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Modelling, simulation and control of multiphase steel production

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Abstract: Multiphase steels combine good formability properties with high strength and have therefore become important construction materials, especially in automotive industry. The standard process route is hot rolling with subsequent controlled cooling to adjust the desired phase mixture. In the first part of the paper a phenomenological model for the austenite ferrite phase transition is developed in terms of a nucleation and growth process, where the growth rate depends on the carbon concentration in austenite. The approach allows for further extensions, e.g., to account for a speed up of nucleation due to deformation of austenite grains.

The model is coupled with an energy balance to describe the phase transitions on a run-out table after hot rolling. Here, the most important control parameters are the amount of water flowing per time and the feed velocity of the strip. The spatial flux profile of the water nozzles has been identified from experiments.

Since the process window for the adjustment of the phase composition is very tight the computation of optimal process parameters is an important task also in practice. This is discussed in the last part of the paper using a classical optimal control approach. To this end a cost functional is defined, which amounts to demanding a desired ferrite fraction and temperature at the end time. The functional is minimized in the set of solutions to the state system such that the control satisfies additional inequality constraints. Numerical results and the convergence history of the developed algorithm are presented for the production of a real dualphase steel with desired phase composition.

Keywords: Hot rolling, multiphase steels, nucleation and growth, phase transition, optimal control

1 Introduction

Despite the development of sophisticated composite materials in recent years, steel is still the basic construction material for industrial societies. Steel is also a modern material, e.g., 80% of the steel grades sold by the German steel producer ThyssenKrupp have been developed in the last 15 years. Fig. 1 shows the strength and formability properties for a number of different steel grades. While classical single phase steels either have good formability (ferritic steels) or strength (martensitic steels), modern multiphase steels like dual-phase (DP) or TRIP-steels have shown high potential especially for automotive applications due to their remarkable properties combining high strength and good formability.

In particular, this development has been triggered by the the demands of automotive industry. In 1999, a group of 33 international steel producers formed the Ultra Light Steel Auto Body - Advanced Vehicle Concepts (ULSAB-AVC) consortium to pursue a steel-intensive family car, fit for the 21st century, that would be safe, affordable and fuel-efficient. Approximately 75 % of the ULSAB-AVC body structure design uses dual-phase (DP) steels.

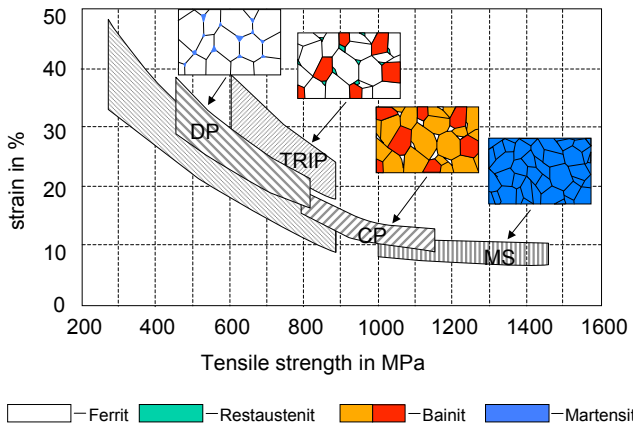

Figure 1. Strength vs. formability for different steel grades

The standard process route for the production of DP steel is by hot rolling and subsequent controlled cooling. It provides good microstructure homogeneity with acceptable surface quality for many applications. The hot rolling process of dual phase steel consists of 4 steps:

Rolling in roughing and finishing stands, which results in the refinement of austenite grain size due to the repeating static recrystallisation (1), laminar cooling into two phase region (2), isothermal holding at ferrite transformation region temperatures, where the temperatures remain relatively constant (3), and finally, fast continuous cooling to the required coiling temperature, during which martensite transformation takes place and bainite transformation can be avoided (4). The controlled cooling of stages (2)–(4) happens on the so-called run-out table. The biggest challenge in producing DP steel in this way is that the process window is very tight as only very short time in order of less than 10 s is allowed on the run out table (ROT) according to its limited length. Hence, there is a strong demand for the online control of the process parameters such as the time and temperature on ROT as well as the cooling rate during cooling down to coiling (step 4 in Figure 1).

The paper is organized as follows. In the next section we derive a phenomenological model for the phase transitions leading to multiphase steel. To simulate a real run-out table, in Section 3 we consider the pilot hot rolling mill at IMF Freiberg, Germany. In Section 4, we outline an optimal control strategy for the production of multiphase steel.

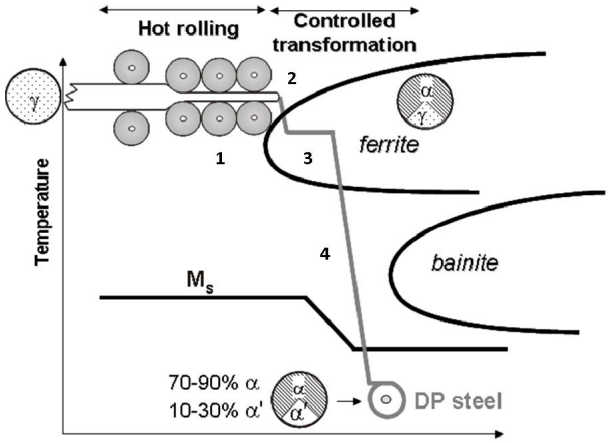

Figure 2. A sketch of the processing scheme for hot rolled dual phase steel.

2 A PHENOMENOLOGICAL MODEL OF PHASE TRANSITIONS IN DUAL PHASE STEEL

DP steels typically consist of 70-80% ferrite and 20-30% martensite formed upon rapid quenching. Hence the main modelling issue is to develop a decent macroscopic austenite – ferrite transformation model. Note that austenite and ferrite are interstitial solutions of carbon in γ (fcc) iron and α (bcc) iron, respectively. This phase transition is governed by the diffusion of carbon from the carbon rich phase austenite to the carbon depleted phase ferrite and stops when equilibrium is reached. To fix some notations, in the sequel, C_γ is the actual carbon concentration in austenite, while C_γ^{eq} and C_α^{eq} are the corresponding equilibrium concentrations in austenite and ferrite, respectively.

To allow for a better model interpretation we seek for a model which explicitly includes the growth rate ρ and nucleation rate ν of the austenite – ferrite transition. Inspired by a paper by Andreucci, Fasano and Primicerio (Andreucci et al. (1991)). we define $\frac{4}{3}\pi\left(\int_\tau^t \rho(s)ds\right)^3$ to be the volume of a ferrite crystal born at time τ. This crystal grows and after some time will also impinge with other crystals. The resulting *virtual volume* of all these interpenetrating volumes is

$$\tilde{f}(t) = \int_0^t \nu(\tau)\frac{4}{3}\pi\left(\int_\tau^t \rho(s)ds\right)^3 d\tau,$$

with growth rate

$$\tilde{f}_t = 4\pi\rho(t)\int_0^t \nu(\tau)\left(\int_\tau^t \rho(s)ds\right)^2 d\tau.$$

Now the question is how to correct for the impingement to get the real volume fraction of the new phase. The classical approach of Avrami (1941) was to say that only growth in the untransformed part contributes to further growth, i.e., to demand that

$$df = (1-f)d\tilde{f}.$$

This leads to the real volume fraction

$$f(t) = 1 - e^{-\tilde{f}(t)},$$

and assuming further constant nucleation and growth rate it gives the classical Johnson-Mehl-Avrami-Kolmogorov law (Avrami (1941), Kolmogorov (1937), Johnson and Mehl (1939))

$$f(t) = 1 - e^{-\frac{1}{3}\nu_0\pi\rho_0^3 t^4}.$$

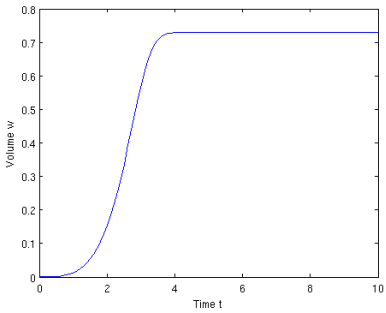

Figure 3. Evolution of ferrite using model (3).

However, here we allow for non-constant growth and nucleation. To correct for impingement we proceed as in Andreucci et al. (1991) and define the nucleation rate as

$$\nu(f,\theta) = \nu_0(\theta)(1-f),$$

where ν_0 might depend on the actual temperature θ. This results in the ferrite growth model

$$f_t = 4\pi\rho(t)\int_0^t \nu(f,\theta(\tau))\left(\int_\tau^t \rho(s)ds\right)^2 d\tau \tag{1a}$$

$$f(0) = f_0. \tag{1b}$$

It is easy to see that the solution to (1a) asymptotically tends to 1 for constant growth rate, i.e. it would always lead to complete transformation disregarding the fact that the growth should stop when the carbon concentration in austenite reaches equilibrium, i.e. $C_\gamma \to C_\gamma^{eq}$.

An easy way to achieve this is by demanding

$$\rho \propto C_\gamma^{eq} - C_\gamma. \tag{2}$$

Assuming tacitly the carbon concentration in ferrite C_α always to be equal to equilibrium concentration C_α^{eq}, conservation of mass gives

$$C_0 = C_\alpha^{eq} f + C_\gamma(1-f) \quad \text{i.e. } C_\gamma = \frac{C_0 - C_\alpha^{eq} f}{1-f},$$

with C_0 the overall mean carbon concentration. This allows to eliminate C_γ in (2) and we end up with the growth rate

$$\rho(f,\theta) = \rho_0(\theta)\frac{\bar{f}-f}{1-f},$$

where again ρ_0 might depend on temperature θ and $\bar{f}$ is the resulting equilibrium fraction of ferrite

$$\bar{f} = \frac{C_\gamma^{eq} - C_0}{C_\gamma^{eq} - C_\alpha^{eq}}.$$

Altogether we have obtained our ferrite growth model

$$f_t = 4\pi\rho(f,\theta(t))\int_0^t \nu(f,\theta(\tau))\left(\int_\tau^t \rho(f,\theta(s))ds\right)^2 d\tau \tag{3a}$$

$$f(0) = f_0. \tag{3b}$$

Using data for a typical carbon steel, Fig. 3 shows the evolution of ferrite to its equilibrium carbon concentration corresponding to an equilibrium phase fraction of 73% in that case. The nice feature of the

model is that the explicit occurrence of nucleation rate allows for an easy extension to account for the so-called austenite conditioning i.e. the speed up of nucleation due to the deformation of the austenite grains by the hot rolling process. For details, we refer to Suwanpinij et al. (2010). Another interesting task could be to study ellipsoidal instead of spherical growth for the ferrite nuclei.

3 A MODEL OF A REAL HOT ROLLING MILL

In a joint project with mechanical engineers from the Institute of Metal Forming (IMF) at TU Bergakademie Freiberg we have identified the process parameter for the pilot hot rolling mill at IMF (cf. Fig. 4). As before, our focus is on the phase transformation, i.e., the growth of ferrite, on the run-out table. After passing the cooling section and a holding section the specimen is quench cooled by manually throwing it into a water bath.

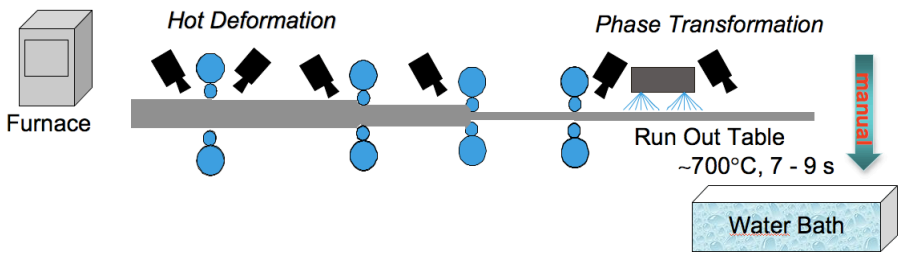

Figure 4. Pilot hot rolling mill at IMF, TU Bergakademie Freiberg, Germany.

To describe the evolution of temperature and ferrite on the run-out table we have to complement (3) with the heat equation. To this end we assume heat conduction to be negligible in the feeding direction of the specimen and write down the system for a 2D cross section Ω, which yields the system

$$f_t = G(\theta, f), \qquad \text{in } Q = \Omega \times (0,T) \tag{4a}$$
$$f(0) = 0, \qquad \text{in } \Omega \tag{4b}$$
$$\rho c \theta_t - \nabla \cdot (k(x)\nabla\theta) = \rho L f_t, \qquad \text{in } Q \tag{4c}$$
$$-k\frac{\partial\theta}{\partial n} = u(t) g(x,y,t;v)(\theta - \theta_w), \qquad \text{on } \Sigma_R = \Gamma \times (0,T) \tag{4d}$$
$$-k\frac{\partial\theta}{\partial n} = 0, \qquad \text{on } \Sigma_D = (\partial\Omega \setminus \Gamma) \times (0,T) \tag{4e}$$
$$\theta(0) = \theta_0, \qquad \text{in } \Omega \tag{4f}$$

The term on the right-hand side of (4c) describes the latent heat of the phase transition. Our main modeling assumption at this point is that the heat transfer coefficient can be multiplicatively decomposed into the amount of water sprayed onto the specimen $u(t)$ and a term g including the normalized water nozzle profile and the feeding velocity v. Fig. 5 shows the effect of varying water amount and strip velocity. From these kind of experiments the function g could be identified.

4 OPTIMAL CONTROL OF THE RUN-OUT TABLE AFTER HOT ROLLING

After the process parameters have been identified we want to compute on optimal amount of water $u(t)$ to achieve a desired distribution of ferrite f_d at the end-time T. At the same time we want to realize a desired end temperature θ_d. To this end, we define a cost functional

$$J(\theta, f, u) = \frac{\alpha_1}{2}\int_\Omega (f(x,T) - f_d(x))^2\,dx + \frac{\alpha_2}{2}\int_\Omega (\theta(x,T) - \theta_d(x))^2\,dx + \frac{\alpha_3}{2}\int_0^T u^2 dt,$$

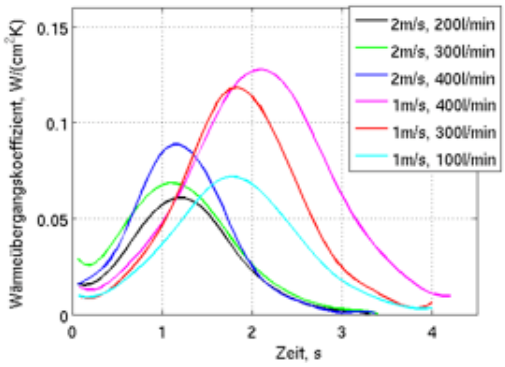

Figure 5. Measured heat transfer coefficient for different amounts of water and strip velocities

where the last regularizing term penalizes high costs. Then we consider the control problem **(CP)**

$$\begin{aligned} \min \quad & J(\theta, f, u) \\ & \text{such that } (\theta,\ f,\ u) \text{ satisfy the state system (4)} \\ & \qquad \text{and the control constraint } u_a \le u \le u_b, \quad t \in (0,T) \quad a.e. \end{aligned}$$

In a forthcoming paper (cf. Hömberg et al. (2011)), we have investigated this control problem both analytically and numerically. For its numerical solution an SQP (sequential quadratic programming) strategy has been developed with a primal-dual active set strategy (PDAS) to account for the inequality constraint in $u(t)$ and a line-search based globalization strategy (see Nocedal and Wright (2006) for algorithmic details). The code has been used to compute the optimal cooling strategy for a DP-steel with 70% ferrite and a desired end temperature after the cooling section of $\theta_d = 680^oC$. Table 1 shows the convergence history of the SQP steps.

The optimal amount of water $u(t)$ is depicted in Fig. 6. Its evolution reflects the presence of the box constraints and the functioning of the actice set method. For the longest part of the time interval the optimal control sticks to the upper bound of the box constraint and then it quickly decreases to zero.

5 Conclusions

The goal of this paper was to show how mathematics can be used for the computation of process conditions to develop multiphase steels with desired composition by controlled cooling on the run-out table of a hot rolling mill. The results have been verified in practice and can be used for the offline optimization of run-out tables. There are two challenging directions of future research. On the one hand the phase transition models have to be complemented with an additional equation for bainite in order to extend the model to other multiphase steels, e.g., TRIP steel. The morphology and kinetics of bainitic growth is between the diffusive ferrite and the non-diffusive martensitic growth. It is fair to say that its modelling has not been fully understood yet and poses a challenging problem for applied mathematicians. On the other hand regarding the industrial employment the development of real-time process control strategies

Iteration	J_i	$\|(u^i, \theta^i, f^i, p^i, q^i) - (u^{i-1}, \theta^{i-1}, f^{i-1}, p^{i-1}, q^{i-1})\|$	Number of PDAS-Loops
1	0.025359	0.24649	7
2	0.021225	0.016189	3
3	0.021237	0.000171	2
4	0.021237	$2.16 \cdot 10^{-6}$	2

Table 1. Value of objective function J_i and relative error in i-iteration of SQP Method.

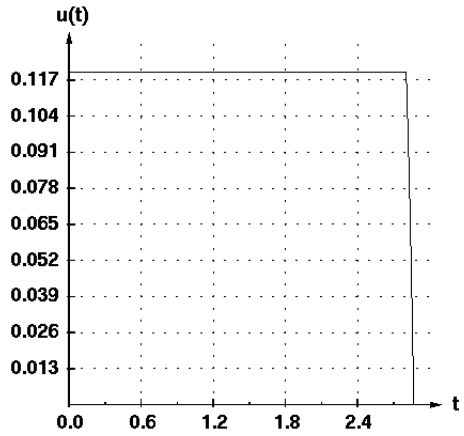

Figure 6. Optimal amount of water $u(t)$.

based on (CP) is a very important task. Here, recent developments in model reduction techniques seem to be a promising tool and will be subject of future research of the authors.

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