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## Irreversible phase transitions in steel

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# Irreversible phase transitions in steel

by D. Hömberg

## Abstract

We present a mathematical model for the austenite-pearlite and austenite-martensite phase transitions in eutectoid carbon steel. The austenite-pearlite phase change is described by the Additivity Rule. For the austenite-martensite phase change we propose a new rate law, which takes into account its irreversibility. We investigate questions of existence and uniqueness for the three-dimensional model and finally present numerical calculations of a continuous cooling transformation diagram for the eutectoid carbon steel C1080.

## 1 Introduction

In this paper we investigate a mathematical model for the phase changes in carbon steel of the so-called eutectoid composition of 0.8 % carbon content. In contrast to a previous paper [9] we now take care of the irreversibility of the austenite-martensite phase change. For the three-dimensional model we end up with a nonlinear evolution equation for the temperature (including a maximal monotone operator of  $\theta_t$ ), coupled with two ordinary differential equations to describe the phase fractions. Related problems have been studied by Colli and Visintin [8], Blanchard, Damlamian and Ghidouche [5], and Blanchard and Ghidouche [6].

We will now give only a brief phenomenological description of the phase transitions. For a more detailed discussion and further references on this subject, we refer to [9].

The kinetics of the phase changes can easily be described using an isothermal-transformation (It-) diagram (see fig.1.1). Above a temperature  $A_s$  eutectoid steel is in the austenitic phase. Below this temperature the formation of pearlite starts. For fixed temperature the bold faced curves indicate the beginning and the end of the austenite pearlite transformation. The reason for the 'nose-shape' of these curves is that this phase change is a nucleation and growth process with opposite temperature dependency of the nucleation and the growth rate. The A-P transformation is driven by the diffusion of carbon atoms, it is time-dependent and irreversible.

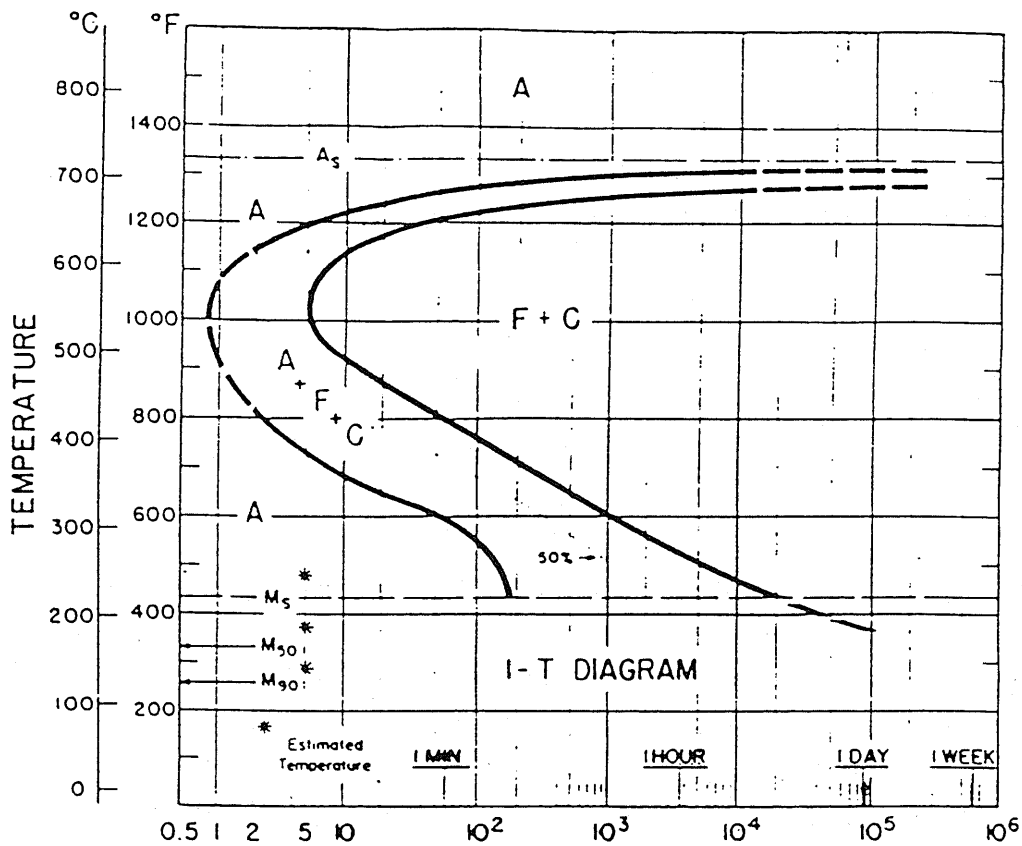


Figure 1.1: Isothermal-transformation diagram for the plain carbon steel C1080 (from [1])

Below a temperature  $M_s$ , the formation of martensite starts. This phase transition is diffusionless and irreversible. It is temperature-dependent in such a way that the fraction of martensite only increases during nonisothermal stages of the cooling process.

Both phase transitions taken together are often referred to as the *eutectoid transformation*. The resulting phases pearlite and martensite have different mechanical properties: pearlite is soft and ductile while martensite is very hard and brittle.

This fact has an important application in the heat treatment of steel. In this process a workpiece is heated up until it is in the austenitic phase. Then it is cooled down in a certain way to get a desired distribution of martensite and pearlite. In a gear wheel, for instance, one wants to have a hard (martensitic) outer part to reduce abrasion and a softer (pearlitic) inner part to minimize fatigue effects.

For planning a heat treatment engineers have to know the nonisothermal evolution of the phases. This is usually depicted in continuous-cooling-transformation (CCT-) diagrams (see fig. 1.2). Deriving a CCT-diagram experimentally is quite costly, thus there is a demand for numerical simulations of these diagrams(cf. [9], [10] and the references given there).

In the next section we formulate an initial value problem which describes the evolution

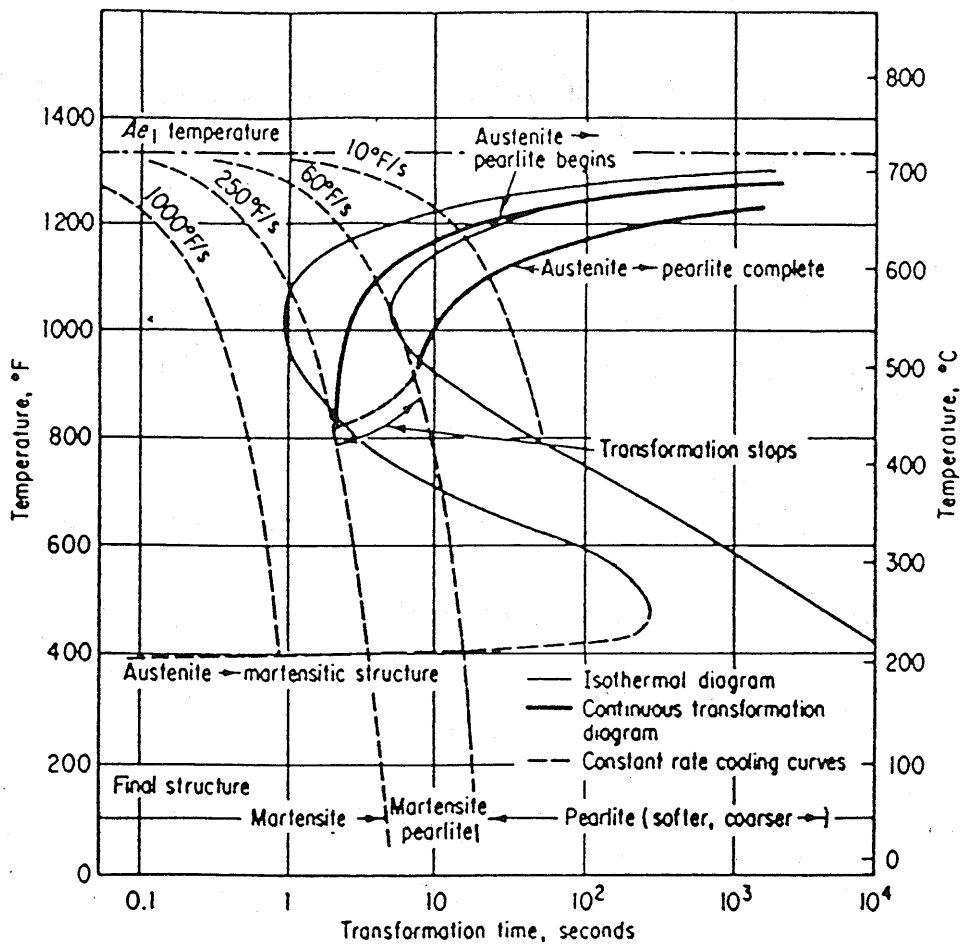


Figure 1.2: Derivation of a continuous-cooling from an isothermal-transformation diagram (from [4])

of the phase fractions of pearlite and martensite. In Section 3 we consider the three-dimensional case. Section 4 is devoted to presenting numerical simulations of CCT-diagrams and some concluding remarks on further research. Finally, in the appendix we list some properties of maximal monotone operators to be used in Section 3.

## 2 Mathematical description of the phase transition kinetics

### 2.1 Austenite – pearlite

The austenite – pearlite phase transition is a nucleation and growth process, which, in the isothermal case, can be described by the generalized Johnson–Mehl equation

$$p(t) = 1 - e^{-b(\theta)t^{a(\theta)}}, \quad (2.1)$$

with temperature dependent coefficients  $a(\theta)$  and  $b(\theta)$ . (For a more detailed exposition we again refer to [9].)

In the nonisothermal case, we use the *Additivity Rule* to describe the formation of pearlite:

$$\int_0^t \frac{1}{\tau(\theta(\xi), p(t))} d\xi = 1. \quad (2.2)$$

Here,  $\tau(\theta, p)$  denotes the time to transform the fraction  $p$  to pearlite at constant temperature  $\theta$ . Thus, by (2.1),

$$\tau(\theta, p) = \left( -\frac{\ln(1-p)}{b(\theta)} \right)^{\frac{1}{a(\theta)}}. \quad (2.3)$$

The Additivity Rule coupled with an energy balance equation has been investigated by Visintin [16]. A different approach to model a nucleation and growth process has been chosen by Andreucci et al. [2] in connection with the solidification of polymers.

Concerning the data functions in (2.1), we make the following assumptions:

(A1)  $a, b \in C^1(\mathbb{R})$ ,

(A2) there exist positive constants  $m, M$ , such that  $a(x) > m, b(x) > m$  for all  $x \in \mathbb{R}$  and  $\|a\|_{C^1(\mathbb{R})} + \|b\|_{C^1(\mathbb{R})} \leq M$ ,

(A3) there exists a constant  $\tilde{M}_s > M_s$ , such that  $a'(x) \geq 0$  for all  $x \leq \tilde{M}_s$ .

**Remark 2.1** *The graph of  $a$  is approximately bell-shaped (cf. [9], fig. 2.1). Therefore, (A3) poses no unphysical restriction on  $a$ .*

As pointed out in [9], the early stages of the pearlitic transformation are inaccurately described by the additivity rule. This led to introducing a fixed incubation time  $t_I$ . During this time small grains of pearlite are formed without knowing the exact evolution kinetics. At the end of this stage the process is gauged by claiming that the additivity rule shall hold for  $t = t_I$ . Thus we consider the following model for the formation of pearlite:

- Let  $\theta : (0, T) \rightarrow \mathbb{R}$  be a given temperature evolution,
- $t_I \in (0, T)$  the fixed incubation time, then, depending on  $\theta$ ,
- $p_0$  is defined by

$$\int_0^{t_I} \frac{1}{\tau(\theta(\xi), p_0)} d\xi = 1. \quad (2.4)$$

- The fraction of pearlite is determined by the following initial value problem (IVP):

$$p(0) = p_0, \quad (2.5a)$$

$$\dot{p}(t) = \begin{cases} 0 & , 0 < t < t_I \\ \hat{f}(t, p(t))H(A_s - \theta(t)) & , t_0 \leq t < T. \end{cases} \quad (2.5b)$$

Here,  $\hat{f}(t, p(t))$  results from a formal differentiation of the additivity rule with respect to time and has the following form:

$$\hat{f}(t, p(t)) = - \left( \int_0^t \frac{\partial}{\partial p} \frac{d\xi}{\tau(\theta(\xi), p(t))} \right)^{-1} \frac{1}{\tau(\theta(t), p(t))}. \quad (2.6)$$

The heaviside function  $H(\cdot)$  prevents the formation of pearlite above the critical temperature  $A_s$ .

## 2.2 Austenite – martensite

While the additivity rule is a well investigated decent tool for describing the pearlitic transformation there seems to be no satisfactory model at hand for the martensitic transformation.

Usually, exponential growth laws like the Koistinen and Marburger formula

$$m(t) = 1 - e^{-c(M_s - \theta(t))} \quad (2.7)$$

are used (cf. [9], [11], [12]).

These equations have all in common that they do not model the irreversibility of the austenite – martensite phase transition. Thus, in numerical simulations based on these models, owing to the release of latent heat, usually a decrease in the martensite fraction is observed (cf. [9] and Section 4).

As mentioned before, the formation of martensite starts below the critical temperature  $M_s$ , and the volume fraction of martensite only grows during nonisothermal stages of a cooling process.

Hence we propose the following rate law for the growth of martensite:

$$m(0) = 0, \quad (2.8a)$$

$$\dot{m}(t) = (1 - m(t))G(\theta(t))H(-\theta_t(t)). \quad (2.8b)$$

Here again  $H$  is the heaviside function. Concerning  $G(\theta)$  we assume:

$$(A4) \quad G \in C^{0,1}(\mathbb{R}),$$

there is a constant  $M > 0$  s.t.  $0 \leq G(x) \leq M$  for all  $x \in \mathbb{R}$

and  $G(x) = 0$  for all  $x \geq M_s$ .

The irreversibility of the martensitic transformation now carries over to the model. We also tacitly assume that we start with a temperature  $\theta(0) \geq M_s$ .

### 2.3 An initial value problem for the eutectoid transformation

In (2.5b) and (2.8b), actually, not the fractions  $p$  and  $m$  occur but the volume fraction of austenite which is  $1 - p$  or  $1 - m$ , respectively. Therefore, to combine both models one only has to replace these terms by the volume fraction of austenite in the case when both pearlite and martensite are present, i.e.  $1 - p - m$ .

So we end up with the following initial value problem for the phase transitions in eutectoid carbon steel:

$$p(0) = p_0, \tag{2.9a}$$

$$m(0) = 0, \tag{2.9b}$$

$$\dot{p}(t) = (1 - p(t) - m(t)) f(t, p(t), m(t), \theta) H(A_s - \theta(t)), \tag{2.9c}$$

$$\dot{m}(t) = (1 - p(t) - m(t)) G(\theta(t)) H(-\theta_t(t)), \tag{2.9d}$$

where we define

$$f(t, p, m, \theta) := - \left( \int_0^t \frac{d\xi}{a(\theta(\xi)) \tau(\theta(\xi), p, m)} \right)^{-1} \frac{\ln(1 - p - m)}{\tau(\theta(t), p, m)} H(t - t_I). \tag{2.10}$$

Here,  $\tau(\theta, p, m)$  is defined by

$$\tau(\theta, p, m) = \left( - \frac{\ln(1 - p - m)}{b(\theta)} \right) \frac{1}{a(\theta)}. \tag{2.11}$$

We have the following result for the complete model:



**Lemma 2.1** Assume (A1) – (A4), let  $\theta \in H^1(0, T)$  with  $\theta(0) = A_s$  and  $t_I \in (0, T)$ . Then the following are valid:

(1)  $p_0$  is uniquely defined by

$$\int_0^{t_I} \frac{1}{\tau(\theta(\xi), p_0)} d\xi = 1.$$

(2) The IVP (2.9a–d) has a unique solution

$$(p, m) \in W^{1,\infty}(0, T) \times W^{1,\infty}(0, T).$$

(3)

$$p_0 \leq p(t) + m(t) \leq c_{t_I, T} < 1 \text{ for all } t \in [0, T].$$

(4) There exists a constant  $M > 0$ , independent of  $\theta$ , s.t.

$$\|\dot{p}\|_{L^\infty(0, T)} + \|\dot{m}\|_{L^\infty(0, T)} \leq M.$$

For proving this lemma, we need the following result:

**Lemma 2.2** Let  $z_0 \in (0, 1)$ ,  $D = [a, b] \times [z_0, 1)$  and  $g : D \rightarrow \mathbb{R}_+$  be given, s.t.  $t \mapsto g(t, z)$  is measurable for all  $z \in [z_0, 1)$ ,  $z \mapsto g(t, z)$  Lipschitz continuous for  $t \in [a, b]$  and  $\text{ess sup}_{(t, z) \in D} g(t, z) \leq M < \infty$ . Then, the IVP

$$z(a) = z_0 \in (0, 1) \tag{2.12a}$$

$$\dot{z}(t) = -(1 - z) \ln(1 - z) g(t, z(t)) \tag{2.12b}$$

has a unique solution on  $[a, b]$  satisfying

$$z_0 \leq z(t) \leq c_{a, b} < 1 \text{ for all } t \in [0, T].$$

*Proof:*

Define  $F : K \subset C[a, b] \rightarrow C[a, b]$  by

$$z := F\bar{z}, \tag{2.13}$$

where  $z$  is the solution of

$$z(a) = z_0, \tag{2.14a}$$

$$\dot{z} = -(1 - z) \ln(1 - z) g(t, \bar{z}(t)) \tag{2.14b}$$

and

$$K := \{f \in C[a, b] \mid z_0 \leq f(t) < 1\}. \quad (2.15)$$

The solution of (2.14) has the following explicit form:

$$z(t) = 1 - e^{\ln(1 - z_0)e^{f(t)}}, \quad (2.16)$$

with

$$f(t) = \int_a^t G(\xi, \bar{z}(\xi)) d\xi. \quad (2.17)$$

Hence it follows that

$$z(t) \leq 1 - e^{\ln(1 - z_0)(b - a)M} =: c_{a,b} < 1. \quad (2.18)$$

Then  $F : \hat{K} \rightarrow \hat{K}$  with  $\hat{K} = \{f \in K \mid f(t) \leq c_{a,b} \text{ for all } t \in [a, b]\}$  is a self-mapping. In view of the assumptions on  $g$  it is easy to see that  $F$  is also a contraction, at least on an interval  $[a, b^+]$ ,  $b^+ \leq b$ . Thus applying Banach's fixed point theorem finishes the proof.  $\square$

*Proof of Lemma 2.1:*

As  $\dot{p}$  and  $\dot{m}$  have discontinuous right-hand sides, we can only obtain absolutely continuous solutions. It is an easy exercise to show that (2.9 a-d) has a unique local solution on an interval  $[0, T^+]$ , with  $T^+ > t_I$ , which we will omit here.

To obtain a priori estimates for the solution, we add the equations for  $\dot{p}$  and  $\dot{m}$  and get the following IVP (with  $z = p + m$ ):

$$z(0) = p_0, \quad (2.19a)$$

$$\dot{z}(t) = (1 - z(t)) \left( f(t, z(t), \theta) + G(\theta(t))H(-\theta_t(t)) \right). \quad (2.19b)$$

In  $[0, t_I]$ , for the solution of (2.20), we get the bound

$$p_0 \leq z(t) \leq 1 - (1 - p_0)e^{-F(t_I)} =: z_I, \quad \text{for all } t \in [0, t_I] \quad (2.20)$$

with  $F(t_I) = \int_0^{t_I} G(\theta(\xi))H(-\theta_\xi(\xi))d\xi$ .

Therefore, we put  $z(t_I) = z_I$  and solve (2.20) only for  $t \geq t_I$ . We distinguish between three cases:

(a)  $G(\theta(t))H(-\theta_t(t)) = 0$  a.e. in  $[t_I, T]$ :

Then we have to solve the IVP

$$z(t_I) = z_I, \quad (2.21a)$$

$$\dot{z}(t) = (1 - z(t))f(t, z(t), \theta)H(A_s - \theta(t)). \quad (2.21b)$$

Using the same argument as in [9], we obtain a unique solution of (2.22) satisfying

$$z_I \leq z(t) \leq c_T < 1, \quad \text{for all } t \in [t_I, T]. \quad (2.22)$$

(b)  $G(\theta(t))H(-\theta_t(t)) \neq 0$  a.e. in  $[t_I, T]$ .

In this case we rewrite (2.20) in the following way:

$$z(t_I) = z_I, \quad (2.23a)$$

$$\dot{z}(t) = -(1 - z(t)) \ln(1 - z(t)) (\tilde{f}_1(t, z(t), \theta) + \tilde{f}_2(\theta(t), \theta_t(t))), \quad (2.23b)$$

where we define

$$\tilde{f}_2(\theta, \theta_t) := -\frac{1}{\ln(1 - z(t))} G(\theta) H(-\theta_t) \quad (2.24)$$

and

$$\tilde{f}_1(t, z(t), \theta) := -\underbrace{\left( \int_0^t \frac{b(\theta(\xi))^{\frac{1}{a(\theta(\xi))}}}{b(\theta(t))^{\frac{1}{a(\theta(t))}}} \left( -\ln(1 - z(t)) \right)^{\frac{1}{a(\theta(t))} - \frac{1}{a(\theta(\xi))}} d\xi \right)^{-1}}_{=:I} H(A_s - \theta(t)). \quad (2.25)$$

We know that

$$\theta \leq M_s \quad \text{and} \quad \theta_t \leq 0 \quad \text{a.e. in } [t_I, T], \quad (2.26)$$

therefore, thanks to (A3), for all  $t_1, t_2 \in [t_I, T]$ ,  $t_1 \leq t_2$  we have

$$0 < a(\theta(t_2)) \leq a(\theta(t_1)). \quad (2.27)$$

Hence utilizing (A2) there exist constants  $c_1, c_2 > 0$ , such that

$$I \geq c_1 t_I \inf_{\substack{t_1, t_2 \in [t_I, T] \\ t_1 \leq t_2}} \inf_{z \in [z_I, 1]} \left( -\ln(1 - z) \right)^{\frac{1}{a(\theta(t_2))} - \frac{1}{a(\theta(t_1))}} \geq c_2. \quad (2.28)$$

Then, in view of (A4) there exists a constant  $c_3 > 0$  s.t.

$$\sup_{(t, z) \in [t_I, T] \times [p_0, 1]} (\tilde{f}_1(t, z(t), \theta) + \tilde{f}_2(\theta(t), \theta_t(t))) \leq c_3. \quad (2.29)$$

Applying Lemma 2.2, we obtain a unique solution of (2.23), satisfying

$$z_I \leq z(t) \leq c_{I, T} < 1, \quad \text{for all } t \in [t_I, T]. \quad (2.30)$$

(c) General case:

Although there may exist infinitely many disjoint intervals  $J_k \subset [t_I, T]$  such that

$$G(\theta(t))H(-\theta_t(t)) \neq 0 \quad \text{a.e. in } J_k$$

(think for instance of  $\theta(t) = M_s + (t - c)^2 \sin(\frac{1}{t-c})$ , and  $c > t_I$ ), since  $\theta$  is of bounded variation and thanks to (A3) we can dissect  $[t_I, T]$  in (finitely many) intervals such that either inequality (2.28) is valid or  $G(\theta(t))H(-\theta(t)) = 0$ . Therefore, alternating between cases (a) and (b) finitely often, we have proved assertion (3). Then assertion (4) is a direct consequence of (A1)–(A4) and (3).

Using the apriori estimates (3) and (4), the solution can be extended to the whole interval  $[0, T]$ .

Assertion (1) finally follows from the strong monotonicity of the function

$$p \mapsto \int_0^{t_I} \frac{1}{\tau(\theta(\xi), p)} d\xi. \quad (2.31)$$

□

For later use, we now replace the Heaviside function  $H$  occurring in the expressions  $H(A_s - \theta)$  and  $H(-\theta_t)$  with the Yosida approximation  $H_\delta$  of the heaviside graph  $\hat{H}$  (c.f. appendix), and obtain the following regularized problem:

$$p(0) = p_0, \quad (2.32a)$$

$$m(0) = 0, \quad (2.32b)$$

$$\dot{p}(t) = (1 - p(t) - m(t)) f(t, p(t), m(t), \theta) H_\delta(A_s - \theta(t)), \quad (2.32c)$$

$$\dot{m}(t) = (1 - p(t) - m(t)) G(\theta(t)) H_\delta(-\theta_t(t)). \quad (2.32d)$$

Of course, Lemma 2.1 still holds for (2.32a–d). Furthermore, we get the following result:

**Lemma 2.3** *Let  $(p_i, m_i)$ ,  $i = 1, 2$  be two solutions of (2.32a–d) corresponding to  $\theta_i \in H^1(0, T)$ ,  $i = 1, 2$ , then under the assumptions of Lemma 2.1, there exist constants  $L_1, L_2$  such that for all  $t \in [0, T]$  the following is valid:*

$$\begin{aligned} & (p_1(t) - p_2(t))^2 + (m_1(t) - m_2(t))^2 \\ & \leq L_1 \int_0^{\max\{t, t_I\}} (\theta_1(\xi) - \theta_2(\xi))^2 d\xi + L_2 \int_0^t (\theta_{1,\xi}(\xi) - \theta_{2,\xi}(\xi))^2 d\xi. \end{aligned} \quad (2.33)$$

*Proof:* Using the implicit function theorem, for the initial values  $p_{0,1}, p_{0,2}$  as defined in (2.4) one easily gets:

$$|p_{0,1} - p_{0,2}| \leq L \int_0^{t_I} |\theta_1(\xi) - \theta_2(\xi)| d\xi. \quad (2.34)$$

Then (2.33) directly follows from (A1)–(A4) and the Lipschitz continuity of the Yosida approximation (cf. Lemma A.3). □

### 3 Three-dimensional model

Let  $\Omega \subset \mathbb{R}^3$  be bounded with smooth boundary  $\partial\Omega =: \Gamma$  and  $Q := \Omega \times (0, T)$ . In a spatial model one has to take into account recalescence effects owing to the latent heat of the phase transitions. As in [9] we consider the following balance of energy:

$$\rho(\theta)c(\theta)\frac{\partial\theta}{\partial t} - \nabla \cdot (k(\theta)\nabla\theta) = \rho(\theta)L_p(\theta)\frac{\partial p}{\partial t} + \rho(\theta)L_m(\theta)\frac{\partial m}{\partial t}, \quad \text{in } Q, \quad (3.1)$$

together with boundary and initial conditions

$$-k(\theta)\frac{\partial\theta}{\partial\nu} = \gamma(\theta)(\theta - \theta_\Gamma), \quad \text{in } \Gamma \times (0, T), \quad (3.2a)$$

$$\theta(\cdot, 0) = A_s, \quad \text{in } \Omega. \quad (3.2b)$$

Here  $\rho$  is the mass density,  $k$  the heat conductivity,  $c$  the specific heat at constant pressure,  $\gamma$  the heat transfer coefficient and  $L_m, L_p$  the latent heats of the austenite–martensite and the austenite–pearlite phase change, respectively.

Concerning these data functions, we assume the following:

(A5)  $\rho, c, k, \gamma > 0$  constants,

(A6)  $L_p, L_m \in C^{0,1}(\mathbb{R})$  satisfying

$$0 \leq L_p(\theta) \leq \eta, \quad 0 \leq L_m(\theta) \leq \eta \text{ for all } \theta \in \mathbb{R} \text{ and a positive constant } \eta.$$

**Remark 3.1** *Assumption (A5) is not essential. Using the Kirchhoff transformation*

$$J(\theta) = \int_{A_s}^{\theta} \rho(x)c(x)dx$$

*one could allow for temperature dependent coefficients  $\rho, c$ .*

Before studying the general case, we consider the following regularized problem ( $P_\delta$ ):

$$\rho c \theta_t + \rho L_m(\theta)(1 - p - m)G(\theta)A_\delta(\theta_t) - k\Delta\theta = \rho L_p(\theta)p_t, \quad \text{in } Q, \quad (3.3a)$$

$$-k\frac{\partial\theta}{\partial\nu} = \gamma(\theta - \theta_\Gamma), \quad \text{in } \Gamma \times (0, T), \quad (3.3b)$$

$$\theta(\cdot, 0) = A_s, \quad \text{in } \Omega. \quad (3.3c)$$

Here,  $(p, m)$  is the solution to (2.32a–d), where we have replaced  $H(A_s - \theta)$  and  $H(-\theta_t)$  with  $H_\delta(A_s - \theta)$  and  $H_\delta(-\theta_t)$  and where  $H_\delta$  again denotes the Yosida approximation of the heaviside graph. Furthermore, we have introduced the notation  $A_\delta(\cdot) := -H_\delta(-\cdot)$ .

We have the following result for the regularized problem:

**Theorem 3.1** *Assume (A1)–(A6) and let  $\theta_\Gamma \in H^1(0, T; H^1(\Omega))$ . Then, if the incubation time  $t_I \in (0, T)$  has been chosen small enough, there exists a unique solution  $\theta_\delta \in H^{2,1}(Q) = H^1(0, T; L^2(\Omega)) \cap L^2(0, T; H^2(\Omega))$  to  $(P_\delta)$ .*

*Proof:*

The proof is carried through using a fixed point argument. To this end, we define the space  $X_T : H^1(0, T; L^2(\Omega))$  endowed with the norm  $\|u\|_{X_T}^2 := \|u\|_{L^2(Q)}^2 + \|u_t\|_{L^2(Q)}^2$  and an operator

$$F : K_T \subset X_T \longrightarrow X_T, \quad \theta = F\hat{\theta}, \quad (3.4)$$

where  $\theta$  is the solution of the following nonlinear parabolic problem:

$$(\rho c \mathbf{I} + D_1(\hat{\theta})A_\delta)(\theta_t) - k\Delta\theta = D_2(\hat{\theta}), \quad \text{in } Q, \quad (3.5a)$$

$$-k\frac{\partial\theta}{\partial\nu} = \gamma(\theta - \theta_\Gamma), \quad \text{in } \Gamma \times (0, T), \quad (3.5b)$$

$$\theta(\cdot, 0) = A_s, \quad \text{in } \Omega. \quad (3.5c)$$

Here we used the abbreviations

$$D_1(\hat{\theta}) = \rho L_m(\hat{\theta})(1 - \hat{m} - \hat{p})G(\hat{\theta}), \quad (3.6)$$

$$D_2(\hat{\theta}) = \rho L_p(\hat{\theta})\hat{p}_t, \quad (3.7)$$

where  $(\hat{p}, \hat{m})$  is the solution to (2.9a–d) corresponding to  $\hat{\theta}$ . Owing to the strong monotonicity of the operator  $\rho c \mathbf{I} + D_1(\hat{\theta})A_\delta$ , using Rothe's method of implicit time discretization, it is not difficult to prove that (3.5a–c) has a unique solution  $\theta$ . Testing (3.5a) with  $\theta_t$  and invoking Gronwall's inequality, we obtain the standard estimate

$$\rho c \int_0^t \int_\Omega \theta_s^2 dx ds + \frac{k}{2} \int_\Omega |\nabla\theta(t)|^2 dx + \frac{\gamma}{2} \int_\Gamma \theta(t)^2 d\sigma \leq M_1, \quad (3.8)$$

where, thanks to (A1)–(A4) and Lemma 2.1(4), the constant  $M_1$  is independent of  $\hat{\theta}$ . Hence,  $F$  is well-defined and a self-mapping on

$$K_T := \{\theta \in X_T \mid \|\theta\|_{X_T} \leq M_2\} \quad (3.9)$$

for some constant  $M_2 > 0$ .

Now, let  $\hat{\theta}_i \in X_T$  and  $\theta_i := F(\hat{\theta}_i)$  for  $i=1,2$ .

Then, owing to Lemma 2.3 and (A1) – (A6), the following Lipschitz conditions hold a.e. in  $Q$ :

$$|D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2)| \leq L_1|\hat{\theta}_1 - \hat{\theta}_2| + L_2 \int_0^{t^*} |\hat{\theta}_1 - \hat{\theta}_2| ds + L_3 \int_0^t |\hat{\theta}_{1,s} - \hat{\theta}_{2,s}| ds \quad (3.10)$$

$$|D_2(\hat{\theta}_1) - D_2(\hat{\theta}_2)| \leq L_1|\hat{\theta}_1 - \hat{\theta}_2| + L_2 \int_0^{t^*} |\hat{\theta}_1 - \hat{\theta}_2| ds + L_3 \int_0^t |\hat{\theta}_{1,s} - \hat{\theta}_{2,s}| ds, \quad (3.11)$$

with  $t^* := \max\{t, t_I\}$ . Inserting  $(\hat{\theta}_i, \theta_i)$ ,  $i = 1, 2$  into (3.5a-d), subtracting both equations and testing with  $\theta_t := \theta_{1,t} - \theta_{2,t}$  we find:

$$\begin{aligned}
& \int_0^t \int_{\Omega} (D_2(\hat{\theta}_1) - D_2(\hat{\theta}_2)) \theta_s \, dx ds \\
&= \rho c \int_0^t \int_{\Omega} \theta_s^2 \, dx ds + \int_0^t \int_{\Omega} D_1(\hat{\theta}_1) (A_\delta(\theta_{1,s}) - A_\delta(\theta_{2,s})) \theta_s \, dx ds \\
&\quad + \int_0^t \int_{\Omega} A_\delta(\theta_{2,s}) (D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2)) \theta_s \, dx ds + \frac{k}{2} \int_{\Omega} |\nabla \theta(t)|^2 \, dx + \frac{\gamma}{2} \int_{\Gamma} \theta^2(t) \, d\sigma \\
&\geq \rho c \int_0^t \int_{\Omega} \theta_s^2 \, dx ds + \int_0^t \int_{\Omega} A_\delta(\theta_{2,s}) (D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2)) \theta_s \, dx ds. \tag{3.12}
\end{aligned}$$

Using Hölder's and Young's inequalities, we get

$$\begin{aligned}
& \int_0^t \int_{\Omega} A_\delta(\theta_{2,s}) (D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2)) \theta_s \, dx ds \\
&\leq \frac{\rho c}{4} \int_0^t \int_{\Omega} \theta_s^2 \, dx ds + \frac{1}{\rho c} \int_0^t \int_{\Omega} (D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2))^2 \, dx ds, \tag{3.13}
\end{aligned}$$

and

$$\begin{aligned}
& \int_0^t \int_{\Omega} (D_2(\hat{\theta}_1) - D_2(\hat{\theta}_2)) \theta_s \, dx ds \\
&\leq \frac{\rho c}{4} \int_0^t \int_{\Omega} \theta_s^2 \, dx ds + \frac{1}{\rho c} \int_0^t \int_{\Omega} (D_2(\hat{\theta}_1) - D_2(\hat{\theta}_2))^2 \, dx ds. \tag{3.14}
\end{aligned}$$

Thanks to (3.10) and the inequality

$$\int_0^t \int_{\Omega} \left( \int_0^{\max\{s, t_I\}} |\hat{\theta}_1 - \hat{\theta}_2| \, d\xi \right)^2 \, dx ds \leq t^{*2} \int_0^t \int_{\Omega} (\hat{\theta}_1 - \hat{\theta}_2)^2 \, dx ds, \tag{3.15}$$

we obtain

$$\begin{aligned}
& \int_0^t \int_{\Omega} (D_1(\hat{\theta}_1) - D_1(\hat{\theta}_2))^2 \, dx ds \\
&\leq 3(L_1 + t^{*2}L_2) \int_0^t \int_{\Omega} (\hat{\theta}_1 - \hat{\theta}_2)^2 \, dx ds + 3L_3 t^2 \int_0^t \int_{\Omega} (\hat{\theta}_{1,s} - \hat{\theta}_{2,s})^2 \, dx ds \tag{3.16}
\end{aligned}$$

$$\leq 3(L_1 + T^2L_2)T \|\hat{\theta}_1 - \hat{\theta}_2\|_{L^\infty(0,T;L^2(\Omega))}^2 + 3L_3 T^2 \int_0^T \int_{\Omega} (\hat{\theta}_{1,s} - \hat{\theta}_{2,s})^2 \, dx ds. \tag{3.17}$$

The same inequality holds for  $D_2(\hat{\theta}_1) - D_2(\hat{\theta}_2)$ . Invoking the Poincaré inequality

$$\int_{\Omega} \theta^2(x, t) dx ds \leq T \int_0^t \int_{\Omega} \theta_t^2(x, s) dx ds, \quad (3.18)$$

we finally obtain

$$\|\theta(t)\|_{X_T}^2 \leq g(T) \|\hat{\theta}_1 - \hat{\theta}_2\|_{X_T}^2, \quad (3.19)$$

with a strictly increasing polynomial  $g$ . Since  $g(t) \rightarrow 0$  for  $t \rightarrow 0$ , there exists  $T^+$  such that  $g(T^+) < 1$ . Choosing  $t_I \in (0, T^+)$  the operator  $F$  is well-defined and a contraction on  $K_{T^+}$ , whereby we have obtained a unique local solution of  $(P_\delta)$  which in view of the a priori estimate (3.8) globally exists.

Standard parabolic regularity results (cf. [14]) finally yield that  $(P_\delta)$  has a strong solution  $\theta$  satisfying

$$\|\theta\|_{H^{2,1}(Q)} \leq M_3, \quad (3.20)$$

with a constant  $M_3 > 0$  independent of  $\theta$ . This finishes the proof of Theorem 3.1.  $\square$

**Remark 3.2** *Instead of assuming the incubation time  $t_I$  to be chosen 'small enough' one could also demand  $\frac{\partial m}{\partial t} = 0$  a.e. in  $(0, t_I)$  or  $p_0 \in (0, 1)$  constant, independent of  $\theta$ .*

*The first case refers to a heat treatment with a moderate cooling rate, producing pearlite and subsequently possibly some martensite.*

*The second condition applies to quench cooling, i.e. very fast cooling to achieve a nearly pure martensitic structure. In this case it is reasonable to assume  $p_0$  to be constant, because no more pearlite will be formed during the cooling process.*

We have the following result for the general case:

**Theorem 3.2** *Under the assumptions of Theorem 3.1, there exists a triple  $(\theta, w, v) \in H^{2,1}(Q) \times L^\infty(Q) \times L^\infty(Q)$ , satisfying*

$$\rho c \theta_t + \rho L_m(\theta) G(\theta) (1 - p - m) w - k \Delta \theta = \rho L_p(\theta) p_t, \quad \text{in } Q, \quad (3.21a)$$

$$-k \frac{\partial \theta}{\partial \nu} = \gamma(\theta - \theta_\Gamma), \quad \text{in } \Gamma \times (0, T), \quad (3.21b)$$

$$\theta(\cdot, 0) = A_s, \quad \text{in } \Omega, \quad (3.21c)$$

and

$$v \in \hat{H}(A_s - \theta), \quad (3.22)$$

$$w \in \hat{A}(\theta_t), \quad (3.23)$$



a.e. in  $Q$ , where  $\hat{A} := -\hat{H}(-\cdot)$ .

Here, for almost all  $x \in \Omega$ ,  $(p(x, \cdot), m(x, \cdot))$  is the solution to the following (IVP):

$$p(x, 0) = p_0(\theta(x, \cdot)), \quad (\text{cf. (2.4)}) \quad (3.24a)$$

$$m(x, 0) = 0, \quad (3.24b)$$

$$p_t(x, t) = (1 - p(x, t) - m(x, t))f(t, p(x, t), m(x, t)\theta(x, \cdot))v(x, t), \quad (3.24c)$$

$$m_t(x, t) = -(1 - p(x, t) - m(x, t))G(\theta(x, t))w(x, t). \quad (3.24d)$$

*Proof:* For  $\delta > 0$  fixed, let  $\theta_\delta$  be the solution to  $(P_\delta)$ . Owing to (3.20), there exists a subsequence

$$\theta_{\delta'} \longrightarrow \theta \quad \text{weakly in } H^{2,1}(Q) \quad (3.25)$$

and, inter alia, strongly in  $L^2(Q)$ . Hence, possibly extracting a further subsequence, we find

$$\theta_{\delta'} \longrightarrow \theta \quad \text{a.e. in } Q. \quad (3.26)$$

Defining  $v_\delta := H_\delta(A_\delta - \theta_\delta)$  and  $w_\delta := A_\delta(\theta_{\delta,t})$  we have

$$v_{\delta'} \longrightarrow v, \quad w_{\delta'} \longrightarrow w \quad \text{weakly}^* \text{ in } L^\infty(Q). \quad (3.27)$$

For  $x \in \Omega \setminus N$  fixed, with a set  $N \subset \Omega$  of measure zero, we call  $(p_\delta(x, \cdot), m_\delta(x, \cdot))$  the solution to (2.32a-d) corresponding to  $\theta_\delta$ . Thanks to Lemma 2.1(3),(4), there exists a constant  $c > 0$  such that

$$\|p_\delta(x, \cdot)\|_{W^{1,\infty}(0,T)} + \|m_\delta(x, \cdot)\|_{W^{1,\infty}(0,T)} \leq c. \quad (3.28)$$

Hence, there exist subsequences

$$p_{\delta'}(x, \cdot) \longrightarrow p(x, \cdot), \quad m_{\delta'}(x, \cdot) \longrightarrow m(x, \cdot) \quad \text{weakly}^* \text{ in } W^{1,\infty}(0, T) \quad (3.29)$$

and uniformly in  $C[0, T]$ . On the other hand, we have

$$\frac{\partial m_{\delta'}}{\partial t}(x, t) = -(1 - p_{\delta'}(x, t) - m_{\delta'}(x, t))G(\theta_{\delta'}(x, t))w_{\delta'}(x, t). \quad (3.30)$$

Thus, possibly extracting a further subsequence, we get

$$w_{\delta'}(x, \cdot) \longrightarrow w(x, \cdot) \quad \text{weakly}^* \text{ in } L^\infty(0, T). \quad (3.31)$$

Moreover, thanks to Lebesgue's theorem, we find

$$(1 - p_{\delta'}(x, \cdot) - m_{\delta'}(x, \cdot))G(\theta_{\delta'}(x, \cdot))\varphi \rightarrow (1 - m(x, \cdot) - p(x, \cdot))G(\theta(x, \cdot))\varphi \quad (3.32)$$

strongly in  $L^1(0, T)$  for any  $\varphi \in L^1(0, T)$ . Hence, the right-hand side of (3.30) converges to  $(1 - m(x, \cdot) - p(x, \cdot))G(\theta(x, \cdot))w(x, \cdot)$  weakly  $*$  in  $L^\infty(0, T)$ . Next, using (3.29) and (A1)–(A3) it is easily confirmed that

$$\frac{\partial p_{\delta'}}{\partial t}(x, \cdot) \longrightarrow (1 - p(x, \cdot) - m(x, \cdot))f(\cdot, p(x, \cdot), m(x, \cdot), \theta(x, \cdot))v(x, \cdot), \quad (3.33)$$

weakly $*$  in  $L^\infty(0, T)$ , and (cf. [9], Lemma 3.1)

$$p_0(\theta_{\delta'}(x, \cdot)) \longrightarrow p_0(\theta(x, \cdot)). \quad (3.34)$$

This means, the limits  $(p(x, \cdot), m(x, \cdot))$  in (3.33) are the solution to the (IVP) (2.32a–d) with respect to the temperature evolution  $\theta(x, \cdot)$ , where we have replaced the terms  $H_\delta(A_s - \theta)$  and  $H_\delta(-\theta_t(x, \cdot))$  with  $v(x, \cdot)$  and  $w(x, \cdot)$ , respectively.

Invoking Lebesgue's theorem once again, we finally obtain:

$$p_{\delta'} \longrightarrow p \quad m_{\delta'} \longrightarrow m \quad \text{strongly in } L^q(Q) \quad (3.35)$$

for any  $q \in [1, \infty)$ . Now we consider the weak formulation of (3.3) for  $\varphi \in L^2(0, T; H^1(\Omega))$  chosen arbitrarily:

$$\begin{aligned} & \int_0^T \int_\Omega (\rho c \theta_{\delta',s} + \rho L_m(\theta_{\delta'})(1 - p_{\delta'} - m_{\delta'})G(\theta_{\delta'})w_{\delta'})\varphi dx ds \\ & + k \int_0^T \int_\Omega \nabla \theta_{\delta'} \nabla \varphi dx ds + \gamma \int_0^T \int_\Gamma (\theta_{\delta'} - \theta_\Gamma)\varphi d\sigma ds = \rho \int_0^T \int_\Omega L_p(\theta_s)p_{\delta',s}\varphi dx ds. \end{aligned} \quad (3.36)$$

In view of (3.20), (3.27) and (3.35), using again Lebesgue's theorem we can pass to the limit in (3.36) and obtain

$$\begin{aligned} & \int_0^T \int_\Omega (\rho c \theta_s + \rho L_m(\theta)(1 - p - m)G(\theta)w)\varphi dx ds \\ & + k \int_0^T \int_\Omega \nabla \theta \nabla \varphi dx ds + \gamma \int_0^T \int_\Gamma (\theta - \theta_\Gamma)\varphi d\sigma ds = \rho \int_0^T \int_\Omega L_p(\theta)p_s\varphi dx ds. \end{aligned} \quad (3.37)$$

Furthermore, since  $v_{\delta'} \rightarrow v$  weakly in  $L^2(Q)$  and  $\theta_{\delta'} \rightarrow \theta$  strongly in  $L^2(Q)$ , using Lemma A.1, we can easily verify (3.22).

Now, the crucial step is to show (3.23), i.e.  $w \in \hat{A}(\theta_t)$ . To this end, we define an operator  $\mathcal{T} : L^2(Q) \rightarrow L^2(Q)$  by

$$\mathcal{T}(u) := \rho L_m(\theta)(1 - m - p)G(\theta)\hat{A}(u). \quad (3.38)$$

According to Lemma A.4,  $\mathcal{T}$  is a maximal monotone operator. Thus, to get

$$\rho L_m(\theta)(1 - m - p)G(\theta)w \in \mathcal{T}(\theta_t), \quad (3.39)$$

we have to show:

$$\int_0^T \int_{\Omega} (\rho L_m(\theta)(1-m-p)G(\theta)w - \eta)(\theta_t - \xi) dx dt \geq 0, \quad (3.40)$$

for all  $(\xi, \eta) \in \text{Graph}(\mathcal{T})$ .

Since  $w_{\delta'} = A_{\delta'}(\theta_{\delta', t}) \in A(J_{\delta'}(\theta_{\delta', t}))$ , we have

$$\rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} \in \mathcal{T}(J_{\delta'}(\theta_{\delta', t})), \quad (3.41)$$

therefore, for all  $(\xi, \eta) \in \text{Graph}(\mathcal{T})$ , the following inequality is valid:

$$\begin{aligned} 0 &\leq \int_0^T \int_{\Omega} (\rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} - \eta)(J_{\delta'}(\theta_{\delta', t}) - \xi) dx dt \\ &= - \int_0^T \int_{\Omega} \rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} \xi dx dt - \int_0^T \int_{\Omega} \eta J_{\delta'}(\theta_{\delta', t}) dx dt \\ &\quad + \int_0^T \int_{\Omega} \eta \xi dx dt + \int_0^T \int_{\Omega} \rho(\theta) L_m(\theta)(1-m-p)G(\theta)w_{\delta'} J_{\delta'}(\theta_{\delta', t}) dx dt. \end{aligned} \quad (3.42)$$

Owing to Lemma A.3, we have

$$\begin{aligned} J_{\delta'}(\theta_{\delta', t}) &= \theta_{\delta', t} - \delta' w_{\delta'} \\ &\longrightarrow \theta_t \quad \text{weakly in } L^2(Q) \end{aligned} \quad (3.43)$$

and

$$\begin{aligned} &\int_0^T \int_{\Omega} \rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} J_{\delta'}(\theta_{\delta', t}) dx dt \\ &= \int_0^T \int_{\Omega} \rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} \theta_{\delta', t} dx dt \\ &\quad - \delta' \int_0^T \int_{\Omega} \rho(\theta) L_m(\theta)(1-m-p)G(\theta)w_{\delta'}^2 dx dt. \end{aligned} \quad (3.44)$$

Therefore, in order to verify (3.40), it suffices to prove

$$\begin{aligned} &\limsup \int_0^T \int_{\Omega} \rho L_m(\theta)(1-m-p)G(\theta)w_{\delta'} \theta_{\delta', t} dx dt \\ &\leq \int_0^T \int_{\Omega} \rho L_m(\theta)(1-m-p)G(\theta)w \theta_t dx dt. \end{aligned} \quad (3.45)$$

To this end, we test (3.5a) by  $\theta_{\delta',t}$  to obtain

$$\begin{aligned}
& \rho c \int_0^T \int_{\Omega} L_m(\theta_{\delta'}) (1 - p_{\delta'} - m_{\delta'}) G(\theta_{\delta'}) w_{\delta'} \theta_{\delta',t} dx dt \\
&= -\rho c \int_0^T \int_{\Omega} \theta_{\delta',t}^2 dx dt - \frac{k}{2} \int_{\Omega} |\nabla \theta_{\delta'}(T)|^2 dx + \frac{k}{2} \int_{\Omega} |\nabla \theta_0|^2 dx \\
&\quad - \gamma \int_0^T \int_{\Gamma} (\theta_{\delta'} - \theta_{\Gamma}) \theta_{\delta',t} d\sigma dt + \rho \int_0^T \int_{\Omega} L_p(\theta_{\delta'}) p_{\delta',t} \theta_{\delta',t} dx dt. \tag{3.46}
\end{aligned}$$

According to Lemma A.5,  $H_{\delta'}(A_s - \cdot)$  is the subdifferential of a convex function  $\mathcal{H}_{\delta'}(A_s - \cdot)$  converging to  $\mathcal{H}(A_s - \cdot)$  and  $\partial \mathcal{H} = \hat{H}$ . Then, in view of (2.9c), defining

$$g_{\delta'} := L_p(\theta_{\delta'}) (1 - p_{\delta'} - m_{\delta'}) f(t, p_{\delta'}, m_{\delta'}, \theta_{\delta'}), \tag{3.47}$$

the last term in (3.46) may be written in the following way:

$$\begin{aligned}
& \int_0^T \int_{\Omega} L_p(\theta_{\delta'}) p_{\delta',t} \theta_{\delta',t} dx dt = - \int_0^T \int_{\Omega} g_{\delta'} \frac{\partial}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) dx dt \\
&= \int_0^t \int_{\Omega} (g - g_{\delta'}) \frac{\partial}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) dx dt - \int_0^T \int_{\Omega} g \frac{\partial}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) dx dt. \tag{3.48}
\end{aligned}$$

Since  $g_{\delta'} \rightarrow g$  strongly in  $L^2(Q)$  we only have to consider the last integral in (3.47), which by integration by parts leads to

$$\begin{aligned}
& \int_0^T \int_{\Omega} g \frac{\partial}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) dx dt \\
&= \int_{\Omega} g \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) \Big|_0^T dx - \int_0^T \int_{\Omega} \frac{\partial g}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta_{\delta'}) dx ds. \tag{3.49}
\end{aligned}$$

On the other hand, thanks to (3.37), (3.22) and Lemma A.5(2), we have

$$\begin{aligned}
& \int_0^T \int_{\Omega} g v \theta_t dx dt = - \int_0^T \int_{\Omega} g \frac{\partial}{\partial t} \mathcal{H}(A_s - \theta) dx dt \\
&= - \int_{\Omega} g \mathcal{H}(A_s - \theta) \Big|_0^T dx - \int_0^T \int_{\Omega} \frac{\partial g}{\partial t} \mathcal{H}_{\delta'}(A_s - \theta) dx ds. \tag{3.50}
\end{aligned}$$

Thus, invoking Lemma A.5(3) we can pass to the limit in (3.48) and obtain (3.50).

For the boundary integral in (3.46) we obtain

$$\int_0^T \int_{\Gamma} (\theta_{\delta'} - \theta_{\Gamma}) \theta_{\delta',t} d\sigma dt = \frac{1}{2} \int_{\Gamma} \theta_{\delta'}^2 \Big|_0^T d\sigma + \int_0^T \int_{\Gamma} \theta_{\Gamma,t} \theta_{\delta'} d\sigma dt - \int_{\Gamma} \theta_{\Gamma} \theta_{\delta'} d\sigma. \tag{3.51}$$

Hence, taking into account (3.48) – (3.51) and the lower semi-continuity of the norm with respect to weak convergence, a comparison with (3.37) shows that we can take lim sup on both sides of equation (3.46) to obtain

$$\begin{aligned} \limsup \rho \int_0^T \int_{\Omega} L_m(\theta_{\delta'}) (1 - p_{\delta'} - m_{\delta'}) G(\theta_{\delta'}) w_{\delta'} \theta_{\delta',t} dx dt \\ \leq \rho \int_0^T \int_{\Omega} L_m(\theta) (1 - m - p) G(\theta) w \theta_t dx dt. \end{aligned} \quad (3.52)$$

This finishes the proof, since the last equation obviously implies (3.45).  $\square$

## 4 Conclusions

Figure 4.1 depicts numerical simulations for the carbon steel C 1080 (cf. Fig. 1.1) using the model under study in this paper (a) in comparison with the model in [9], which was based on the Koistinen and Marburger formula (b). Owing to the irreversibility of our new model for the austenite–martensite phase transition, the cooling curves intersect the dotted  $M_s$ –line without showing unphysical heating–up effects seen in the old model.

Now that an appropriate model for the complete eutectoid transformation is at hand, we see two directions for further research:

- extending the model to a broader class of steels; i.e. incorporating the formation of ferrite and bainite;
- taking into account mechanical effects, which play an important role at least for the austenite–martensite phase transition.

Finally, one could think of modelling the reverse transformation to austenite (although there still seem to be some open questions concerning metallurgy). Then one would be able to describe the complete heat treatment cycle.

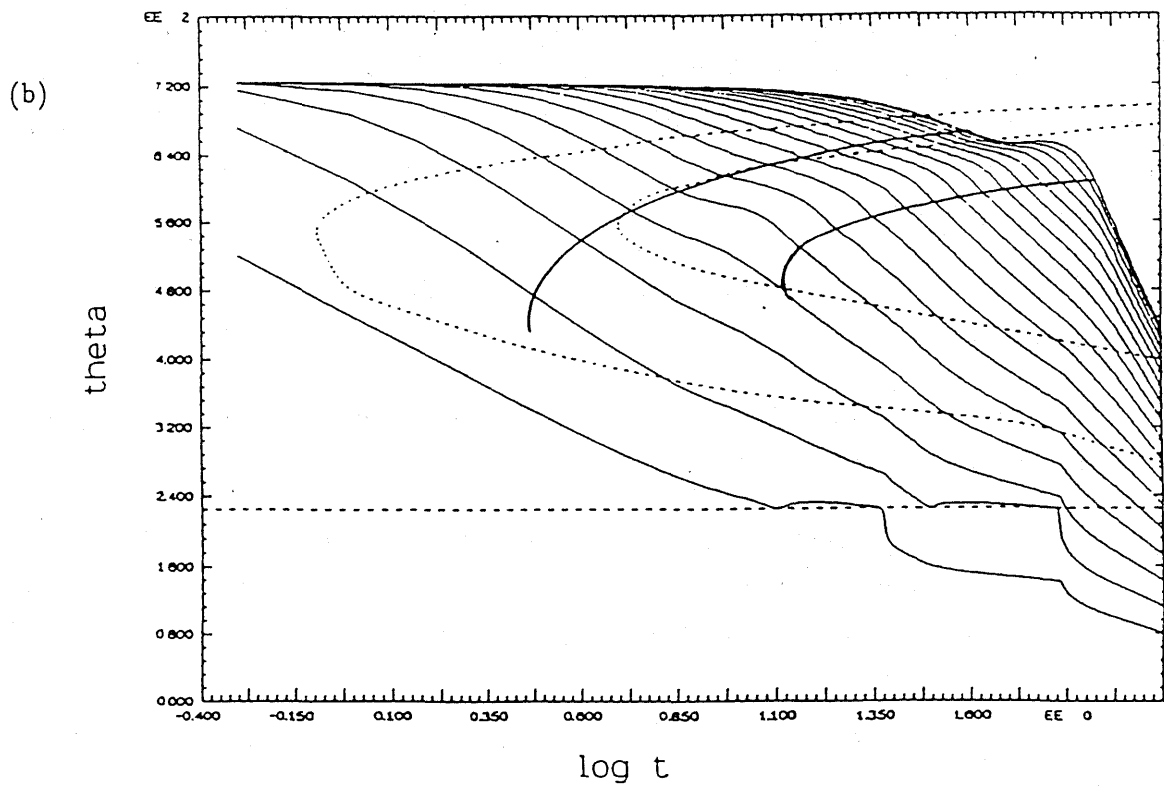
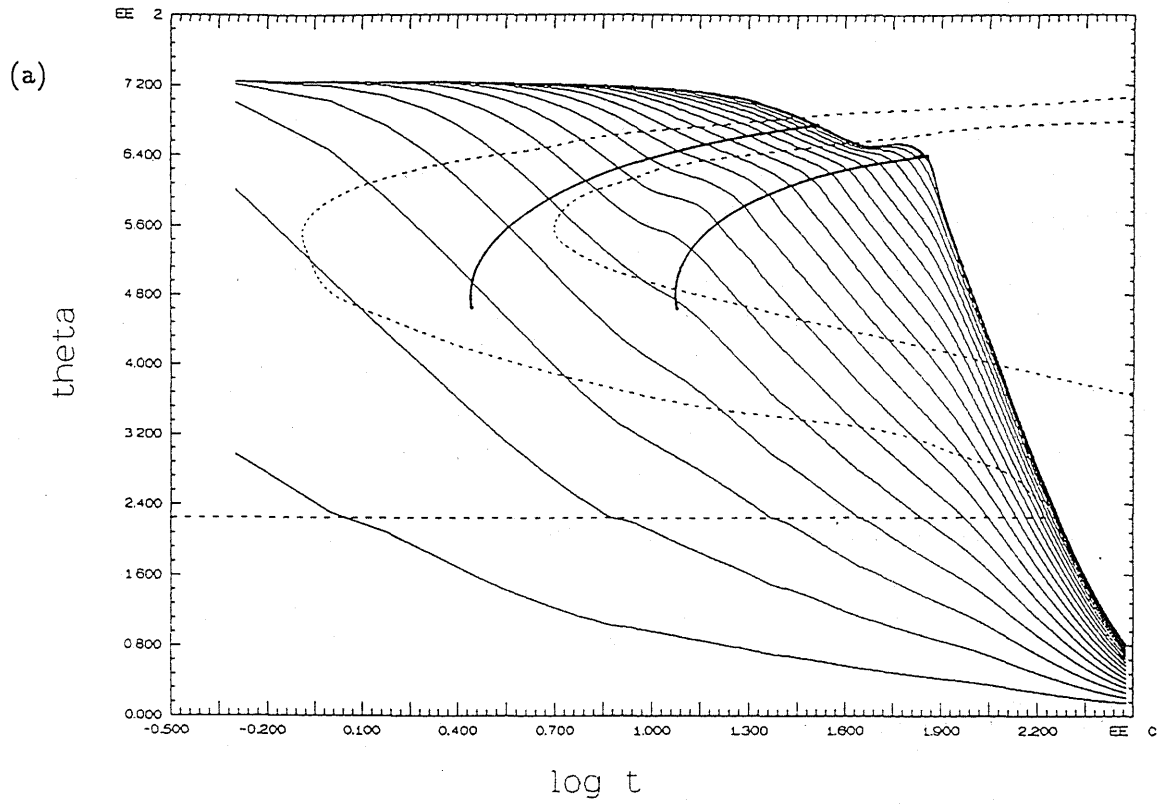


Figure 4.1: Numerical simulations of a CCT diagram: (a) new model, (b) old model, using Koistinen and Marburger formula.

## Appendix

Here we will briefly summarize some basic results about maximal monotone graphs, which can be found, e.g., in the monographs [3], [7] and in [8]. Throughout this section, we will assume that  $X$  is a Hilbert space, which we identify with its dual  $X^*$ .

**Lemma A.1**  $B : X \rightarrow 2^X$  is maximal monotone, if and only if the statements (a) and (b) are equivalent:

(a) For every  $(y, v) \in \text{Graph}(B)$ ,  $\langle u - v, x - y \rangle \geq 0$ .

(b)  $u \in B(x)$ .

**Lemma A.2 (Minty)**

Let  $B : X \rightarrow 2^X$  be monotone. It is maximal monotone if and only if  $I + B$  is surjective.

**Lemma A.3** Let  $B : X \rightarrow 2^X$  be maximal monotone. Then, for all  $\delta > 0$  the following are valid:

(1) The resolvent  $J_\delta := (I + \delta B)^{-1}$  of  $B$  is a non-expansive single valued map from  $X$  to  $X$ .

(2) The Yosida approximation  $B_\delta := \frac{1}{\delta}(I - J_\delta)$  of  $B$  satisfies

(i)  $B_\delta(x) \subset B(J_\delta(x))$ ,  $\forall x \in X$ ,

(ii)  $B_\delta$  is Lipschitzian with constant  $\frac{1}{\delta}$  and maximal monotone.

(3) For all  $x \in \text{Dom}(B)$

(i)  $J_\delta(x) \rightarrow x$ ,

(ii)  $B_\delta(x) \rightarrow m(B(x))$ , where  $m(B(x))$  is the element of  $B(x)$  with minimal norm.

**Lemma A.4** Let  $\hat{H} : \mathbb{R} \rightarrow 2^{\mathbb{R}}$  be the heaviside graph

$$\hat{H}(x) = \begin{cases} \{1\} & , x > 0, \\ [0, 1] & , x = 0, \\ \{0\} & , x < 0, \end{cases}$$

and  $f \in L^2(\Omega)$ ,  $\Omega \subset \mathbb{R}^n$  satisfying  $f(\xi) \geq 0$  a.e. in  $\Omega$ . Then,  $\mathcal{T} : L^2(\Omega) \rightarrow 2^{L^2(\Omega)}$ , defined by

$$(\mathcal{T}(x))(\xi) = f(\xi)\hat{H}(x(\xi))$$

is maximal monotone.

*Proof:*

It is easy to see that  $\mathcal{T}$  is monotone. We apply Lemma A.2 to verify that  $\mathcal{T}$  is maximal monotone. Let  $J_\delta, H_\delta$  denote the resolvent and the Yosida approximation of  $\hat{H}$ , respectively.

Given  $y \in L^2(\Omega)$ , for  $\xi \in \Omega \setminus N$ , with  $N$  of measure zero, we define

$$x(\xi) = \begin{cases} y(\xi) & , \text{ if } f(\xi) = 0, \\ J_{f(\xi)}(y(\xi)) & , \text{ if } f(\xi) > 0. \end{cases}$$

Then  $x$  is measurable and, since

$$|J_{f(\xi)}(0)| = |f(\xi)A_{f(\xi)}(0)| \leq |f(\xi)|,$$

using Lemma A.3(1),(2) we have

$$\|x\|_{L^2(\Omega)}^2 \leq \|y\|_{L^2(\Omega)}^2 + \|f\|_{L^2(\Omega)}^2,$$

i.e.  $x \in L^2(\Omega)$ .

Moreover, by its definition it is clear that  $x$  is a solution of  $y \in (I + \mathcal{T})(x)$ .  $\square$

**Lemma A.5** *Let  $\hat{H}$  again denote the heaviside graph, then:*

(1)  $\hat{H}$  is the subdifferential of the convex function

$$\mathcal{H}(x) := \begin{cases} 0 & , x < 0 \\ x & , x \geq 0. \end{cases}$$

(2) Let  $f \in H^1(a, b)$ , then

$$\frac{\partial}{\partial t} \mathcal{H}(f(t)) = \alpha t'(t), \quad \forall \alpha \in \hat{H}(f(t)).$$

(3) Let  $\mathcal{H}_\delta(x) := \frac{\delta}{2} H_\delta^2(x) + \mathcal{H}(x)$ , then  $\partial \mathcal{H}_\delta = H_\delta$  and  $\mathcal{H}_\delta(x) \rightarrow \mathcal{H}(x)$ .

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