, from arbitrariness of $p > 0$ we have during the phase transition

$$\frac{\dot{\rho}}{\rho} + \lambda\rho\dot{\boldsymbol{G}}(\alpha) = 0 \tag{3.15}$$

The free energy will be a state function depending on $(\theta,\alpha,\rho,\nabla\alpha)$

$$\psi = \int e_{r,\theta}(\theta)\,d\theta - \theta\int\frac{e_{r,\theta}(\theta)}{\theta}d\theta$$
$$+\frac{\alpha\mathbf{A}(x)}{\Gamma(1-\alpha(x,t))}\int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}}ds + \theta G(\alpha) + \frac{\varkappa}{2\rho}(\nabla\alpha)^2 \tag{3.16}$$

Then, the entropy is given by

$$\eta = \int \frac{e_{r,\theta}}{\theta} d\theta - G(\alpha) \tag{3.17}$$

Now, we arrive to the differential system connected with melting and solidification of pure metals. Then from the equation (3.9) on the temperature we have

$$\begin{aligned} \rho \dot{e}_r(\theta(x,t),\alpha(x,t)) - \frac{\alpha \mathbf{A}(x)(1+\alpha(x,t))}{2\Gamma(1-\alpha(x,t))} \int_0^\infty \frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha(x,t-s)}} \\ \times \tilde{\alpha}(x,t-s)\, ds - \theta(x,t)\dot{\boldsymbol{G}}(\alpha(x,t)) - \gamma \dot{\alpha}^2(x,t) \\ = -\nabla \cdot \mathbf{q}(x,t) + \rho(x) r(x,t) \end{aligned} \tag{3.18}$$

Moreover, the differential problem is completed by the motion equation (2.7) and the continuity equation (3.15).

4. Constitutive equation by a CF fractional derivative

In this Section, we use the new definition of time fractional derivative of order $\alpha \in (0,1)$ proposed in [4], by CF fractional derivative

$$\mathscr{D}_t^\alpha f(t) = \frac{1}{1-\alpha} \int_0^t e^{-\frac{\alpha}{1-\alpha}(t-\tau)} f'(\tau)\, d\tau \tag{4.1}$$

whose meaning and properties was discussed also in [5]. So, the stress is defined by

$$\boldsymbol{\sigma}(x,t) = -p_{\alpha(x,t)}(\theta)\boldsymbol{I} + \boldsymbol{A}(x)\mathscr{D}_t^{\alpha(x,t)}\boldsymbol{\varepsilon}(x,t)$$

If we suppose that the parameter α is a function of (x,t) we obtain the stress-strain constitutive equation

$$\begin{aligned} \boldsymbol{\sigma}(x,t) &= -p_{\alpha(x,t)}(\theta(x,t))\boldsymbol{I} + \frac{\boldsymbol{A}(x)}{1-\alpha(x,t)} \int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)} \boldsymbol{\varepsilon}'(x,\tau)\, d\tau \\ &= -p_{\alpha(x,t)}(\theta(x,t))\boldsymbol{I} + \boldsymbol{\sigma}_E(x,t) \end{aligned} \tag{4.2}$$

Also for this model, for $\alpha = 1$ we obtain a viscoelastic fluid, while for $\alpha(x,t) \in (a,1)$ we have the phase transition, the viscoplastic solid phase is represented by $\alpha = a$.

In order to prove that this new system by constitutive equation (4.2) satisfies the restrictions of the Thermodynamic Laws is necessary to study the representation of the internal mechanical power $\mathscr{P}_m^i(s,P)$ given by

$$\mathscr{P}_m^i(s,P) = \left(-p_a(\theta(x,t))\boldsymbol{I} + \frac{\boldsymbol{A}(x)}{(1-\alpha(x,t))}\int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}\boldsymbol{\varepsilon}'(x,\tau)\,d\tau\right)\cdot\dot{\boldsymbol{\varepsilon}}(x,t) \tag{4.3}$$

$$= \left(-p_a(\theta(x,t))\boldsymbol{I} + \frac{\alpha\boldsymbol{A}(x)}{(1-\alpha(x,t))^2} \times \int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}(\boldsymbol{\varepsilon}(x,\tau)-\boldsymbol{\varepsilon}(x,t))\,d\tau\right)\cdot\frac{d}{dt}\boldsymbol{\varepsilon}(x,t)$$

$$= -p_a(\theta(x,t))\boldsymbol{I} + \frac{\alpha\boldsymbol{A}(x)}{(1-\alpha(x,t))^2} \times \int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t)) \cdot\frac{d}{dt}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds - \frac{\alpha\boldsymbol{A}(x)}{(1-\alpha(x,t))^2} \times \int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t)) \cdot\frac{d}{ds}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds$$

So,

$$\mathscr{P}_m^i(s,P) = -p_a(\theta(x,t))\boldsymbol{I} + \frac{\alpha\boldsymbol{A}(x)}{2(1-\alpha(x,t))^2}\frac{d}{dt}\int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t)) \cdot(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds - \frac{\alpha^2\boldsymbol{A}(x)}{(1-\alpha(x,t))^3}\int_0^t e^{-\frac{\alpha(x,\tau)}{1-\alpha(x,\tau)}(t-\tau)}(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t)) \cdot(\boldsymbol{\varepsilon}(x,t-s)-\boldsymbol{\varepsilon}(x,t))\,ds \tag{4.4}$$

5. Simulations

In the previous section we have seen that the transition of a pure metal between the viscous fluid phase and the viscoplastic solid phase can be modelled by using a stress-strain relation that makes use of a fractional derivative, together with a Ginzburg–Landau type phase transition model. We used two different types of fractional derivative, the usual Caputo fractional time derivative and the new fractional time derivative, recently introduced in [4].

Now, we would like to apply previous results to understand up to what point they are in agreement with the experimental knowledge that we have of the phenomena involved. For this purpose we performed some simulations considering a situation in which, for the sake of simplicity, the geometry of the problem is one-

dimensional, and further limiting our considerations to the time dependence: this means that we consider all involved functions as homogeneous with respect to space.

In detail, we consider the following reduced stress-strain relation

$$\sigma_E(t) = \frac{A}{\Gamma(1-\alpha(t))} \int_0^t \frac{1}{(t-\tau)^{\alpha(\tau)}} \varepsilon'(\tau)\, d\tau \tag{5.1}$$

when using a stress-strain relation with the usual Caputo fractional time derivative.

For the stress, we consider an harmonic oscillating function, while for the phase α we consider a function increasing from a to 1 with the time t, built by an appropriate scaling and translation of a sinusoidal function.

The obtained result for the usual Caputo fractional time derivative are reported, for two different values of the fixed parameter a, in Fig. 3.

As we can see, from the start of the curve, near the origin of the axes, the stress-strain relation is not a linear one, and this corresponds to a plastic material. This effect is more evident in the first of the two graphs, where the parameter a is greater. Moreover, we see that for high values of α the curve follows a sort of elliptic curve, typical of a viscous fluid.

For a stress-strain relation that make use of the new fractional time derivative we have the following reduced stress-strain relation

$$\sigma_E(t) = \frac{A}{1-\alpha(t)} \int_0^t \exp\Big(-\frac{\alpha(\tau)}{1-\alpha(\tau)}(t-\tau)\Big)\varepsilon'(\tau)\, d\tau. \tag{5.2}$$

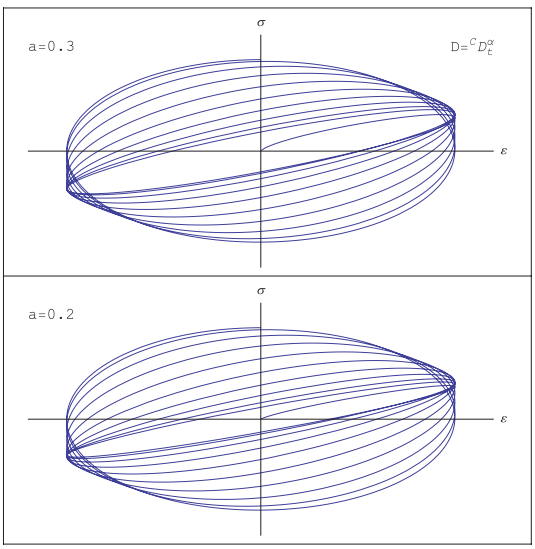

Figure 3. Stress vs. strain in a phase transition from $\alpha = a$ to $\alpha = 1$, for two different values of a and using the usual Caputo fractional time derivative

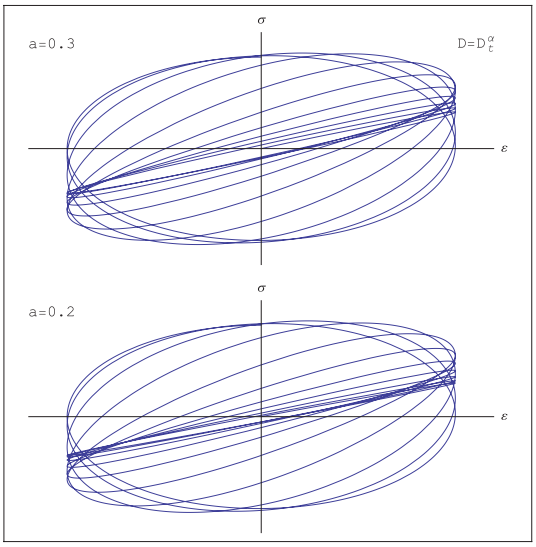

Figure 4. Stress vs. strain in a phase transition from $\alpha = a$ to $\alpha = 1$, for two different values of a and using the new fractional time derivative

In the next figure, we show the results obtained for the new fractional time derivative, also in this case for the same two different values of the fixed parameter a (see Fig. 4).

In this graphs we can see a behavior similar to the previous ones, but with a slower adapting of the curve to the phase α.

It is the case to observe that the representations of phenomena by the constitutive equations (5.1) and (5.2) are rather similar to each other. However we observe that the simulations of the strain-stress graphs considered in Fig. 3 and Fig. 4, have similar behaviors. The graphs show as the first model presents a more evident memory effects compared with the corresponding graph of the second model.

We finally show a last figure (see Fig. 5) in which we let the phase α to reach 0, so as to model a material that in the solid phase is elastic.

We can clearly see that in both graphs the start of the curve, near the origin of the axes, is compatible with a straigth line through the origin, representing the usual elastic stress-strain relation, in which the stress is proportional to the strain (Hooke law). Again, the two graphs are different in the rapidity with which the moving point follow the increasing of the transition phase α: the new fractional time derivative retains a certain memory and it is slower in adapting to the phase.

6. Phase model with finite deformations

In this Chapter, we consider finite deformations, so that we do not unify the lagrangian and eulerian view point, as considered in the first part of the paper.

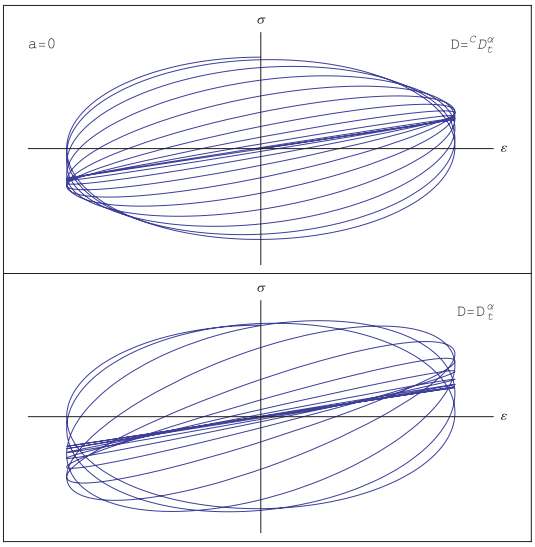

Figure 5. Stress vs. strain in a phase transition from $\alpha = a = 0$ to $\alpha = 1$, for the two different types of Caputo fractional time derivative

Because, during the melting-solid transition, we need to change the view point. So, for this reason we cannot use the classical motion equation

$$x = \hat{\chi}(X, t) \tag{6.1}$$

where $X \in \mathscr{B}$ denotes the material point of the body $\mathscr{B}$ and x is localization of X, i.e. the position occupied by the particle X at the instant t. As consequence of the phase transition the equation (6.1) has to be replaced by the new function

$$x_\alpha(X, t) = \tilde{\chi}(X, f(\alpha)t)$$

where $f(t)$ is a monotone function, such that $f(a) = 0$, $f(1) = 1$. So, when $\alpha = a$, we obtain the Lagrangian view point, while if $\alpha = 1$ we have the Eulerian point of view. Then, the constitutive equation (2.4) assumes the form

$$\boldsymbol{\sigma}(x_\alpha, t) = -p_\alpha(\theta)\boldsymbol{I} + \frac{1}{\Gamma(1-\alpha)}\mathbf{F}\Big(\int_0^t \frac{\boldsymbol{\varepsilon}'(x_\alpha, \tau)}{(1-\tau)^\alpha}\, d\tau\Big) \tag{6.2}$$

where $\mathbf{F}$ is a smooth second order tensor defined in a subset of a tensor space $\boldsymbol{T}$. Moreover, the Ginzburg–Landau equation assumes the equivalent form

$$\lambda(x_\alpha)\frac{\partial}{\partial t}\alpha(x_\alpha,t)=\kappa(x_\alpha)\nabla^2\alpha(x_\alpha,t)-\theta_T(x_\alpha)F'(\alpha(x_\alpha,t))-\left(\theta(x_\alpha,t)-\frac{1}{\gamma}(p(x_\alpha,t)-p_T)\right)G'(\alpha(x_\alpha,t)) \tag{6.3}$$

moreover, the motion equation is given by

$$\rho(x_\alpha)\frac{\partial}{\partial t}\mathbf{v}(x_\alpha,t)=-\nabla p_\alpha(x_\alpha,t)+\nabla\cdot\boldsymbol{\sigma}_E(x_\alpha,t)+\rho(x_\alpha)\mathbf{b}(x_\alpha,t) \tag{6.4}$$

while from (3.18) we have the heat equation

$$\rho(x_\alpha)\dot{\boldsymbol{e}}_r(\theta(x_\alpha,t),\alpha(x_\alpha,t))-\frac{\alpha\mathbf{A}(x_\alpha)(1+\alpha(x_\alpha,t))}{2\Gamma(1-\alpha)}\int_0^\infty\frac{(\varepsilon^t(x,s)-\varepsilon(x,t))^2}{s^{2+\alpha}}ds$$
$$-\theta\dot{\boldsymbol{G}}(\alpha(x_\alpha,t))-\gamma\dot{\alpha}^2(x_\alpha,t)=-\nabla\cdot\mathbf{q}(x_\alpha,t)+\rho(x_\alpha)r(x_\alpha,t)$$

Finally, the free mechanical energy $\Psi_E(\varepsilon^t(x_\alpha,s))$ is defined by the functional

$$\Psi_E(\varepsilon^t(x_\alpha,s))=\frac{\alpha\mathbf{A}(x_\alpha)}{2\rho(x)\Gamma(1-\alpha)}\int_0^\infty\frac{(\varepsilon^t x_\alpha x,s)-\varepsilon(x_\alpha,t))^2}{s^{1+\alpha}}ds. \tag{6.5}$$

whereby we have by (6.5)

$$\rho(x_\alpha)\dot{\boldsymbol{\Psi}}_E(\varepsilon^t(x_\alpha,s))=\sigma_E(x_\alpha,t)\cdot\dot{\varepsilon}(x_\alpha,t)-\frac{\alpha\mathbf{A}(x)(1+\alpha)}{2\Gamma(1-\alpha)}\int_0^\infty\frac{(\varepsilon^t(x_\alpha,s)-\varepsilon(x_\alpha,t))^2}{s^{2+\alpha}}ds. \tag{6.6}$$

7. Conclusions

We presented a phase field model useful for the study of phase transitions related with melting and solidification of metals. This model applies to pure metals, as aluminum, iron, copper, zinc, silver, etc., which in the solid phase show a pastic beavior.

We first considered a constitutive equation related with Caputo fractional derivative, whose coefficient is a new variabile of the problem, which satifies the Ginzburg–Landau equation. Then, we supposed that along the transition there are only small deformations. We proved the compatibility of the model with the First and Second Laws of Thermodynamics. We then repeat the same analysis for a new definition of time fractional derivative.

Next, we proposed some numerical simulations in a simplified situation, to verify the obtained results in comparison with the experimental evidence.

In the last part of the paper, by a suitable use of the phase parameter α, we generalized the mechanical processes, in order to consider also finite deformations.

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REFERENCES

[1] M. CAPUTO, *Linear models of dissipation whose Q is almost frequency independent*, part II, Geophys. J. R. Astron. Soc., 13, (1967), 529–539.

[2] M. CAPUTO, *Wavenumber-independent rheologies in a sphere*, Rendic. Acc. Naz. Lincei, 81, (1987), 175–207.

[3] M. CAPUTO - M. FABRIZIO, *Damage and fatigue by a fractional derivative model*, J. Comput. Phys., 293, (2015), 400–408.

[4] M. CAPUTO - M. FABRIZIO, *A new definition of fractional derivative without singular kernel*, Progr. Fract. Differ. Appl., 1, (2015), 73–85.

[5] M. CAPUTO - M. FABRIZIO, *Applications of new time and spatial fractional derivatives with exponential kernels*, Progr. Fract. Differ. Appl., 2, (2016), 1–11.

[6] M. DI PAOLA - M. ZINGALES, *Exact mechanical models of fractional hereditary materials*, J. Rheol., vol. 56, (2012), 983–1004.

[7] M. FABRIZIO, *Plasticity, internal structures and phase field models*, Mechanics Research Communications, 43, (2012), 29–33.

[8] M. FABRIZIO, *Ginzburg–Landau equations and first and second order phase transitions*, Int. J. Eng. Sci., 44(8), (2006), 529–539.

[9] M. FREMOND - B. NEDJAR, *Damage, gradient of damage and principle of virtual power*, Int. J. Solids Structures, 33, (1996), 1083–1103.

[10] V. L. GINZBURG - L. D. LANDAU, *On the theory of superconductivity*, Zh. Eksp. Teor. Fiz., 20, (1950), 1064–1072.

[11] D. GRAFFI, *Sui problemi della ereditarietà lineare*, Il Nuovo Cimento, 5(1), (1928), 53–71.

[12] L. LANDAU, *On the theory of phase transitions*, Zh. Eksp. Teor. Fiz, 7, (1937), 19–32, Translated and reprinted from L. D. Landau "Collected Papers" (Nauka, Moscow), 1, (1969), 234–252.

[13] W. SUMELKA, *Fractional viscoplasticity*, Mech. Research Comm, 56, (2014), 31–36.

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