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Abstract

Phase transformations (PT) are an important phenomenon in the material behaviour of steel. There is a large number of models mostly based on the Johnson-Mehl-Avrami-Kolmogorov kinetics for diffusive transformations, and based on the Koistinen-Marburger equation for martensitic transformation. Besides this, generalisations have been developed in order to get more practicable tools for simulations, and to deal with the multi-phase case. It is the main aim of the current paper to develop a quite general phenomenological model of PT based on differential equations, generalising the proposals presented before in a suitable manner. The usual well-known models of PT are included in our general approach. The necessary parameters can be obtained from dilatometer experiments or from transformation diagrams. We present examples for that, based on real data, and perform simulations.

In a further paper [Wol07c], we evaluate the proposed phenomenological model, comparing it with several other PT models. These results show that the proposed model gives a good approximation to experiments.

Keywords

Modelling, phase transformations, steel, multi-phase models, parameter identification, simulations

1 Introduction

Phase transformations (PT) in steel represent a wide field of investigation. The *isothermal* diffusive PT is well described by the Johnson-Mehl-Avrami-Kolmogorov (JMAK) kinetics, there are essential open questions in modelling of *non-isothermal* PT as well as of PT under stress or pre-deformation of austenite, e.g. As a consequence of this there are many proposals for modifications of PT models. For this matter we refer to [Böh03], [Den97], [Leb84, 85], [Lem01], [Rét87, 97], [Ron00] for overview and for [Böh04], [Cab01], [Dac03], [Den92], [Fer85], [Gar98], [Hou86], [Hun99], [Leb84, 85], [Mio04], [Mit92, 02], [Rét98, 99a, 99b, 01], [Sur04], [Sys03], [Wil86], [Wol03a, 03c, 07b, 07c] for investigations and discussions of stress-free PT. There are proposals in order to generalise the classical approach due to JMAK [Avr39, 40, 41], [Joh39] to take the multi-phase case into account, and, last but not least, to obtain practicable tools for simulations (cf. [Leb84, 85], [Rét98, 99b, 01], [For00]).

To investigate stress-free phase transformations one usually performs tests with dilatometers. Stress-dependent phase transformations are investigated with special devices under controlled temperature and stress, measuring length and diameter of the specimen (cf. [Ahr00, 02, 03], [Dal04] for experimental device, and [Ahr00, 02, 03], [Dal04], [Shi04], [Wol03a, 03b, 03c, 05a, 06b, 06c, 06d, 06e, 07b] for experiments and data processing, e.g.). In real processes like heat treatment we normally encounter a situation in which the evolution of phase fractions, temperature and mechanical entities (and sometimes of the carbon content in austenite) is mutually influenced. Thus, modelling and simulation of complex material behaviour like heat-treatment processes of work-pieces generally requires the implementation of PT models describing the multi-phase case in more general situations. We refer to [Ald06], [Bes93], [Ber99], [Dav94], [Den97, 02], [Fuh99], [Höm96, 02, 04, 06a, 06b], [Ino85, 89], [Kim05], [Pie00], [Ron00], [Sch06], [Sjö84], [Suh05], [Vid94], [Wol04, 05b, 06a, 06g], [Yu77] for modelling and/or simulation of complex material behaviour of steel. There are many textbooks and monographs dealing with iron and steel in the context of physics and engineering. Examples are: [Ber06], [Bur65], [Chr75], [Hor92], [Koh94], [Lem01], [Pol88], [Ros56, 72], [Sei99], [Van91]. For modelling of PT in mesoscopic and microscopic context we additionally refer to [Ant04], [Avr39, 40, 41], [Dac04], [Fis03], [Joh39], [Lev98], e.g.

Here our main goals are

- to develop a quite general phenomenological model of PT in steel in the multi-phase case, owing else a simple structure and being suitable for application in simulations,
- to show the relation of this general model to some well-known models like those ones due to Leblond-Devaux (LD) [Leb84, 85] or Johnson-Mehl-Avrami-Kolmogorov [Avr39, 40, 41], [Joh39],
- to give some remarks about interactions between phase evolution, temperature, and mechanical movement,
- to give examples how to obtain the needed parameters from dilatometer data and from transformations diagrams, respectively, and to perform simulations, using these parameters,
- to present some results demonstrating the advantage of the proposed model, referring to our detailed paper [Wol07c].

In section 2 we will deal with modelling of PT. Some remarks about interactions between phase evolution, temperature, and mechanical movement will be given in section 3. In section 4, we will speak in short about mathematical questions arising from PT. Finally, in section 5, we will deal with parameter identification. Using real data, we will simulate examples of the multi-phase case.

2 Phase transformations in steel in the multi-phase case

2.1 General aspects

The subsequent considerations up to formula (2.12) are valid not only for phase transformations (PT) in steel, but also for special (chemical or other) reactions in coexisting mixtures. In the context of macroscopic modelling we regard steel as a coexisting mixture of m ($m \geq 2$) phases (constituents), which may transform into one another under appropriate conditions. Furthermore, we neglect any diffusion of these phases, assuming that they remain at their original places of formation.

Let be p_i ($i = 1, ..., m$) the mass fraction of the i^th^ phase. We write in short $p = (p_1, \ldots, p_m)$. While in the general theory of mixtures mass fractions are used for modelling, volume fractions are mostly preferred when dealing with steel. Fortunately, due to small density differences of the steel phases (for the same temperature) the differences between mass and volume fractions are in the region of one-two percent in the case of steel (cf. [Wol03a, 03c, 07a]). So we will often speak only about “phase fractions”. The number of phases, m, depends on the sort of steel and on the circumstances.

Independent of concrete models of PT we assume the subsequent general balance and non-negativity relations

$$(2.1) \qquad \sum_{i=1}^{m} p_i(x, t) = 1,$$

(2.2) $p_i(x, t) \geq 0$ for $i = 1, ..., m$,

where x is the general spatial point of the body (work piece) Ω and $t \geq 0$ is the time. A general macroscopic model of PT based on ordinary differential equations (ODE) (with the parameter x) usually reads as (cf. [Böh03, 04], [Den97], [For00], [Fuh99], [Höm95, 96, 97], [Hun99], [Ino89], [Leb84, 85], [Mio04], [Mit92, 02], [Rét97, 98, 99a, 99b, 01, 04], [Ron00], [Sur04], [Sys03] e.g.)

$$(2.3) \qquad \frac{\partial p_i}{\partial t}(x, t) = f_i(x, t, p, \theta, \frac{\partial \theta}{\partial t}, S, \xi),$$

completed by the initial conditions

(2.4) $p_i(x, 0) = p_{0i}(x)$ for all x,

where θ - temperature, S - stress tensor, ξ - further possible parameters interpreted as internal variables (all depending on x and t) (cf. section 3), $p_0 = (p_{01}, \ldots, p_{0m})$ – initial phase fractions fulfilling (2.1) and (2.2). In the sequel, time derivatives will be denoted by dots ($\dot{\theta}$ e.g.) as well as by the symbol in (2.3).

Remark 2.1. (i) It is well-known, that the transformation behaviour essentially depends on the carbon content of the parent phases. Thus, in the case of inhomogeneous carbon content, the right-hand side of (2.3) additionally depends on $u_c = (u_{c1}, u_{c2}, \ldots, u_{cm})$, where u_{ci} is the carbon content in the i^{th} phase. This situation arises, when case hardening is modelled (cf. [Ber99], [Ino89], [Wol06g], e.g.). Formally, we can include u_c into the variable ξ.

(ii) For physical reason the dependence of S in (2.3) takes place through its invariants, the von Mises stress and the mean principal stress, e.g. For simplicity, except in section 3, we keep the notation as in (2.3).

(iii) Generally, there is an interaction of mechanical movement, temperature and phase evolution. Thus, the stress tensor S implicitly depends on other entities, possibly on phase fractions via integral terms. We return to this in section 2.7. Hence, instead of the ODE in (2.3), some integro-differential equations might be more appropriate. Since the subsequent discussion would be analogous, we focus on ODE's for describing PT. We refer to [Ahr00, 02, 03], [Dal04], [Den97], [Ino85, 89], [Shi04], [Wol03b, 05a, 06d, 06f] for investigations of PT under stress.

(iv) Generally, in (2.3), we allow an explicit dependence on x and t. Thus, it is possible to model spatial non-homogeneities (after chemical treatment, e.g., cf. [Fre06]). Moreover, one could use special PT models depending explicitly on time. For convenience, we suppress this in the forthcoming discussion.

(v) As (macroscopic spatial) diffusion of the phases is neglected, the equations in (2.3) do not contain *spatial partial derivatives* like in diffusion equations. Hence, the spatial variable x plays only the role of a parameter. Therefore, in the subsequent models, it will be often suppressed in notation.

A further consequence of (2.1) is the subsequent assumption for $f = (f_1, \ldots, f_m)$

$$(2.5) \qquad \sum_{i=1}^{m} f_i = 0 \qquad \text{for all possible arguments.}$$

Obviously, the considerations above are valid for chemical reactions or general phase changes without diffusion of the constituents.

We note, that the (macroscopic) model given by (2.3), (2.4) can be included into a general model of material behaviour of steel in the frame work of continuum mechanics. In this context the phase fractions are regarded as internal variables and the equations in (2.3) become their evolution equations. We refer to [Wol05b, 06a, 06h] for details and discussion. We note, that the dependence on the time derivative $\dot{\theta}$ of the temperature θ in (2.3) is not compatible with the standard internal-variable setting and requires additional efforts. Here we want to focus on PT themselves, and so we suppress this discussion.

Now, we want to specialise f in order to obtain applicable PT models for multi-phase simultaneous and consecutive reactions, respectively. Following [Leb84, 85], [Rét98, 99b, 01], [For00], we assume, that the transformation of the i^{th} phase into the j^{th} phase ($i \neq j$) abbreviated as $i \to j$ has the transformation rate $-a_{ij}$, i.e., for the transformation $i \to j$ (for $i, j = 1, \dots, m$, $i \neq j$) the change of p_i in favour to p_j can be described by the transformation law in rate form

(2.6) $\dot{p}_i = -a_{ij}$.

In accordance with (2.6) the growth of p_j at expense of p_i is expressed as

(2.7) $\dot{p}_j = a_{ij}$.

As a consequence of (2.6) and (2.7) we set

(2.8) $a_{ii} := 0 \qquad i = 1, \dots, m$

and

(2.9) $a_{ij} \geq 0 \qquad i, j = 1, \dots, m.$

If the transformation $i \to j$ does not take place, we have $a_{ij} = 0$. Generally, the a_{ij} depend on the same variables as the f_i in (2.3). In case of

(2.10) $a_{ij} = a_{ij}(p_i, p_j, \theta, \dot{\theta}, S, \xi)$

the PT $i \to j$ is *not* influenced by the presence of the remaining phases. But generally, there may be an influence of further present phases. In this case, we have

(2.11) $a_{ij} = a_{ij}(p_i, p_j, p_k, \theta, \dot{\theta}, S, \xi) \qquad k \neq i, j.$

Here, we do not specify the rates a_{ij} in accordance with the JMAK kinetics or with other approaches as in [Leb84, 85], [Rét98, 99b, 01, 04], [For00]. Later on (cf. (2.22)), we propose a more general ansatz leading to differential equations with several (possibly five) parameters.

Based on the above considerations, the system (2.3) can be specialised in the following manner

(2.12) $\dot{p}_i = -\sum_{j=1}^{m} a_{ij} + \sum_{j=1}^{m} a_{ji} \qquad i = 1, \dots, m,$

fulfilling the condition (2.5) (taking (2.8) into account). These equations are still quite general. Similarly as in [Leb84, 85], [Rét98, 99b, 01], [For00], we formulate two general assumptions for *phase transformations in steel*:

(2.13) For each $i, j \in \{1, ..., N\}$, $i \neq j$, there exists a quantity $\overline{p}_{ij} = \overline{p}_{ij}(\theta, S, \xi, p_k, p_0)$ ($k \neq i, j$), such that the transformation $p_i \to p_j$ may only occur under the condition

$$p_i > 0 \quad \text{and} \quad \overline{p}_{ij} - p_j > 0.$$

If a particular transformation can not occur under any conditions, we set $\overline{p}_{ij} = 0$.

(2.14) For each phase j, there exist two temperatures θ_{jf} and θ_{js} generally depending on S, ξ (and possibly on $\dot{\theta}$ and on p_k, $k \neq i, j$) such that the transformation $i \to j$ may only occur, if $\theta_{jf} \leq \theta < \theta_{js}$. This last condition can be taken into account by a switch-off function G_{ij}, which is one, if the condition is fulfilled, and which is zero otherwise.

We want to comment on these last two assumptions.

Remarks 2.2. (i) The quantity $\overline{p}_{ij}$ plays the role of a “limit value” of the j^{th} phase fraction which can be obtained from phase i (cf. [For00]). That means, for the transformation $i \to j$ the maximal possible fraction p_j is $\overline{p}_{ij}$, and $\overline{p}_{ij}$ depends on the current values of θ, S, ξ, the remaining phases p_k, and possibly on the initial values p_0 (cf. section 2.6.2). Sometimes, there was introduced an equilibrium value $\overline{p}_j$ of the j^{th} phase which can be obtained under given θ, S, ξ from all possible phases (cf. [Leb84, 85], [Rét98, 01]).

(ii) Of course, sometimes the limit values are equilibrium values, too. For instance, this is the case for the PT austenite into ferrite and vice versa in an non-alloyed hypoeutectoid steel for temperatures higher than 723 °C. The equilibrium values can be obtained from the Fe-Fe_3C diagram, using the lever rule (cf. [Ber06], [Hor92], [Koh94], [Pol88], [Ros56, 72], [Wev54], [Van91]).

(iii) The assumption (2.14) does *not* exclude a simultaneous forming and dissolution of a phase at the same time. Assuming *additionally* for a pair i, j

$$(2.15) \qquad \theta_{is} \leq \theta_{jf} \qquad \text{or} \qquad \theta_{js} \leq \theta_{if},$$

the transformations i → j and j → i cannot be performed simultaneously. The condition (2.15) describes the typical situation for steel.

Let be the Heaviside function H defined by

$$(2.16) \qquad H(s) := 0 \qquad \text{for } s \leq 0, \qquad H(s) = 1 \qquad \text{for } s > 0.$$

Taking the assumptions (2.13) and (2.14) into account, we propose the subsequent general model for PT in steel

$$(2.17) \qquad \dot{p}_i = -\sum_{j=1}^{m} a_{ij}\, H(p_i)\, H(\overline{p}_{ij} - p_j)\, G_{ij} + \sum_{j=1}^{m} a_{ji}\, H(p_j)\, H(\overline{p}_{ji} - p_i)\, G_{ji} \qquad i = 1, \ldots, m.$$

Clearly, if there are only two phases, i and j, and if the conditions (2.13) and (2.14) are fulfilled, (2.17) reduces to (2.6) and (2.7). As the functions a_{ij} may be quite general, one has to propose an ansatz. After this, the needed parameters must be determined by additional considerations, using dilatometer data or transformation diagrams. We will deal with this in the points 2.2 – 2.6.

Remarks 2.3. (i) The condition (2.5) is fulfilled for the right-hand sides of (2.17).

(ii) The number of phases under consideration depends on the specific situation of modelling. On one side, this number depends on the steel category (eutectoid, hypoeutectoid e.g.). On the other side, sometimes it may be convenient to deal with additional artificial phases (see section 2.6).

(iii) The Heaviside function in (2.16) is not continuous in s = 0. Thus, for mathematical reason it could be necessary to regularise it (cf. section 4). The same concerns to the switch-off functions G_{ij}.

(iv) Experiments show, that PT in steel are generally not symmetric, i.e. in general, we have

$$(2.18) \qquad a_{ij} \neq a_{ji}.$$

(v) From the balance relations (2.1) it follows that the ODE in (2.3) (as well as in (2.12) and (2.17)) are not independent from each other. Thus, for convenience one can drop one ODE, as the one for austenite, e.g.

Example 2.4. A simple specialisation of (2.6) consists in assuming

$$(2.19) \qquad a_{ij} = \mu_{ij}\, p_i,$$

where the non-negative μ_{ij} may depend on the same arguments as a_{ij}. The last equation means, that the rate of decomposition of i into j is proportional to the fraction of i available for decomposition. In case of only two present phases 1 and 2 this leads to (cf. (2.6))

$$(2.20) \qquad \dot{p}_1 = -\, \mu_{12}\, p_1.$$

Using (2.1), we obtain for the forming phase

(2.21) $\dot{p}_2 = \mu_{12}\,(1 - p_2)$.

Hence, in this case the entities $\bar{p}_{12}$ and $\bar{p}_{21}$ are 1 and 0, respectively. Thus, the ansatz (2.19) does *not* allow arbitrary “equilibrium” values. A slight generalisation of (2.19) leads to the approach developed in [Leb84, 85] (see section 2.3).

2.2 A general phenomenological multi-phase model for PT in steel

We are going to present proposals for the functions a_{ij} in (2.17) which determine the PT. As mentioned in the introduction, the PT laws presented before do not fit very well with available data in the case of varying temperature, under stress and after pre-deformation of austenite, respectively. Therefore, we present a phenomenological model owing else a simple structure and being capable for extensions (stress dependence, e.g.) as well as for possible simplifications, and, moreover, for applications in simulations. The involving parameters have to be identified at best by experimental data (see section 5.1). Slightly extending the suggestions in [Höm06a], we assume for the (*both* diffusive and martensitic) PT $i \to j$ the growth rate a_{ij} (of p_j) (cf. (2.6))

(2.22) $a_{ij} := (e_{ij}(\theta, S, \xi) + p_j)^{r_{ij}(\theta, S, \xi)}\,(\bar{p}_{ij} - p_j)^{s_{ij}(\theta, S, \xi)}\,g_{ij}(\theta, S, \xi)\,h_{ij}(\dot{\theta})$ for $i, j = 1, \ldots, m$.

The parameters e_{ij}, r_{ij}, s_{ij}, g_{ij}, and h_{ij} have to fulfil

(2.23) $e_{ij} \geq 0,\ r_{ij} \geq 0,\ s_{ij} > 0,\ g_{ij} \geq 0,\ h_{ij} \geq 0,\ h(0) = 1$ for all admissible arguments.

Remarks 2.5. (i) (Motivation of (2.22)) The ansatz in (2.22) is motivated by the subsequent considerations. Generally, a diffusive transformation begins and ends slowly. Thus, we may assume that the production rate of p_j is proportional to p_j itself as well as to the difference to the limit value. This leads to

(2.24) $a_{ij} := p_j\,(\bar{p}_{ij} - p_j)\,g_{ij}$,

and in generalisation to (2.22). The (small) parameter e_{ij} has been introduced for mathematical reason (see section 4). For martensitic transformation one can set $r_{ij} = 0$, because there is no delay at the beginning. This leads to the ansatz by Leblond and Devaux [Leb84, 85] (see section 2.3).

(ii) The ansatz in (2.22) works well, if the phase j forms *only* from phase i (as a ferritic phase from austenite). Contrary to this, the forming of austenite from several ferritic phases may lead to some problems when defining the limit values. We will return to this in section 2.6.2.

(iii) Furthermore, it is possible, that the parameters in (2.22) depend on the remaining phases p_k, $k \neq i, j$. In this case, the parameter identification is more complicated. But even in this case, the subsequent discussions remain valid with adequate modifications. Therefore, we focus on the approach in (2.22).

In accordance with (2.8) we set

(2.25) $e_{ii} = r_{ii} = s_{ii} = g_{ii} = h_{ii} := 0$ for $i = 1, \ldots, m$.

For completely non-occurring transformations we set $g_{ij} = 0$. In section 4 we discuss further restrictions to the parameters e_{ij}, r_{ij} and s_{ij} coming both from physical and mathematical reasons. Depending on the circumstances, one can deal without the parameter h in (2.22) or not. In section 5, we return to this, using real data. But, anyway, we assume

(2.26) $h_{ij}(0) = 1$ for diffusive PT, $h_{ij}(0) = 0$ for the martensitic PT.

Hence, for *isothermal* diffusive PT (under constant stress) there are the four parameters e_{ij}, r_{ij}, s_{ij} and g_{ij} which have to be identified, using experimental data obtained from special testing machines like dilatometer. After this, the parameter h can be optimised for linear cooling.

Alternatively, transformation diagrams can be used for determining the needed parameters. We will discuss these questions of parameter identification in section 5.

Finally, combining (2.17) and (2.22), we obtain a quite general mathematical model for multi-phase transformations in steel:

$$(2.27)\qquad \dot{p}_i = -H(p_i) \sum_{j=1}^{m} (e_{ij} + p_j)^{r_{ij}} (\max\{\overline{p}_{ij} - p_j, 0\})^{s_{ij}} g_{ij} h_{ij} G_{ij} +$$

$$+ \sum_{j=1}^{m} (e_{ji} + p_i)^{r_{ji}} (\max\{\overline{p}_{ji} - p_i, 0\})^{s_{ji}} g_{ji} h_{ji} G_{ji} H(p_j) \qquad i = 1, \ldots, m.$$

As we will show in the next sections, some well-known PT laws are included in the ansatz (2.22) as special cases.

2.3 The Leblond-Devaux proposal

In [Leb84, 85] the authors proposed a model for anisothermal phase transformations in steel in the case of more than one phase for diffusive as well as for martensitic transformations. (In [For00], a generalisation was presented.) The goal in [Leb84, 85] was to present a model being "nearly" linear, taking (2.13) into account and generalising the simplest possible transformation in case of two phases. Contrary to our more general approach, Leblond and Devaux [Leb84, 85] assumed that each phase i has its equilibrium value $\overline{p}_i$, and that the transformation i → j is only possible, if

$$(2.28)\qquad p_i > \overline{p}_i \text{ and } \overline{p}_j > p_j.$$

In this case they proposed for two existent phases:

$$(2.29)\qquad \dot{p}_j = \frac{\overline{p}_j - p_j}{\tau_{ij}},$$

where the non-negative parameter τ_{ij} has the dimension of time ("delay time") and characterises the speed of the transformation. In the simplest case, $\overline{p}_j$ and τ_{ij} are only regarded as temperature dependent. Obviously, the phenomenological model defined by (2.22) includes the ansatz in (2.29) for the parameter choice $r_{ij} := 0$, $s_{ij} := 1$ and $g_{ij} := \tau_{ij}^{-1}$, $h_{ij} = 0$. Clearly, $p_j(t)$ tends to $\overline{p}_j$ for $t \to \infty$ for constant temperature. For convenience, we introduce the reciprocal value

$$(2.30)\qquad \mu_{ij} := \tau_{ij}^{-1}.$$

We define

$$(2.31)\qquad a_{ij} := \mu_{ij}(\overline{p}_j - p_j), \qquad \mu_{ii} := 0 \qquad i, j = 1, \ldots, m.$$

Assuming independence like in (2.10), and regarding (2.28) as a side condition, the ansatz (2.31) leads to the subsequent system for the multi-phase system

$$(2.32)\quad \dot{p}_i = -H(p_i - \overline{p}_i) \sum_{j=1}^{m} \mu_{ij} \max\{\overline{p}_j - p_j, 0\}\, G_{ij} + \max\{\overline{p}_i - p_i, 0\} \sum_{j=1}^{m} \mu_{ji} H(p_j - \overline{p}_j)\quad G_{ij}$$

$$i = 1, \ldots, m.$$

Additionally, if the μ_{ij} are independent of the phase fractions, the system (2.32) is "nearly" linear.

Remarks 2.6 (i) Alternatively to (2.31), Leblond and Devaux [Leb84, 85] propose

$$(2.33) \qquad a_{ij} := \mu_{ij}\,(\overline{p}_j\, p_i - \overline{p}_i\, p_j), \qquad \mu_{ii} := 0 \qquad i, j = 1, \ldots, m.$$

Using (2.1) and (2.31), *in case of only two phases*, the equation (2.29) can be rewritten as

$$(2.34) \qquad \dot{p}_1 = -\,\mu_{12}\,(\overline{p}_2\, p_1 - \overline{p}_1\, p_2).$$

Generalising this ansatz in [Leb84, 85], the subsequent system for the multi-phase case reads as

$$(2.35) \quad \dot{p}_i = -\,H(p_i - \overline{p}_i) \sum_{j=1}^{m} \mu_{ij}\,(\overline{p}_j\, p_i - \overline{p}_i\, p_j)\, H(\overline{p}_j - p_j) + $$

$$+\, H(\overline{p}_i - p_i) \sum_{j=1}^{m} \mu_{ji}\,(\overline{p}_i\, p_j - \overline{p}_j\, p_i)\, H(p_j - \overline{p}_j) \qquad i = 1, \ldots, m.$$

Clearly, if $p_i > \overline{p}_i$ and $p_j < \overline{p}_j$, then the a_{ij} in (2.33) are non-negative. We note, that in the case of simultaneous PT the model (2.34) does not recover a single transformation like (2.29).

(iv) Generally, the parameters μ_{ij} in (2.30) as well as the equilibrium values $\overline{p}_i$ may depend on the same variables as a_{ij} in (2.10). Furthermore, it is possible to consider the system (2.32) or (2.35) in the more general case (2.11) (cf. remark 2.5).

2.4 A multi-phase model based on the Johnson-Mehl-Avrami-Kolmogorov kinetics

Now we want to show how to specialise the general model in (2.17) to the JMAK kinetics for diffusive PT (cf. the pioneering works [Avr39, 40, 41], [Joh39] as well as [Böh03], [Bur65], [Chr75], [Lem01], [Rét97] e.g.). As in section 2.3 we begin with the case of a single transformation, for instance with the transformation of austenite into ferrite for a hypoeutectoid low alloyed steel at a temperature where both phases may exist in equilibrium.

At constant temperature θ the forming phase 2 of this transformation 1 → 2 grows according to the JMAK formula

$$(2.36) \qquad p_2(t) = \overline{p}_{12}\,\Big(1 - \exp\Big(-\Big(\frac{t}{\tau_{12}(\theta)}\Big)^{n_{12}(\theta)}\Big)\Big)$$

where $\tau_{12} > 0$ and $n_{12} > 1$ are temperature-dependent material parameters characterising the PT 1 → 2. Usually, in the JMAK approach, the value $\overline{p}_{12}$ stands for the equilibrium value (as in the LD approach) and will be denoted by $\overline{p}_2$. To be in accordance with our more general approach, we regard this value as “limit value” (cf. (2.13) and remark 2.2 (i)). Clearly, (2.36) implies for the initial time

$$(2.37) \qquad p_2(0) = 0.$$

Taking the time derivative (for constant θ) and excluding the exponential and the explicit time dependence, we obtain from (2.36) the autonomous ODE for the PT 1 → 2

$$(2.38) \qquad \dot{p}_2(t) = (\overline{p}_{12} - p_2(t))\,\frac{n_{12}}{\tau_{12}}\,\big(-\ln(1 - p_2(t)\,\overline{p}_{12}^{\,-1})\big)^{1 - \frac{1}{n_{12}(\theta)}}\,.$$

Therefore, assuming the JMAK kinetics for all possible PT i → j and for varying temperature, we define

$$(2.39)\qquad a_{ij} := (\overline{p}_{ij} - p_j(t))\,\frac{n_{ij}}{\tau_{ij}}\,(-\ln(1 - p_j(t)\,\overline{p}_{ij}^{\,-1})\,)^{1 - \frac{1}{n_{ij}(\theta)}} \qquad \text{for } i, j = 1, \ldots, m,\ i \neq j.$$

$$a_{ii} := 0 \qquad \text{for } i = 1, \ldots, m.$$

This and (2.17) imply

$$(2.40)\quad \dot{p}_i = -\,H(p_i) \sum_{j=1,\, a_{ij} \neq 0}^{m} \max\{\,\overline{p}_{ij} - p_j(t), 0\}\,\frac{n_{ij}}{\tau_{ij}}\,(-\ln(1 - p_j(t)\,\overline{p}_{12}^{\,-1}\,)^{1 - \frac{1}{n_{ij}(\theta)}}\,G_{ij}\, +$$

$$+ \sum_{j=1,\, a_{ij} \neq 0}^{m} H(p_j) \max\{\,\overline{p}_{ji} - p_i(t), 0\}\,\frac{n_{ji}}{\tau_{ji}}\,(-\ln(1 - p_i(t)\,\overline{p}_{12}^{\,-1}\,)^{1 - \frac{1}{n_{ji}(\theta)}} \qquad \text{for } i = 1, \ldots, m.$$

We conclude this point with some remarks again.

Remarks 2.7 (i) The JMAK model (2.39) is *not* a special case of the general ansatz (2.22). A linearisation of the logarithm in (2.39) yields the following approximation for small values of p_2

$$(2.41)\qquad \dot{p}_2(t) = (\overline{p}_{12} - p_2(t))\,\frac{n_{12}}{\tau_{12}}\,(\,p_2(t)\,\overline{p}_{12}^{\,-1}\,)^{1 - \frac{1}{n_{12}(\theta)}}.$$

Obviously, (2.41) *is a special case* of (2.22).

(ii) The solution of the problem (2.36), (2.37) is *not* unique. Besides the obvious solution $p_2 = 0$, there exist non-zero solutions. An example is p given by (2.35) in the case of constant temperature. This is an un-pleasant *mathematical* disadvantage of the JMAK model. Therefore, for calculations one usually takes a small value for $p_2(0)$, 10^{-5}, e.g., instead of zero. Another way out consists in using the more general ansatz in (2.22) with a small positive parameter e_{ij}.

(iii) Experiments show that for non-isothermal diffusive transformations the model (2.38) (as well as (2.40)) does *not* approximate the reality sufficiently well (cf. [Böh04], [Fer85], [Hun99], [Hou86], [Rét97] e.g.). Therefore, there are several proposals in order to extend the ODE (2.38), or to use other approaches (cf. [Ber99], [Böh03, 04], [Cah56], [Dac03], [Den92], [Höm97], [Ino85, 89], [Leb84, 85], [Lem01], [Mit92, 02], [Rét97, 99a, 04], [Sys03], [Ver87] e.g.). This *physical* disadvantage of the JMAK kinetics was the reason for introducing our general model based on (2.17), (2.22). For constant transformation temperature the JMAK model (2.38) describes the diffusive PT more correctly than the linear equation (2.29) proposed in [Leb84, 85]. We will return to this in section 5, when dealing with simulations. Contrary to this, under non-isothermal conditions the LD model (2.29) (and therefore (2.32), (2.35)) has a simpler structure.

(iv) Clearly, the LD model (2.29) comes from the JMAK model (2.39) for $n_{ij} = 1$. Only in this case the parameters τ_{ij} in (2.29) and (2.39) are the same.

2.5 The martensitic transformation

For the multi-phase models presented in 2.2, 2.3 and 2.4 each PT $i \to j$ has the same structure as its inverse $j \to i$. There are only differences in the values of material parameters. However, one can include arbitrary PT laws into the general concept presented above. We demonstrate this with the martensitic transformation.

It is well known, that the formation of martensite does not follow the JMAK kinetics. Due to Koistinen and Marburger (cf [Koi59], [Lem01]) the martensite fraction forming from a given austenite fraction $p_1(t_{ms})$ at the temperature θ less than the martensite-start temperature θ_{ms} reads as

$$(2.42)\qquad \overline{p}_{1m}(\theta) = p_1(t_{ms})\,(1 - \exp(-\,\frac{\theta_{ms} - \theta}{\theta_{m0}}\,)),$$

where t_{ms} is the time when the martensite-start temperature θ_{ms} is reached, and θ_{m0} is a positive material parameter (depending on the steel sort and on stress (cf. [Ahr03], [Den97], [Shi04], [Wol06f] e.g.), and usually being independent of temperature). In the sequel we indicate the martensite by the number m and the austenite by 1. Of course, if the martensitic transformation starts with pure austenite, we have $p_1(t_{ms}) = 1$. The formula (2.42) does not contain any information about the martensite evolution. It is known by experiments that the formation of martensite is very fast (with the speed of sound). This fact suggests the following approach: Assuming a monotone decreasing temperature $\theta = \theta(t)$ (below θ_{ms}), we regard the current martensite fraction as the final fraction at $\theta(t)$, i.e.,

$$(2.43) \qquad p_m(t) := \bar{p}_{1m}(\theta(t)).$$

In this case equation (2.42) also describes the martensite evolution, i.e. we have

$$(2.44) \qquad p_m(t) = p_1(t_{ms})\,(1 - \exp(-\frac{\theta_{ms} - \theta(t)}{\theta_{m0}})),$$

where the corresponding initial conditions are

$$(2.45) \qquad p_m(t_{ms}) = 0, \qquad \theta(t_{ms}) = \theta_{ms}.$$

Taking the time derivative and excluding the exponential, we obtain from (2.42)

$$(2.46) \qquad \dot{p}_m(t) = (p_1(t_{ms}) - p_m(t))\,\frac{-\dot{\theta}\,(t)}{\theta_{m0}}\,.$$

Furthermore, experiments show that martensite can only form if the temperature decreases, and if the current temperature is not higher than the minimum temperature during the cooling (cf. [Ant04] e.g.). To be more precise, we have instead of (2.46) the extended version (cf. [Böh03], [Wol07a])

$$(2.47) \qquad \dot{p}_m(t) = (p_1(t_{ms}) - p_m(t))\,\frac{-1}{\theta_{m0}}\,\frac{d}{dt}(\min_{0 \le s \le t}\{\theta(s)\})\,H(\theta_{ms} - \theta(t)).$$

The minimum function in (2.47) can be regarded as an internal variable, when dealing with the bulk behaviour of steel (cf. [Wol05b, 06a, 06h], e.g.). Of course, (2.46) is numerically more convenient than (2.47). In the case of (rapid) quenching one can assume that θ falls approximately monotonously. Thus, (2.46) seems to be applicable in special situations (cf. [Wol07a] for experiments and evaluations). Strictly spoken, t_{ms} is the last time when the martensite-start temperature was reached. Below the martensite-start temperature, practically no other phases form. Hence, we can write

$$(2.48) \qquad p_1(t_{ms}) - p_m(t) = 1 - \sum_{j=2}^{m-1} p_j(t) - p_m(t),$$

and we obtain the equation

$$(2.49) \qquad \dot{p}_m(t) = (1 - \sum_{j=2}^{m-1} p_j(t) - p_m(t))\,\frac{-1}{\theta_{m0}}\,\frac{d}{dt}(\min_{0 \le s \le t}\{\theta(s)\})\,H(\theta_{ms} - \theta(t)).$$

Thus, the “limit value” of martensite can be defined as (cf. (2.13) and remark 2.2 (i)) by

$$(2.50) \qquad \bar{p}_{1m}(t) := 1 - \sum_{j=2}^{m-1} p_j(t).$$

Moreover, we can define the rate a_{1m} for the martensite formation

$$(2.51) \qquad a_{1m} = (1 - \sum_{j=2}^{m-1} p_j(t) - p_m(t))\,\frac{-1}{\theta_{m0}}\,\frac{d}{dt}(\min_{0 \le s \le t}\{\theta(s)\}),$$

where the switch-off function $H(\theta_{ms} - \theta(t))$ is included in G_{1m} (cf. (2.17)). As above (cf. (2.46), (2.47)), in the case of (rapid) quenching, the time derivative in (2.51) can be approximately replaced by $\dot{\theta}(t)$.

Finally, we note that Leblond and Devaux [Leb84, 85] suggested applying the linear approach in (2.29) to the martensitic transformation, too. In this case, one has

$$(2.52) \qquad a_{1m} = (\overline{p}_{1m} - p_m(t))\, \mu_{1m},$$

with

$$(2.53) \qquad \overline{p}_{1m}(t) = \Big(1 - \sum_{j=2}^{m-1} p_j(t)\Big)\Big(1 - \exp\Big(-\frac{\theta_{ms} - \theta(t)}{\theta_{m0}}\Big)\Big)$$

in accordance with (2.42). The parameter can be fitted by dilatometer data (cf. [Wol07a]). We refer to [Böh03], [Wil86], [Yu77] for modifications of the KM approach.

2.6 Special cases of PT

In general, the multi-phase models presented above allow arbitrary transformations. But for steel most of the formally possible phase transformations do not materialise. Moreover, in many practical situations like quenching, one is faced with transformations in only one direction. Thus, one often has to deal with simpler cases than described above.

2.6.1 Dissolution of austenite

During quenching processes austenite normally undergoes only a (complete or incomplete) dissolution, while the ferritic phases can only grow. That means, that the temperature path and other influences *only* allow austenite to decrease and the ferritic phases to increase. Let us assume that we have m relevant phases. For instance, for an hypoeutectoid steel we have austenite (labelled in all cases by the index 1), ferrite, pearlite, bainite and martensite (labelled by m). For an hypereutectoid steel one has austenite, cementite, pearlite, bainite, martensite, sometimes upper and lower bainite. As assumed, austenite can only dissolute, the remaining phases can only form. In section 5, we consider concrete examples. Thus, specialising (2.17), we have

$$(2.54) \qquad \dot{p}_1 = -H(p_1) \sum_{j=2}^{m} a_{1j}\, H(\overline{p}_{1j} - p_j)\, G_{1j},$$

$$(2.55) \qquad \dot{p}_k = a_{1k}\, H(p_1)\, H(\overline{p}_{1k} - p_k)\, G_{1k} \qquad \text{for } k = 2, \ldots, m.$$

The limit values $\overline{p}_{1k}$ must be determined for the steel sort under consideration, using information from the Fe-Fe$_3$C diagram and/or from the transformation diagrams. In section 5.2 we will go into details. Besides this, in [Rét01] e.g. this procedure is done for concrete steels. The limit value $\overline{p}_{1m}$ for martensite may be chosen differently, depending on the model used. In the case of the Leblond-Devaux approach (2.52), we have (cf. (2.53))

$$(2.56) \qquad \overline{p}_{1m}(t) = \Big(1 - \sum_{j=2}^{m-1} p_j(t)\Big)\Big(1 - \exp\Big(-\frac{\theta_{ms} - \theta(t)}{\theta_{m0}}\Big)\Big).$$

But for the Koistinen-Marburger approach (2.51) one has

$$(2.57) \qquad \overline{p}_{1m}(t) = 1 - \sum_{j=2}^{m} p_j(t).$$

The switch-off functions G_{ij} have to be determined by special considerations, too (cf. [Wol06g] for an example).

Remark 2.8. Clearly, due to (2.5), the equations (2.54), (2.55) are dependent. For practical use, one normally only works with the equations in (2.55).

The transformation rates a_{1k} (k = 2, …, m) in (2.54), (2.55) have to be determined by dilatometer data or by transformation diagrams, using alternatively the general ansatz (2.22) or the special ones by JMAK (2.39), by LD (2.31), and by KM (2.46), respectively. In our situation, the initial conditions are

$$p_{10} = 1, \qquad p_{k0} = 0 \qquad \text{for } k = 2, \ldots, m. \tag{2.58}$$

Thus, the phase fractions are determined for a given temperature path (see section 4). Generally, we have a coupled problem with temperature, mechanics and, possibly carbon diffusion (see section 3).

Remark 2.9. Another model describing the dissolution of austenite (into several phases) based on JMAK kinetics was developed in [Rét98, 99b].

2.6.2 Formation of austenite

This case exhibits some differences to the one considered in section 2.6.1. More than one phase are now sources for the austenite. Besides this, the dissolution of the ferritic phases is a complex physical phenomenon. Especially, when taking into account the changes which martensite undergoes (tempering effects). The possible presence of retained austenite has an essential influence of the forthcoming PT. For this matter we refer to [Pet89], [Yan89], e.g. Here, we want to focus more on the phenomenological side of modelling. As before, austenite is labelled by “1”. For the initial condition (2.4), we assume

$$p_{01} < 1, \qquad \sum_{j=1}^{m} p_{0j} = 1, \qquad p_{0j} \geq 0 \qquad \text{for } j = 1, \ldots, m. \tag{2.59}$$

If there is no retained austenite, we will have $p_{01} = 0$. Neglecting tempering effects (cf. [Wan04] for modelling and discussion), we assume that each phase j = 2, …, m completely transforms into austenite. If there are *only* two phases 1 and j, the transformation $j \rightarrow 1$ can be modelled (cf. (2.22) and remark 2.5 (i)) as

$$\dot{p}_1 = (e_{j1} + p_1)^{r_{j1}(\theta)} (1 - p_1)^{s_{j1}(\theta)} g_{j1} h_{j1}(\dot{\theta}). \tag{2.60}$$

The equation (2.60) has the same structure as (2.22) with $\overline{p}_{j1} = 1$. Clearly, we have $p_j = 1 - p_1$. The generalisation to m – 1 ferritic phases consists in replacing $1 - p_1$ by p_j in (2.60). This corresponds to the fact that the austenite production due to the j^th^ phase ends, if p_j becomes zero. Thus, we have for the PT $j \rightarrow 1$

$$\dot{p}_1 = (e_{j1} + p_1)^{r_{j1}(\theta)} p_j^{s_{j1}(\theta)} g_{j1} h_{j1}(\dot{\theta}) \qquad \text{for } j = 2, \ldots, m. \tag{2.61}$$

Summing up the equations in (2.61), and introducing suitable switch-off functions, we obtain for the *whole* austenite

$$\dot{p}_1 = \sum_{j=2}^{m} (e_{j1} + p_1)^{r_{j1}(\theta)} p_j^{s_{j1}(\theta)} g_{j1} h_{j1}(\dot{\theta}) G_{j1} \tag{2.62}$$

as well as for the ferritic phases

$$\dot{p}_j = -(e_{j1} + p_1)^{r_{j1}(\theta)} p_j^{s_{j1}(\theta)} g_{j1}(\theta) h_{j1}(\dot{\theta}) G_{j1} \qquad \text{for } j = 2, \ldots, m. \tag{2.63}$$

Clearly, we assume that the temperature path does *not* allow a dissolution of austenite.

Remarks 2.10. (i) Due to (2.61), a later dissolution of a ferritic phase is influenced by the dissolution of a former one. For instance, let us assume, that the process starts without retained austenite. Then the first PT j → 1 starts slowly (because, generally, e_{j1} is quite small). After that, the next PT starts with the already formed austenite, i.e. that PT has no "incubation" (cf. remark (iii), too). Of course, here is not the place to discuss the physical background. Nevertheless, the system (2.62), (2.63) has its advantages: Its structure is simple, it does not depend on the initial values p_{0j}.

(ii) When using JMAK kinetics, the initial value p_{01} must be positive (cf. remark 2.7 (ii)).

(iii) The model in (2.61), (2.62) starts with the formation of austenite from each ferritic phase (cf. [Mio04], e.g.). Another approach can be found in [Sur04]. There the authors start with the JMAK kinetics applied to the decomposition of the ferritic phases, i.e. they assume for isothermal decomposition

$$(2.64) \qquad p_j(t) = p_{0j} \exp(-(\frac{t}{\tau_j(\theta)})^{n_j(\theta)}).$$

Taking the time derivative (for constant θ), one obtains the subsequent JMAK like differential equations

$$(2.65) \qquad \dot{p}_j = -p_j \frac{n_j}{\tau_j} (-\ln(p_j\, p_{0j}^{-1}))^{1-\frac{1}{n_j}}. \qquad \text{in case of } p_{0j} > 0,$$

which will be applied to non-isothermal transformation, too. At the beginning, i.e. for $p_{0j} - p_j$ small, one can linearise the logarithm, obtaining an approximation of (2.65)

$$(2.66) \qquad \dot{p}_j = -p_j \frac{n_j}{\tau_j} (p_{0j}^{-1})^{1-\frac{1}{n_j}} (p_{0j} - p_j)^{1-\frac{1}{n_j}}.$$

The term $p_{0j} - p_j$ stands for the austenite (newly) formed from p_j, whereas, in (2.61), p_1 stands for the *whole current* austenite. That means, (2.66) takes incubation into account (cf. remark (i)). Nevertheless, if $e_{j1} = 0$, (2.66) and (2.61) have the same structure. But, for $n_j > 1$, (2.66) depends on the initial values.

2.6.3 The general case of PT

Of course, the general case of PT can be dealt with by combining the approaches in the sections 2.6.1 and 2.6.2. Thus, one gets ("1" stands for austenite again)

$$(2.67) \quad \dot{p}_1 = \sum_{j=2}^{m} (e_{j1} + p_1)^{r_{j1}(\theta)} p_j^{s_{j1}(\theta)} g_{j1} h_{j1}(\dot{\theta}) G_{j1} - H(p_1) \sum_{j=2}^{m} a_{1j} H(\overline{p}_{1j} - p_j) G_{1j},$$

$$(2.68) \quad \dot{p}_j = a_{1k} H(p_1) H(\overline{p}_{1k} - p_k) G_{1k} - (e_{j1} + p_1)^{r_{j1}(\theta)} p_j^{s_{j1}(\theta)} g_{j1}(\theta) h_{j1}(\dot{\theta}) G_{j1} \quad \text{for } j = 2, \ldots, m.$$

Clearly, we have to add the initial conditions (2.4) fulfilling (2.1) and (2.2). The system (2.67), (2.68) has the same property as described in remark 2.10 (i). The presence of "retained fractions" at the beginning of a PT influences substantially the subsequent forming. A model which excludes such effects requires internal variables in order to take an "incubation" for diffusive transformations into account.

3 Some remarks on interaction of phase evolution, mechanical movement and temperature

Up to this time we have investigated phase transformations assuming given paths of temperature and of stress, and possibly of other quantities. Of course, in reality, we have an interaction of mechanical movement, temperature, phase evolution, and possibly of other quantities. In this context, there are two specific issues related with PT:

- Transformation-induced plasticity (TRIP). This macroscopic phenomenon leads to a permanent deformation, if PT occur under non-vanishing deviatoric stress. We refer to [Ahr03], [Ant04], [Bes93], [Cor02, 04], [Dal04, 06a, 06b], [Dav94], [Den97], [Fis96, 00], [In096], [Leb86a, 86b, 89a, 89b], [Lem01], [Nag00, 01, 02], [Sjö94], [Pet04], [Tal03, 06], [Wol03b, 05a, 06b, 06c, 06d, 06e, 07a] and the literature cited therein.
- Stress-dependent PT. An applied stress (as well as a possible pre-deformation of the parent phase) essentially influences the kinetics of PT. For this matter we refer to [Ahr00, 02, 03], [Ant04], [Dal04], [Den97], [Shi04], [Wol03b, 05a, 06b, 06d, 06e].

Thus, the modelling and simulation of the bulk behaviour of steel must take these phenomena into account. The following references are examples: [Ald06], [Bes93], [Ber99], [Dav94], [Den97, 02], [Fuh99], [Höm96, 02, 04, 06a, 06b], [Ino85, 89], [Kim05], [Pie00], [Ron00], [Sch06], [Sjö84], [Suh05], [Vid94], [Wol04, 05b, 06a, 06g], [Yu77]. As we want to focus on PT, we only show how their laws may be modified in this more general situation, giving a very short outline.

In case of small deformations, we have the well-known balance equations for linear momentum and energy (tacitly assuming Fourier's law of heat conduction)

$$(3.1)\qquad \rho_0 \frac{\partial^2 u}{\partial t^2} - \operatorname{div} S = f,$$

$$(3.2)\qquad \rho_0 \frac{\partial e}{\partial t} - \operatorname{div}(\lambda_\theta \nabla\theta) = S : \frac{\partial \varepsilon}{\partial t} + r.$$

These equations (as well as the subsequent ones) have to be satisfied in the space-time domain $\Omega\times]0, T[$, where Ω is the body under consideration, and $T > 0$ is a fixed time. The notations are standard ones: ρ_0 - bulk density in the reference configuration, that means for $t = 0$, u – displacement vector, S – (symmetric) Cauchy stress tensor, f – volume density of external forces, ε – linearised Green strain tensor, θ - absolute temperature, e – mass density of internal energy, λ_θ – heat conductivity, r – volume density of heat supply. Besides this, we have the well-known defining relation for ε:

$$(3.3)\qquad \varepsilon = \varepsilon(u) := \frac{1}{2}(\nabla u + \nabla u^T) \qquad\qquad (\nabla u^T \text{ – the transposed of } \nabla u).$$

In (3.2) we employ the following abbreviation for the scalar product of tensors:

$$(3.4)\qquad \alpha : \beta := (\alpha \mid \beta) := \operatorname{tr}(\alpha\, \beta^T) = \sum_{i,\, j = 1}^{3} \alpha_{ij}\, \beta_{ij},$$

with tr(α) – trace of α, i.e. the sum of diagonal elements.

In the framework of small deformations we decompose ε additively in accordance with

$$(3.5)\qquad \varepsilon = \varepsilon_{te} + \varepsilon_{trip} + \varepsilon_{cp},$$

where ε_{te} is the thermoelastic strain (including isotropic strain due to phase transformations), ε_{trip} is the (non-isotropic) strain due to transformation-induced plasticity (TRIP) (cf. further on), and ε_{cp} is the strain due to classical plasticity (CP) (i.e. usual plasticity in metal behaviour). Viscous effects can be taken into account, too. As usual, we assume volume conservation for the TRIP- and classical inelastic deformation, i.e.

$$(3.6)\qquad \operatorname{tr}(\varepsilon_{cp}) = 0, \qquad\qquad \operatorname{tr}(\varepsilon_{trip}) = 0.$$

The stress tensor S and the thermoelastic part ε_{te} of the strain tensor are connected by the law of thermoelasticity taking density changes due to phase transformations into account

$$(3.7)\qquad S = 2\,\mu\, \varepsilon_{te}^* + K \operatorname{tr}(\varepsilon_{te})\, I - 3K_\alpha\, (\theta - \theta_0)\, I - K \sum_{i=1}^{m} \Big(\frac{\rho_0}{\rho_i(\theta_0)} - 1\Big)\, p_i\, I,$$

where μ (shear modulus), K (compression modulus) and K_α can be defined via linear mixture rules:

$$(3.8) \quad \mu(\theta, p) := \sum_{i=1}^{m} \mu_i(\theta)\, p_i, \quad K(\theta, p) := \sum_{i=1}^{m} K_i(\theta)\, p_i, \qquad K_\alpha(\theta, p) := \sum_{i=1}^{m} K_i(\theta)\, \alpha_i(\theta)\, p_i,$$

where the μ_i, K_i and α_i are shear modulus, compression modulus and heat-dilatation coefficient of the ith phase, respectively. Moreover, I is the unity tensor, $\rho_i(\theta_0)$ is the density of the ith phase at initial temperature θ_0, i.e. for t = 0. As usual, the deviator ε_{te}^* of the tensor ε_{te} is defined by

$$(3.9) \qquad \varepsilon_{te}^* := \varepsilon_{te} - \frac{1}{3}\, \mathrm{tr}(\varepsilon_{te})\, I \qquad \text{(in 3d case).}$$

The (classical) inelastic part ε_{cp} of the deformation tensor ε is connected by a special material law with the remaining quantities, for instance by a flow rule in plasticity (see [Leb86a, 86b], [Vid94], [Wol05b, 06a, 06g], e.g., for details in this context). We drop this here. But, we will give some explanation of transformation-induced plasticity (TRIP). If PT occur under non-vanishing deviatoric stress, there will be a permanent non-isotropic deformation (TRIP) which cannot be described by CP at the macroscopic level. Usually one assumes that TRIP has *no yield condition* (cf. [Leb86a, 86b], [Fis96] for discussions, [Azz01], [Ino06] for possible alternative approaches). As in [Wol05b, 06a, 06b, 06g], we propose

$$(3.10) \qquad \dot{\varepsilon}_{trip} = \frac{3}{2}\, (S^* - X_{trip}^*) \sum_{i=1}^{m} \kappa_i(\theta, S, \xi)\, \frac{\partial \phi_i}{\partial p_i}(p_i)\, \max\{\, \dot{p}_i, 0\},$$

where κ_i is the Greenwood-Johnson parameter (generally depending on temperature, stress, and possibly other quantities), and ϕ_i is the saturation function of the ith phase, respectively, fulfilling for all i = 1, …, m

$$(3.11) \qquad \kappa_i \geq 0, \qquad \phi_i(0) = 0, \qquad \phi_i(1) = 1, \qquad \frac{\partial \phi_i}{\partial p}(p) \geq 0 \qquad \text{for all } 0 < p < 1.$$

X_{trip} is a backstress associated with TRIP (cf. [Azz01], [Fis00], [Leb89b], [Nag00, 01, 02], [Tan03], [Wol05b, 06a, 06b, 06g] for discussion). Clearly, from (3.5) – (3.7) we get

$$(3.12) \qquad S^* = 2\,\mu\, \varepsilon_{te}^* = 2\,\mu\, (\varepsilon^*(u) - \varepsilon_{trip} - \varepsilon_{cp}), \qquad \mathrm{tr}(S) = 2\,\mu\, \mathrm{tr}(\varepsilon(u)) = 2\,\mu\, \mathrm{div}(u).$$

We only want to demonstrate how the PT laws (2.3) may be specialised in case of modelling interactions of PT and mechanics. Therefore, we assume that there is *no* classical inelastic deformation ε_{cp}, and that there is *no* backstress X_{trip}. Otherwise, the explanations would be more complicated (cf. [Wol06b, 06g]). Moreover, letting $\kappa_i = \kappa_i(\theta)$, we obtain from (3.10), (3.11)

$$(3.13) \qquad \dot{\varepsilon}_{trip}(t) = 3\,\mu\, (\varepsilon^*(u) - \varepsilon_{trip}(t)) \sum_{i=1}^{m} \kappa_i(\theta)\, \frac{\partial \phi_i}{\partial p_i}(p_i)\, \max\{\, \dot{p}_i(t), 0\},$$

suppressing the dependence on the spatial variable $x \in \Omega$. Assuming the initial value $\varepsilon_{trip}(0) = 0$, and using the abbreviation

$$(3.14) \qquad a(\theta(t), \dot{p}(t)) := 3\,\mu \sum_{i=1}^{m} \kappa_i(\theta)\, \frac{\partial \phi_i}{\partial p_i}(p_i(t))\, \max\{\, \dot{p}_i(t), 0\},$$

we obtain the subsequent relation for ε_{trip}:

$$(3.15) \qquad \varepsilon_{trip}(t) = \int_0^t a(\theta(s), \dot{p}(s))\, \varepsilon^*(u(s))\, \exp\Big(-\int_s^t a(\theta(\tau), \dot{p}(\tau))\, d\tau\Big)\, ds.$$

Finally, (3.12) and (3.15) lead to

$$(3.16) \qquad S^*(t) = 2\,\mu\, \Big(\varepsilon^*(u(t)) - \int_0^t a(\theta(s), \dot{p}(s))\, \varepsilon^*(u(s))\, \exp\Big(-\int_s^t a(\theta(\tau), \dot{p}(\tau))\, d\tau\Big)\, ds\Big).$$

We write (2.3) in the subsequent form (cf. remark 2.1 (ii))

$$(3.17) \qquad \dot{p}_i(t) = f_i(p(t), \theta(t), \theta'(t), \sigma(S), tr(S), \xi)$$

where $\sigma(S)$ is the von Mises equivalent stress

$$(3.18) \qquad \sigma(S) := \left(\frac{3}{2} S^* : S^*\right)^{\frac{1}{2}}.$$

Sometimes, when performing mathematical investigations and simulations, the stress tensor S will be eliminated via (3.12) and (3.16). Hence, if TRIP and stress dependence of PT are taken into account, from (3.17), one obtains implicit integro-differential equations of the subsequent structure

$$(3.19) \quad \dot{p}_i(t) = F_i(p(t), \theta(t), \dot{\theta}(t), 2\mu\, div(u(t)), \int_0^t a(\theta(s), \dot{p}(s))\, \varepsilon^*(u(s)) \exp\left(-\int_s^t a(\theta(\tau),\dot{p}(\tau))\, d\tau\right) ds, \xi).$$

Clearly, the structure of (3.19) will be transmitted to the functions a_{ij} in the specialisation (2.10), and, finally, to the coefficients of the model presented in (2.22).

As mentioned above, a (inelastic) pre-deformation of the parent phase generally influences the subsequent PT (as well as the subsequent TRIP behaviour) (cf. [Ahr03], [Pet04], [Tal06]). This phenomenon (“strain-dependent PT”) can be modeled by internal variables. We introduce the (classical) plastic strain of the parent phase (austenite, e.g.) and its corresponding accumulated strain by

$$(3.20) \qquad \varepsilon_{cp}^{(1)}(t) := \int_0^t \dot{\varepsilon}_{cp}(\tau)\, p_1(\tau)\, d\tau, \qquad s_{cp}^{(1)}(t) := \int_0^t \left(\frac{2}{3}\, \dot{\varepsilon}_{cp}(\tau) : \dot{\varepsilon}_{cp}(\tau)\right)^{\frac{1}{2}} p_1(\tau)\, d\tau,$$

where the index 1 stands for the parent phase. Clearly, if only the parent phase is present during pre-deformation, we have the ε_{cp} and the usual accumulated plastic strain s_{cp}. Thus, in the case of pre-deformation, the variable ξ in (2.3) (and (3.17) and (3.19)) reads as

$$(3.21) \qquad \xi = (\varepsilon_{cp}^{(1)}, s_{cp}^{(1)}).$$

4 Some remarks concerning mathematical questions

Here is not the place for mathematical investigations in detail. And so we only want to give some remarks concerning mathematical aspects of PT. In practice, one expects that for a given path of temperature (and possibly of stress and other variables) there exists a unique solution of the initial-value problem (2.3), (2.4) for all time fulfilling (2.1), (2.2). The same concerns to the more general initial-value problem (3.19), (2.4). The mathematical kernel of this question is, under which assumptions about the right-hand side f (or a_{ij}) and about the initial value one can prove the existence of a global unique solution of the problem (2.3), (2.4) fulfilling (2.1), (2.2).

Let us consider the general initial problem (2.17), (2.4). We remember it:

$$(4.1) \quad \dot{p}_i = -\sum_{j=1}^{m} a_{ij}\, H(p_i)\, H(\bar{p}_{ij} - p_j)\, G_{ij} + \sum_{j=1}^{m} a_{ji}\, H(p_j)\, H(\bar{p}_{ji} - p_i)\, G_{ji} \qquad i = 1, \dots, m,$$

$$(4.2) \quad p_i(0) = p_{0i} \qquad i = 1, \dots, m.$$

An essential problem is that the spatial variable x (stands for a body point) occurs as a parameter in (4.1), (4.2). Thus, it is helpful to formulate this problem as an equivalent operator equation in a suitable function space (cf. [Höm97], [Hüß07], [Ver87], [Vis87] e.g.). At first, one can prove the existence of a unique local (in time) solution. After having proven that this solution fulfils (2.1), (2.2), one gets its boundedness, and can apply continuation arguments (cf. [Hüß07] e.g.). The main mathematical assumptions consist in:

- The initial value p_0 fulfils (2.2).
- The functions a_{ij} have suitable continuity, measurability and growth properties. Besides this, they are locally Lipschitz continuous with respect to p.
- The Heaviside function H and the switch-off functions G_{ij} must be substituted by suitable continuous regularisations. For instance, instead of H one can use $H_\varepsilon(s) := 0$ for $s \leq 0$, $H_\varepsilon(s) := s/\varepsilon$ for $0 < s < \varepsilon$, $H_\varepsilon(s) := 1$ for $s \geq \varepsilon$.
- The functions a_{ij} and (the regularisations of) G_{ij} must be non-negative.

We refer to [Höm97], [Hüß07] for detailed explanations and mathematical results. Mathematical results taking phase transformations and mechanical behaviour (in steel) into account can be found in [Höm04, 06b], [Boe07].

Finally, the subsequent additional assumptions (besides (2.23)) for the parameters of the proposal (2.22) follow from the theory of ODE (existence of global solutions):

(4.3) $s_{ij} \geq 1$ for all arguments.

In order to ensure a unique solution for all possible initial values p_{0i}, it is convenient to assume

(4.4) $e_{ij} \geq e_{ij0} > 0$ for all arguments.

In case of $e_{ij} = 0$, there must be $0 \leq r_{ij} \leq 1$. Moreover, for the initial value $p_{0j} = 0$, in this case, there is no unique solution (cf. remark 2.7 (ii)).

5 Parameter identification and numerical examples

In this section, we demonstrate how to obtain the needed parameters. This can be done, using experimental data (see section 5.1) or transformation diagrams (see section 5.2). Clearly, the information being in experimental data is more complete than this one extracted from transformation diagrams.

5.1 Parameter identification using experimental data

At first, we deal with stress-free transformation of austenite into pearlite of the bearing steel 100Cr6 (SAE 52100). Neglecting carbide precipitation, we regard this transformation as complete in the temperature region between 550°C and 734°C. At first, one performs some dilatometer experiments for isothermal transformation. From the measured length of the probes one obtains the phase evolution of pearlite, and the parameters of the model chosen can be determined by optimisation. Clearly, in case of the complete transformation austenite into pearlite, the evolution of pearlite p is given by

(5.1) $$\dot{p}(t) = (e(\theta) + p(t))^{r(\theta)} (1 - p(t))^{s(\theta)} g(\theta).$$

At first, θ will be kept constant. Analogously, the models by JMAK and by LD read as

(5.2) $$\dot{p}(t) = (1 - p(t)) \frac{n(\theta)}{\tau(\theta)} (-\ln(1 - p(t)))^{1 - \frac{1}{n(\theta)}}$$

and

(5.3) $$\dot{p}(t) = (1 - p(t))\, \mu(\theta),$$

respectively. The dilatometer data allows to determine the pearlite evolution independently of any PT model assumed. Thus, the parameters e, r, s and g in (5.1), the parameters τ and n in (5.2) as well as the parameter μ in (5.3) can be calculated by optimisation procedures. Using data provided by the Institut für Werkstofftechnik Bremen (IWT), we have obtained the following parameter values for the pearlitic transformation (see table 1, cf. [Wol07c] for details).

θ [°C]	Parameter in (5.1)				Parameter in (5.2)		… in (5.3)
	e	r	s	g	n	τ	μ
550	$0.34 \cdot 10^{-3}$	0.26	1,02	$2.90 \cdot 10^{-2}$	1.25	49.70	$2.094 \cdot 10^{-2}$
600	$17.04 \cdot 10^{-3}$	0.83	1,00	$19.58 \cdot 10^{-2}$	2.22	16.91	$6.231 \cdot 10^{-2}$
650	$1.97 \cdot 10^{-3}$	0.76	1,00	$29.59 \cdot 10^{-2}$	2.49	12.15	$8.425 \cdot 10^{-2}$
700	$1000.00 \cdot 10^{-3}$	3.52	1,00	$0.17 \cdot 10^{-2}$	1.85	218.18	$0.4910 \cdot 10^{-2}$

Table 1: Fitted parameters of the models (5.1), (5.2) and (5.3) for isothermal pearlitic transformations.

Using these values obtained for discrete temperatures, one can construct piece-wise linear parameter functions of the temperature θ. (These functions are regarded as constantly continued up to the ends of the temperature interval [550, 734].) Therefore, one obtains the corresponding models (5.1), (5.2) and (5.3) for non-isothermal transformations (in the given temperature range).

In case of necessity, the parameter $h = h(\dot{\theta})$ in (2.22) can be added in all three differential equations (5.1), (5.2) and (5.3). Hence, we obtain

$$\dot{p}(t) = (e(\theta) + p(t))^{r(\theta)}\,(1 - p(t))^{s(\theta)}\,g(\theta)\,h(\dot{\theta}), \tag{5.4}$$

$$\dot{p}(t) = (1 - p(t))\,\frac{n(\theta)}{\tau(\theta)}\,(-\ln(1 - p(t))\,)^{1 - \frac{1}{n(\theta)}}\,h(\dot{\theta}), \tag{5.5}$$

$$\dot{p}(t) = (1 - p(t))\,\mu(\theta)\,h(\dot{\theta}). \tag{5.6}$$

For determining h (at first for constant cooling rates $\dot{\theta}$), one needs dilatometer data for linear cooling. Using the already determined parameter functions e, r, s, g (or τ, n or μ), the parameter h can be obtained for some values of cooling rates via optimisation. The results are in table 2.

$\dot{\theta}$ [°C/s]	0	-0.17	-0.50	-0.80	-1.00	-1.60	-2.00	-2.67	-4.01	-8.00
$h(\dot{\theta})$ for (5.1)	1.00	0.24	0.50	0.68	0.40	1.00	0.37	0.87	0.75	1.00
$h(\dot{\theta})$ for (5.2)	1.00	0.65	1.69	4.33	2.00	3.29	1.73	3.17	2.50	3.95
$h(\dot{\theta})$ for (5.3)	1.00	0.71	2.02	4.69	2.52	4.15	1.90	3.01	2.48	3.45

Table 2: Parameter h for the models (5.4), (5.5) and (5.6).

Finally, from the discrete values of h, one can obtain a function by interpolation (note $h(0) = 1$). Thus, one has PT models taking the current temperature and its current derivative into account. We present some plots comparing the models in (5.1), (5.2) and (5.3) as well as (5.4), (5.5) and (5.6). In the subsequent figures, the curves are denoted by the abbreviations:

- data – phase fraction calculated by measured data (cf. [Wol07c] for details)
- ODE – phase fraction predicted by our proposal (5.1)
- JMAK-DE – phase fraction predicted by the JMAK model (5.2)
- LD-DE – phase fraction predicted by the LD model (5.3)
- ODE h – phase fraction predicted by our proposal (5.4)
- JMAK-DE h – phase fraction predicted by the JMAK model (5.5)
- LD-DE h – phase fraction predicted by the LD model (5.6)

In accordance with [Wol07c] (cf. table 3), the model (5.4) yields the second best least-square approximation of the curve “data”. Figure 1 (right) shows that, nevertheless, there is a larger point-wise abbreviation before the end of the transformation. Zooming near the beginning (see figure 2), one sees that the model (5.4) gives a better agreement at the beginning of PT.

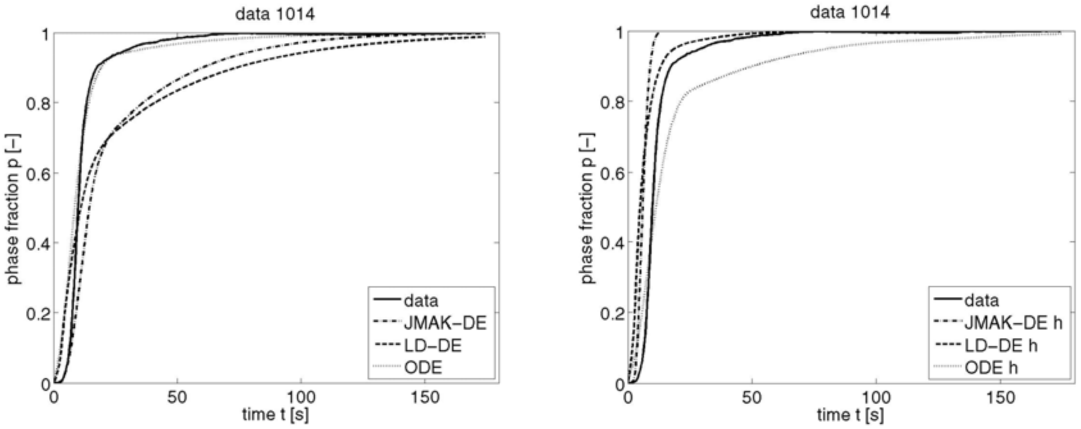

Figure 1: Evolution of pearlite for exponential cooling – calculated by measured data and predicted by the models (5.1) – (5.6)

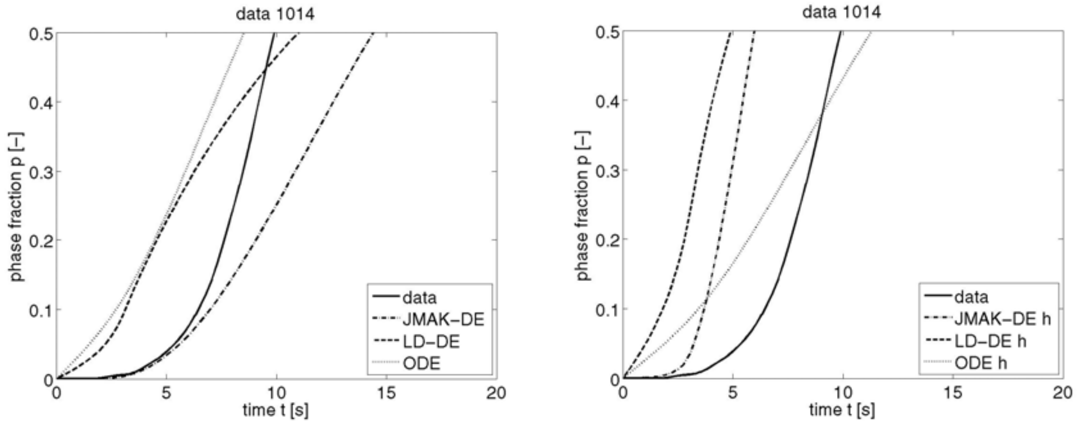

Figure 2: Zoom of the pictures in fig. 1 near the beginning of PT.

Figure 3 shows that the modified models (5.4) – (5.6), in particular (5.4), gives a better approximation.

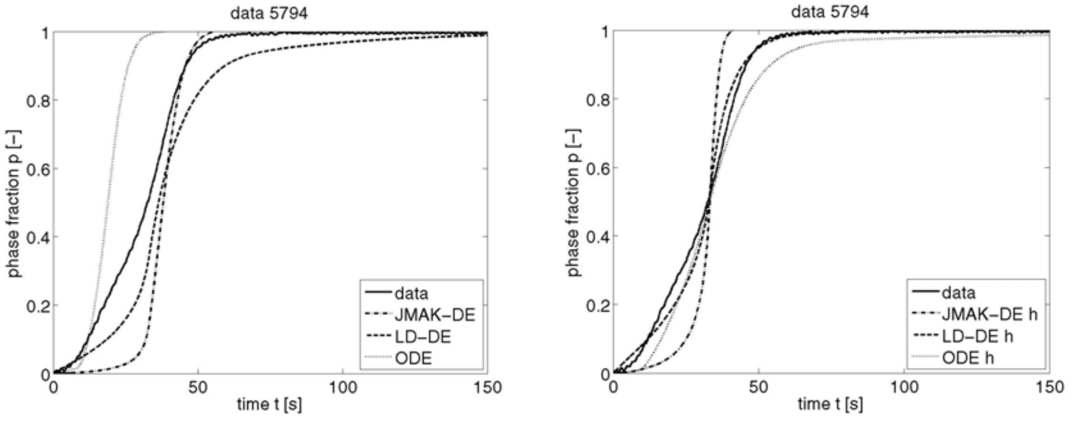

Figure 3: Evolution of pearlite for linear cooling – calculated by measured data and predicted by the models (5.1) – (5.6)

In order to get a qualitative criterion, one can compare the least-square deviations between the curve obtained from the data and the curves predicted by the models ((5.1) – (5.6), e.g.) In [Wol07c] have compared a lot of models for PT. Here we only present the comparison of the six models (5.1) – (5.6) in table 3.

PT model	(5.1)	(5.2)	(5.3)	(5.4)	(5.5)	(5.6)
∅ deviation	$6.53 \cdot 10^{-2}$	$9.46 \cdot 10^{-2}$	$12.08 \cdot 10^{-2}$	$5.53 \cdot 10^{-2}$	$3.82 \cdot 10^{-2}$	$8.72 \cdot 10^{-2}$
ranking	3	5	6	2	1	4

Table 3: Average least-square deviation and ranking for the PT models (5.1) – (5.6) for 25 dilatometer experiments for isothermal transformations (4), linear (9) and exponential (12) cooling path for the pearlitic transformation of the steel 100Cr6 (SAE 52100).

The general results of the comparison are (cf. [Wol07c] for details):

- Among all tested models which *do not contain* the time derivative $\dot{\theta}$, the phenomenological model (5.1) gives the best least-square approximation of the phase evolution.
- Among all tested models, the model (5.4) gives the second best least-square approximation of the phase evolution. For moderate cooling rates, the model (5.4) gives the best least-square approximation of the phase evolution.

For comparison of different PT models we also refer to [Rét97], [Böh04], [Dac03]. As pointed out in section 3, PT generally depend on stress. For determining the stress dependence of the coefficients e, r, s, g in (5.1) as well as of n, τ in (5.2) and μ in (5.3), one needs further experimental data from special devises (Gleeble machine, e.g.) which can perform PT under controlled temperature and stress, measuring length and diameter (cf. [Ahr00, 03], [Dal04, 06a, b], [Nag00, 01, 02], [Wol03b, 05a, 06b] for details). For the same discrete transformation temperature as when having determined the values e, r, s, g, one can perform experiments under different stresses (tension and compression, if possible under torsion, too). As a result, by interpolation again one obtains the parameters as function on stress and stress direction (cf. [Wol06e] for details). Finally, after performing this procedure for different temperatures, one gets the parameters as functions of temperature and stress (and stress direction). After this, the obtained PT model can be tested with data obtained from experiments with different temperature-stress paths. If necessary, in this direction one can proceed, taking $\dot{\theta}$ (and possibly pre-deformation of austenite) into account.

Knowing the transformation parameters, one can simulate the phase evolution in work pieces. Here, we present some calculations for dilatometer probes, assuming spatial homogeneity. Contrary to usual dilatometer experiments with controlled temperature, we calculate it simultaneously together with the phase fractions. For this, we need the transformation parameters of bainitic and martensitic transformation of the steel 100Cr6 (SAE 52100). Analogously as for the pearlitic transformation, we get the parameters for the bainitic transformation, using dilatometer data for constant transformation temperature (see table 4).

θ [°C]	Parameter in (5.1)				Parameter in (5.2)		… in (5.3)
	e	r	s	g	n	τ	μ
300	$1.1 \cdot 10^{-4}$	0.666	1.18	$1.26 \cdot 10^{-2}$	2.02	268.69	0.003921
350	$1.82 \cdot 10^{-3}$	0.741	1.00	$2.33 \cdot 10^{-2}$	2.42	148.46	0.007028
400	$5.52 \cdot 10^{-3}$	0.818	1.00	$6.93 \cdot 10^{-2}$	2.52	54.23	0.019238
450	$9.8 \cdot 10^{-4}$	0.460	1.00	$13.14 \cdot 10^{-2}$	1.59	15.07	0.070788
500	$1.55 \cdot 10^{-3}$	0.363	1.70	$12.43 \cdot 10^{-2}$	1.00	20.59	0.048557

Table 4: Fitted parameters of the models (5.1), (5.2) and (5.3) for isothermal bainitic transformations of the steel 100Cr6 (SAE52100).

The pearlitic and bainitic transformations are alternatively calculated with the aid of the model (5.1) (i.e. (2.22)) as well as with the JMAK and LD kinetics. The martensitic transformation is calculated by the Leblond-Devaux approach in any case. We apply the multi-phase case as in section 2.6.1 (cf. [Boe07] for details). The parameter μ = 5,95 of the martensitic transformation (cf. (2.29), (2.30), (2.52)) as well as the martensite start-temperature θ_{ms} = 260°C and the parameter θ_{m0} = 102°C (cf. (2.42), (2.53)) are taken from [Wol07b]. We consider three cooling scenarios determined by the heat-exchange coefficient. At first, $\delta = 20$ W/(m^2 K) yields a complete transformation into pearlite (see figures 4, 5 and 6).

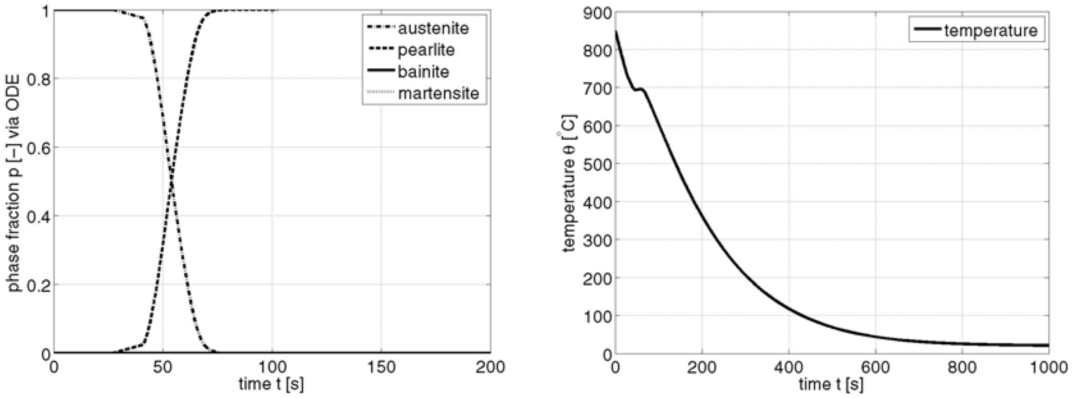

Figure 4: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 20$ W/(m^2 K). Pearlite is calculated by the phenomenological model (5.1)

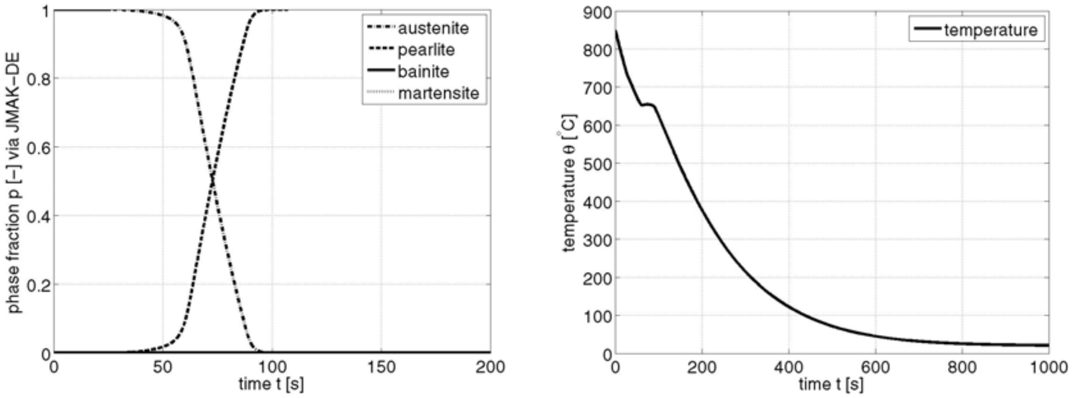

Figure 5: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 20$ W/(m^2 K). Pearlite is calculated by the JMAK kinetics (5.2)

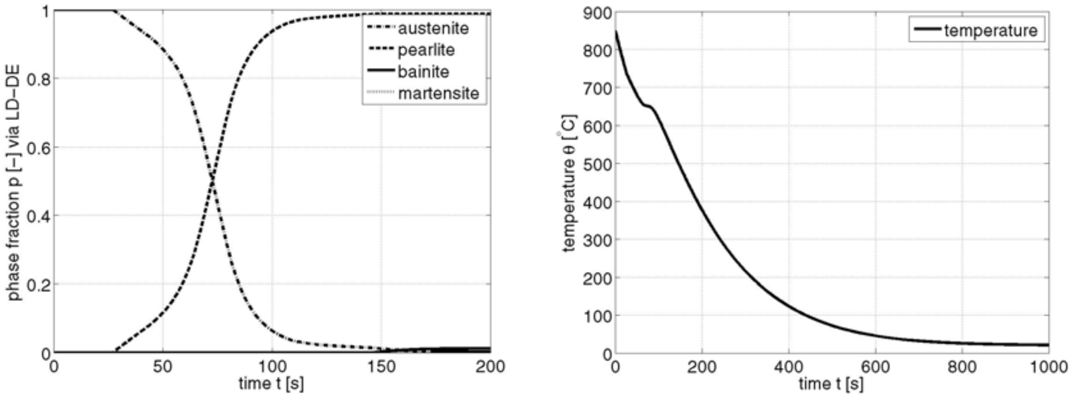

Figure 6: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 20$ W/(m^2 K). Pearlite is calculated by the LD kinetics (5.3)

The heat-exchange coefficient $\delta = 200$ W/(m^2 K) leads to a mixture of all phases (see figures 7, 8, 9).

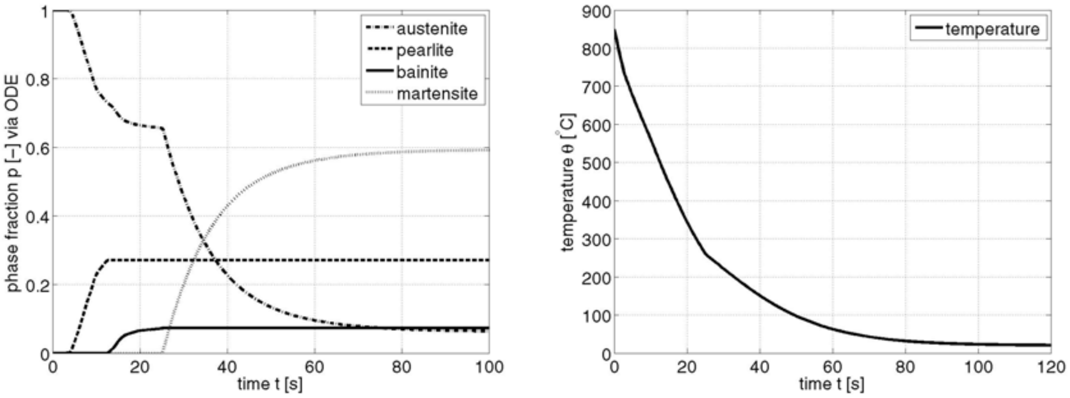

Figure 7: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 200$ W/(m^2 K). Pearlite and bainite are calculated by the phenomenological model (5.1)

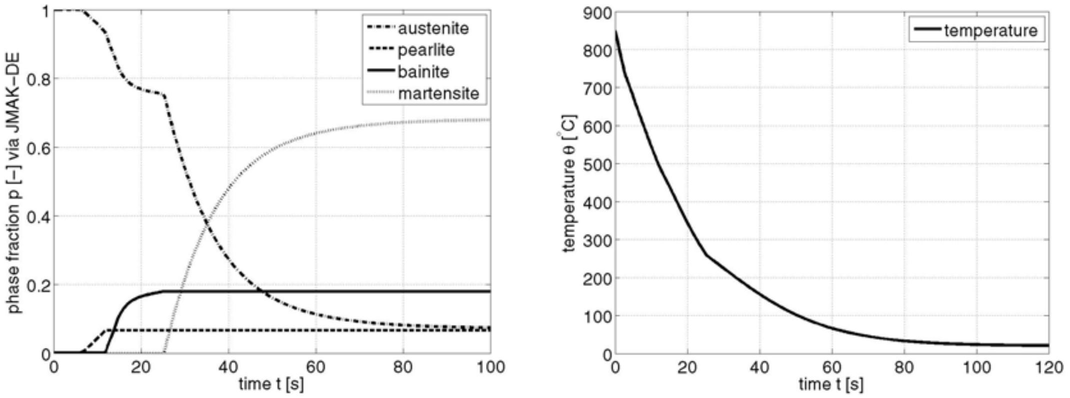

Figure 8: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 200$ W/(m^2 K). Pearlite and bainite are calculated by the JMAK kinetics (5.2)

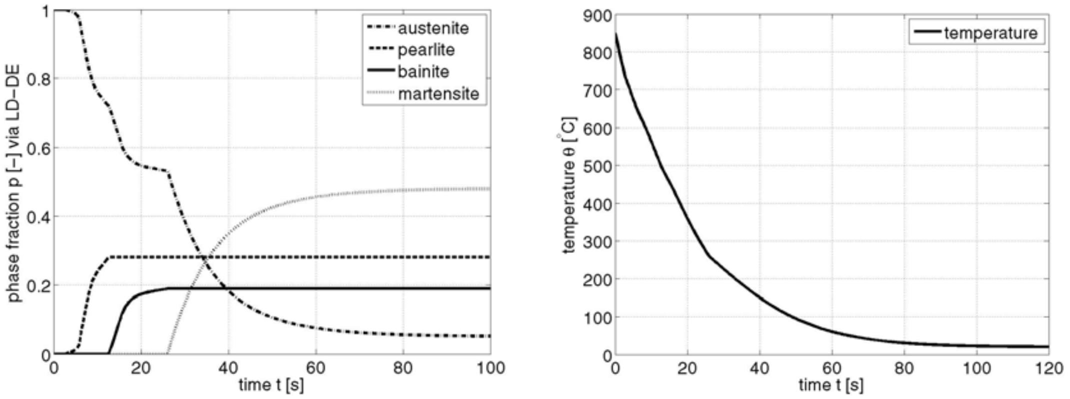

Figure 9: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 200$ W/(m^2 K). Pearlite and bainite are calculated by the LD kinetics (5.3)

The heat-exchange coefficient $\delta = 600$ W/(m^2 K) also leads to a mixture of all phases with a larger part of martensite (see figures 10, 11, 12).

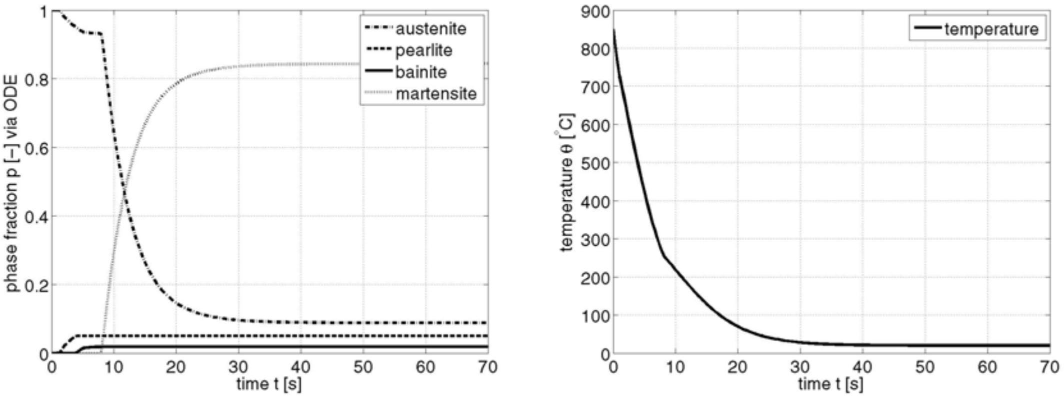

Figure 10: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 600$ W/(m^2 K). Pearlite and bainite are calculated by the phenomenological model (5.1)

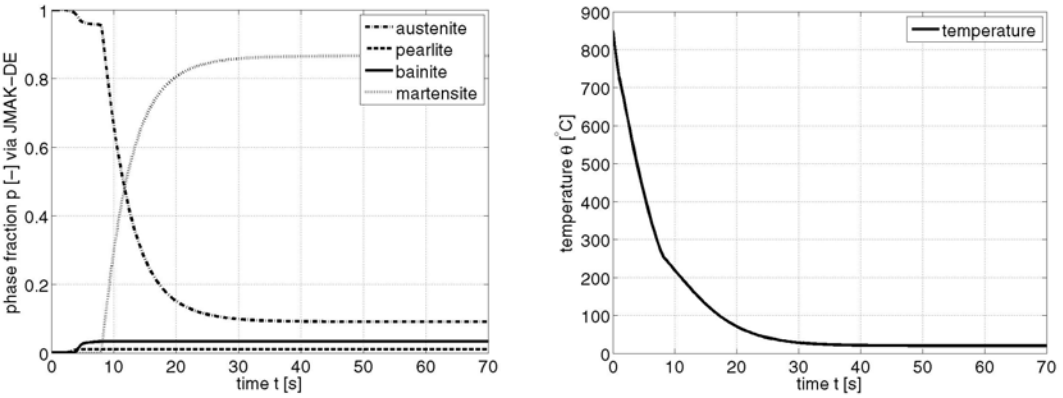

Figure 11: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 600$ W/(m^2 K). Pearlite and bainite are calculated by the JMAK kinetics (5.2)

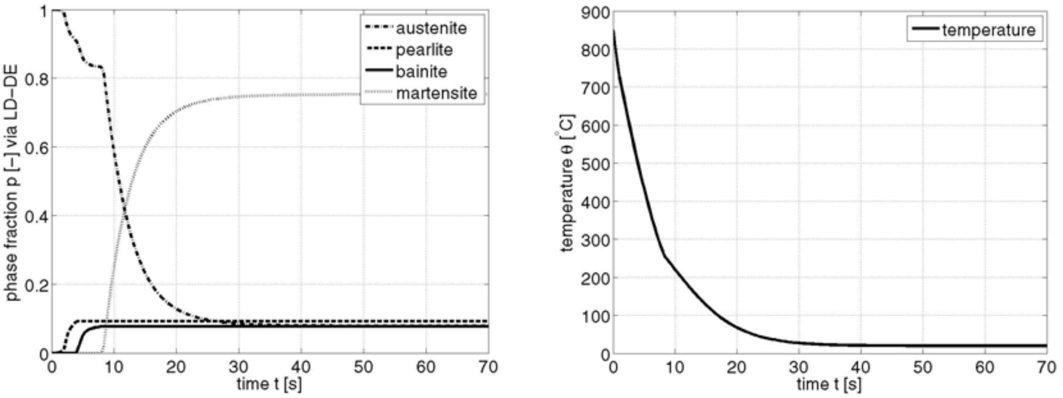

Figure 12: Evolution of phases and temperature for a dilatometer probe, using the heat-exchange coefficient $\delta = 600$ W/(m^2 K). Pearlite and bainite are calculated by the LD kinetics (5.3)

5.2 Parameter identification using transformation diagrams

If there are no experimental data, one can get some information about PT from IT and CCT diagrams (cf. [Wev54], [Ros56], [Ros72], [Pol88], [Van91], [Koh94], [Sei99], [Ber06], for details). Clearly, experimental data contains more information about PT. Therefore, it is difficult to determine the parameters e, r, s, g of the phenomenological model (5.1), using only transformation diagrams. But the JMAK parameters n and τ can be determined, using the 1% and 99% curves in the IT diagrams. For an example of this parameter identification and of simulations, we refer to [Hüß07]. Here we want only sketch the general way.

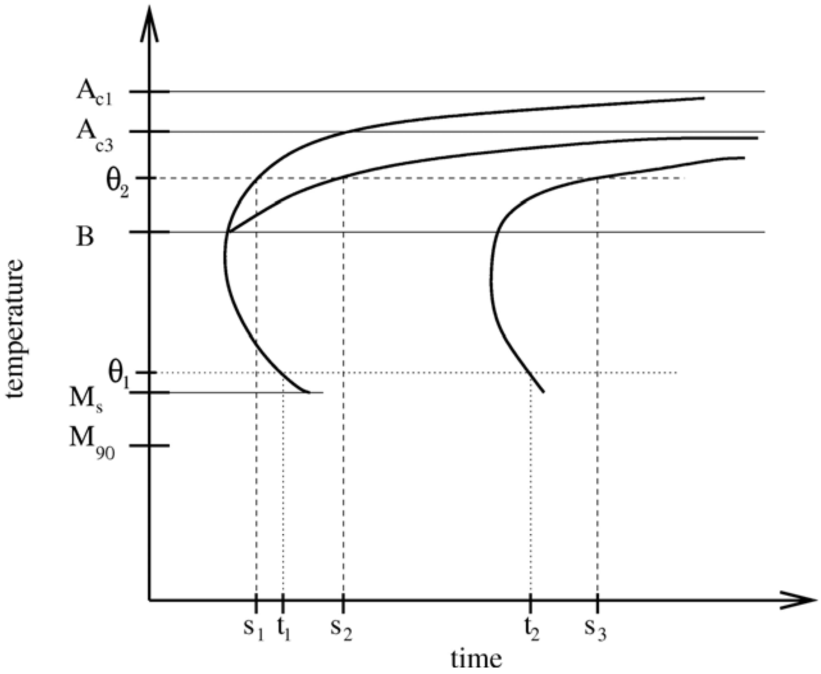

Figure 13: Scheme of an IT diagram for an unalloyed hypoeutectoid steel

Let us consider an unalloyed hypoeutectoid steel with its schematic isothermal transformation diagram (IT diagram) in figure 13. The curves are interpreted by many authors as 1% and 99% curves. That means the left curve indicates the time after which 1% of the corresponding phase is formed. For example, for *constant* transformation temperatures in the region between B and M_s this curve indicates 1% of bainite. And the right curve (in the same region) indicates the time after which 99% of bainite is formed (it corresponds to 1% of remaining austenite). Thus in such regions the JMAK coefficients n and τ can be determined in an easy way. For a chosen temperature θ_1 one can extract the corresponding times t_1 and t_2 to the 1% and 99% curves, respectively (see figure 13). The JMAK approach leads to two equations for determining n and τ:

$$(5.7) \quad 0.01 = 1 - \exp(-(\frac{t_1}{\tau(\theta)})^{n(\theta)}), \quad 0.99 = 1 - \exp(-(\frac{t_2}{\tau(\theta)})^{n(\theta)}).$$

Applying this procedure to some temperature values in the transformation region (of austenite into bainite, e.g.), one obtains temperature-dependent values of n and τ. After interpolation, one gets functions of θ.

In regions with more than two phases, this procedure must be modified. In the region between A_{c3} and B, pre-eutectoid ferrite and pearlite can be formed. In the IT diagram, three curves are plotted. Clearly, the left one indicates 1% of ferrite, the right 99% of ferrite and pearlite (=1% of austenite). Sometimes, the middle curve is simultaneously regarded as the 99% curve of maximally possible ferrite and as 1% curve of pearlite. The fraction of maximally possible ferrite $\bar{p}_{12}(\theta)$ at the corresponding transformation temperature θ_2 must be determined by the lever rule, using an Fe-Fe$_3$C diagram (cf. [Pol88], [Hor92], [Koh94], [Sei99], [Ber06], e.g.). Thus, one obtains

$$(5.8) \qquad \bar{p}_{12}(\theta) = \frac{f_{SE}^{-1}(\theta) - u}{f_{SE}^{-1}(\theta) - f_{QP}^{-1}(\theta)},$$

with the given carbon content u. The values of the curves f_{SE} (“cementite line”) and f_{QP} (“ferrite line”) must be taken from the Fe-Fe$_3$C diagram. After this, one has the following equations for determining the JMAK parameters n_2, τ_2, n_3, τ_3:

$$(5.9)\quad 0.01 = 1 - \exp(-(\frac{s_1}{\tau_2(\theta)})^{n_2(\theta)}), \qquad 0.99 \cdot \bar{p}_{12}(\theta) = 1 - \exp(-(\frac{s_2}{\tau_2(\theta)})^{n_2(\theta)}),$$

$$(5.10)\quad 0.01 = 1 - \exp(-(\frac{s_2}{\tau_3(\theta)})^{n_3(\theta)}), \qquad 0.99 \cdot (1 - \bar{p}_{12}(\theta)) = 1 - \exp(-(\frac{s_3}{\tau_3(\theta)})^{n_3(\theta)}).$$

We refer to [Hüß07] for concrete examples and calculations. Unfortunately, the IT diagrams usually do not give information about the transformation of austenite into ferrite above the eutectoid temperature A_{c3}. The 99% curve is missing. Finally, the IT diagram gives the martensite-start temperature M_s and the temperature θ_{90} of 90% of martensite forming. Thus, the Koistinen-Marburger parameter θ_{m0} (cf. (2.42)) can be determined by

$$(5.11)\qquad 0.90 = 1 - \exp(-\frac{M_s - \theta_{90}}{\theta_{m0}}).$$

This information is sufficient for applying the KM differential equation (2.46), but not for applying the Leblond-Devaux approach (2.52). For this one needs experimental (dilatometer) data (cf. [Wol07b], e.g.). This procedure of determining parameters can be repeated for steels with different carbon content. After interpolating over the carbon content, one obtains the transformation parameters as a function of temperature and carbon content. Thus, processes like case hardening can be modelled. In [Wol06f] we have modelled this situation and performed simulations for a hypoeutectoid steel with varying carbon content over the depth of the work piece. This leads to partial differential equations in one space dimension. Additionally, in [Wol06f] different quenching scenarios (by air and like during the Jominy test) have been considered.

Finally, we remark that continuous cooling temperature diagrams (CCT diagrams) can be exploited for determining transformation parameters, using optimisation procedures (cf. [For00] e.g.).

6 Summary and conclusions

1) We have developed a quite general phenomenological model of phase transformations (PT) in steel in the multi-phase case (see sections 2.1 and 2.2). This proposal generalises approaches presented in [Leb84, 85], [Rét98, 99b, 01], [For00]. Its advantages are:

- simple structure capable for extensions (stress dependence, e.g.)
- easy handling in simulations, in particular in 3d simulations.
- The dependence on the temperature rate can be taken into account or not without changing the basic structure of the model.
- First evaluations yield good results (see section 5.1).

The involving parameters have to be identified at best by experimental data (see section 5.1).

2) We have discussed the relation of our approach to other existing models, giving a survey (see sections 2.3, 2.4, 2.5). Besides this, the multi-phase case of dissolution and of forming of austenite has been considered (see section 2.6).

3) Some remarks about interaction of PT with mechanical movement and temperature have been given, in particular concerning transformation-induced plasticity (TRIP) and stress-dependent PT (see section 3). Additionally, some questions arising from the mathematical side of dealing with PT have been touched (see section 4).

4) We have dealt with parameter identification and simulations. Using experimental data, we have determined the parameter set of the model presented in (2.22). Based on this data, we have performed some calculations for PT of dilatometer probes made of the steel 100Cr6 (SAE

52100). Besides this, we have given an outline for determining transformation parameters from IT diagrams. Unfortunately, this information is normally incomplete.

Performing 3d simulations and comparing with experimental data, we will test our proposal in more general situations, in experiments with 3d work-pieces e.g.

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