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Comparison of several kinetic equations for pearlite transformation in 100Cr6 steel

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Comparison of several kinetic equations for pearlite transformation in 100Cr6 steel

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Abstract

The kinetics of phase transformation in steel under continuous cooling is considered. The aim is to find a model precise as possible for pearlite transformation in 100Cr6 steel comparing different known equations with some extensions. Here we consider only the stress free dilatometer experiments with continuous cooling. The Leblond model is compared with an Johnson-Mehl-Avrami-type equation taking the temperature history into account.

Keywords: kinetic of phase changes, pearlite transformation.

1 Introduction

The classical Johnson-Mehl-Avrami equation [JM39]

$$p(t) = 1 - \exp\left(- \left(\frac{t}{\tau(T)}\right)^{n(T)}\right) \tag{1.1}$$

is in a good agreement with experiment in case of isothermal phase transformation, however it gives only a qualitative description in the non-isothermal case. Here τ and n are two temperature dependent parameters, p is the product phase fraction, t is time and T is temperature. To achieve the high accuracy in simulation of the diffusion phase transformation a lot of attempts have been undertaken in the last decades. The motivation is to have a better control of the additional distortions due to phase transformation during thermal treatment of workpieces. In general stresses affect the phase transformation and the elasto-plastic problem is coupled with evolution of phases, we refer to [DAG+02] and [ABM02]. In this paper we consider the simplest

case (no temperature gradient, stress free) of austenite-pearlite transformation as a starting point for further investigations of a coupled problem. This paper can be considered as a supplement of [BHSW03] where the comparison of five different procedures for kinetic simulation was considered. We used the same experimental data as in [BHSW03] and two kinetic equations. One of them takes into account the history of the temperature evolution, another is the model of Leblond. There are many kinetic equations based on the differential form of the JMA-equation

$$\frac{dp}{dt} = (1-p)\frac{n(T)}{\tau(T)}\Big(-\ln(1-p(t))\Big)^{1-\frac{1}{n(T)}} \tag{1.2}$$

combined sometimes with the additive Scheil rule, see [RHF97], [BHSW03], [Höm95], [LD84] and [BDH$^+$03] for plenty of examples.
We are going to compare some of these methods for pearlite transformation in 100Cr6 steel. The evaluation of five procedures (JMA-equation, Denis model [FDS85],[DFS92], [DAG$^+$02], Hougardy model [HY86] and two generalizations [HLHM99], [SYS00] of JMA-equation with additional factors) has been presented in [BHSW03]. In that paper the best accuracy was obtained with the Model B, which is an extension of (1.2) with a factor

$$(1-g(T))\frac{dT}{dt}, \tag{1.3}$$

where the function $g(T)$ is to be fitted. In the current paper we are going to continue the evaluation and compare two other procedures with the five mentioned above. For this purpose we consider the same steel 100Cr6 and use the same set of continuous cooling experiments with different temperature rates.

2 Phase transformation models

In this paper we concentrate on the transformation of austenite to pearlite under a non-isothermal cooling process free of stresses. The full transformation to the product phase at the end of the process is assumed. The first equation we are going to consider is the equation proposed by Leblond and Devaux in [LD84]

$$\frac{dp}{dt} = \frac{1-p(t)}{\mu(T)}, \quad \mu(T) > 0, \tag{2.1}$$

where $T(t)$ is a given temperature variation, $p(t)$ is the pearlite fraction and $\mu(T)$ is a temperature dependent parameter representing the characteristic

time of the transformation. The initial condition is $p(0) = 0$. We remark that for a single experiment with strictly monotone $T(t)$ one can always find such a function $\mu(T(t))$ that the simulation performs a prescribed accuracy. However it is desired to find a universal $\mu(T)$ for a range of temperature rates.
The second model is the following. We are going to take the history of the temperature evolution into account. For this purpose we introduce the averaged temperature $\theta(t)$ by the following formula

$$\theta(t) = \alpha(1 - e^{-\alpha(t-t_0)})^{-1} \int_{t_0}^{t} T(s)\, e^{-\alpha(t-s)}\, ds, \quad t > t_0, \tag{2.2}$$

$\alpha > 0$ is the parameter of the weight function. Then we use the classical differential equation (1.2) with $\theta(t)$ on the place of $T(t)$. The advantage of this approach is that we can use the same material parameters τ and n obtained in isothermal experiments. We remark that for constant temperature we obtain the same JMA differential equation (1.2).

3 Experimental data

We consider the exponential cooling curves with different rates starting from 850°C to 100°C. The duration $t_{850/100}$ of cooling is respectively 2000s, 1000s, 500s and 300s. The method of calculation of the pearlite fraction from the dilatometer test is described in [BHSW03] and we used the same result from this paper. We confine the consideration on the temperature interval from 800° to 500° as in [BHSW03]. It corresponds to the durations $t_{800/500}$ of 413s, 206s, 103s and 62s. We use also $\tau(T)$ and $n(T)$ from the same paper:

$$\tau(T) = \tau_0 \exp\left(\frac{Q}{T}\right) \exp\left(\frac{P}{T(T_P - T)^2}\right), \quad n(T) = n_0 + n_1 T, \tag{3.1}$$

with $\tau_0 = 0.0018s$, $Q = 7000K$, $P = 1.3 \cdot 10^7 K^3$, $T_P = 760°C$, $n_0 = -16.04$, $n_1 = 0.0324\frac{1}{K}$.

4 Simulation results

The mean square error (or L_2-norm of the deviation) scaled by the length of the correspondent time-interval was used to compare the models (the same as in [BHSW03]), see the Table 1. Here time intervals correspond to the cooling from 850°C to 500°C.

4.1 Leblond model

For the Leblond model we assume the following form of $\mu(T)$

$$\mu(T) = a(850 - T)^2, \quad (T \text{ in } {}^\circ C) \tag{4.1}$$

where $a > 0$ has to be fitted from the experimental data. For this simple model we found that the optimal a for these experiments is $a = 8.8$ in the sense of the L_2-norm of the deviation between the simulation and the experiment.

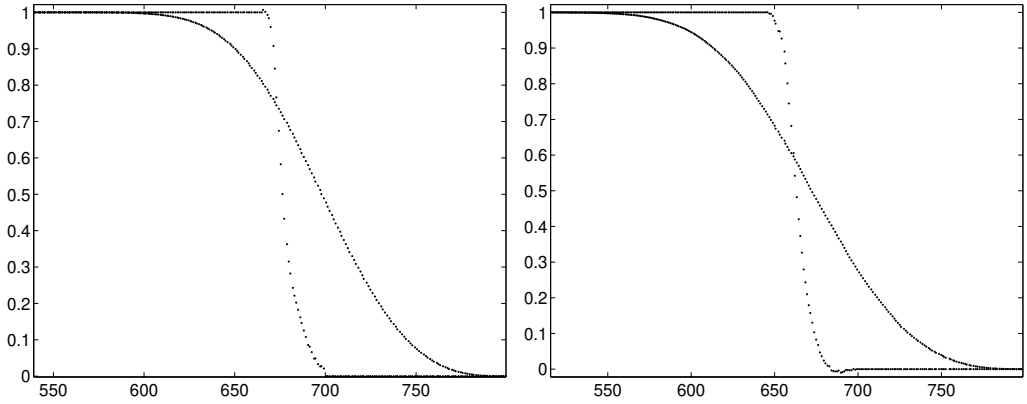

Figure 1: (Leblond model) The dotted line represents the experiment, the solid line corresponds to the simulation. Left – $t_{850/500} = 2000s$, right – $t_{850/500} = 1000s$ (Vertical is volume fraction of pearlite, horizontal is temperature in ${}^\circ C$.)

We see that the result is qualitative good, but the L_2-norm deviation between simulation curves and experimental curves averaged over four processes was found to be 0.177. That is bigger as in the simulations performed in [BHSW03]. For more accuracy one needs to use better parametrization of the function $\mu(T)$ in the Leblond equation.

4.2 Simulation with averaged temperature

Now let us proceed to the second method (1.2), (2.2). The optimal α was found as $\alpha = 0.713\frac{1}{s}$ and the corresponding results are presented on the Figures 3-6. We see essentially a better agreement with the experiment in comparison with the Leblond model. The average L_2-error

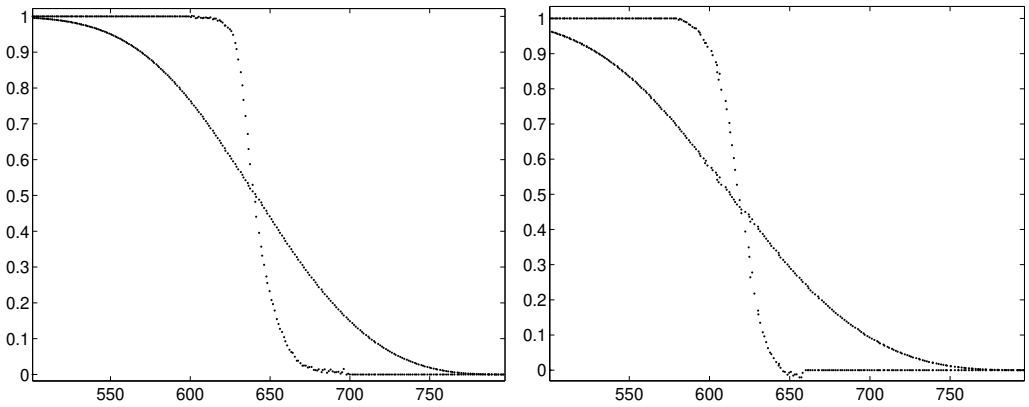

Figure 2: (Leblond model) The dotted line represents the experiment, the solid line corresponds to the simulation. Left – $t_{850/500} = 500s$, right – $t_{850/500} = 300s$ (Vertical is volume fraction of pearlite, horizontal is temperature in $^\circ C$.)

$\left(\frac{1}{k}\sum_{j=1}^{k}\delta_j^2\right)^{\frac{1}{2}}$, (here $k = 4$), where the sum is taken over all considered processes and δ_j are the L_2 norms of the difference between the correspondent experimental curve and its simulation curve, for this model is 0.032, that is better in comparison to the JMA-simulation presented in [BHSW03]. In the first line in the following table we quote results from there. The second and the third line show the L_2-error for each single experiment with the same α (or respectively a) for all processes. In the last line we quote the results for the Model B (see (1.3) from [BHSW03]

We would like to remark that equation (1.2) with initial condition $p(0) = 0$ has two solutions, one of them is trivial. Hence for simulation one have to use $p(0) = \varepsilon$ with a small ε. Then one has a unique solution, but of course it depends on ε. We chose ε small enough so that for smaller values of ε the difference between the simulated solutions is negligible, so we took $\varepsilon = 10^{-7}$.

Table 1: JMA, JMA-α and Leblond models: Mean square errors.

	2000s	1000s	500s	300s
JMA	0.0375	0.0271	0.0627	0.0877
JMA-α	0.0417	0.0306	0.0283	0.0225
Leblond	0.1781	0.1681	0.1711	0.1934
Model B	0.0313	0.0198	0.0164	0.0078

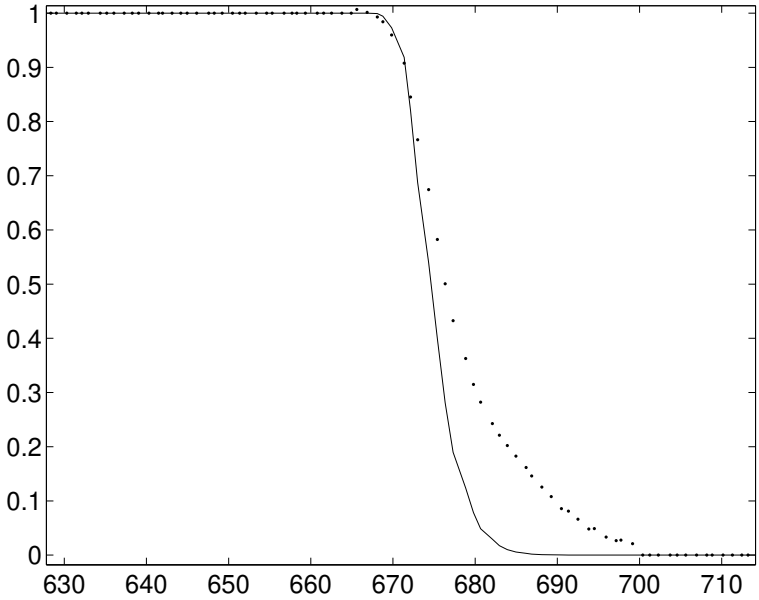

Figure 3: $t_{850/500} = 2000s$ - the dotted line represents the experiment, the solid line corresponds to the simulation (Vertical is volume fraction of pearlite, horizontal is the temperature in $^\circ C$).

5 Discussion and conclusions

The advantage of these two methods considered above is the simplicity of the equations, where only one additional parameter has been introduced. The results performed here yield a qualitatively good agreement with the experiment, however the Leblond model with only one parameter remains to be quantitatively imprecise. One has to find some better formulas for the time-scale parameter $\mu(T)$ to reach a better agreement with experiments.
The second method has better average approximation than the JMA-equation. For higher cooling rates it yields essentially better precision than JMA, but worse for lower ones. It could be probably improved by a more sophisticated functional taking the history of the temperature evolution into account. We conclude that both methods can be used for the kinetic simulation of the pearlite phase transformation, however some improvements of (4.1) are still needed in case of the Leblond model. We also remark that due to essentially higher freedom in fitted parameters (function g from (1.3) in comparison to one parameter a or α from (2.1) or (2.2)) the Model B has a better accuracy then both models discussed above, see Table 1. With reference to [BHSW03] we can also conclude that for a given material and a short range of temperature variation one can always find some extension of the classical models to

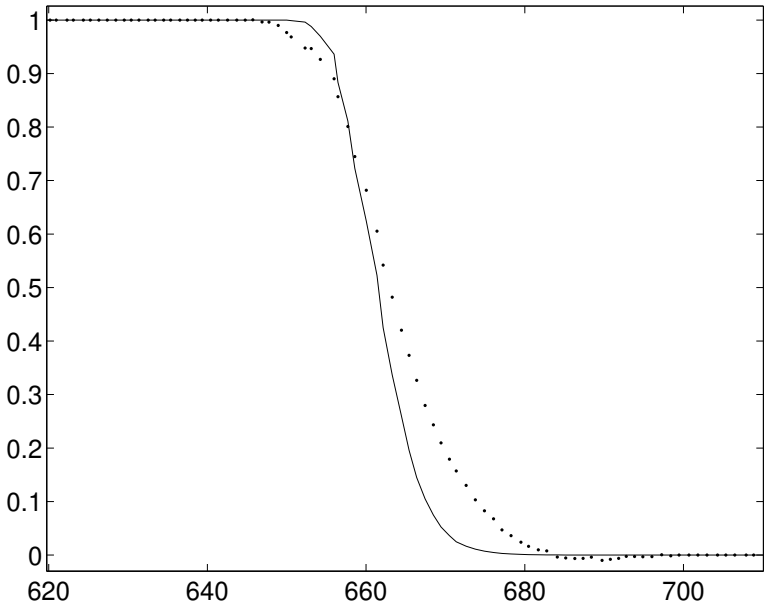

Figure 4: $t_{850/500} = 1000s$ - the dotted line represents the experiment, the solid line corresponds to the simulation (Vertical is the volume fraction of pearlite, horizontal is the temperature in $^\circ C$).

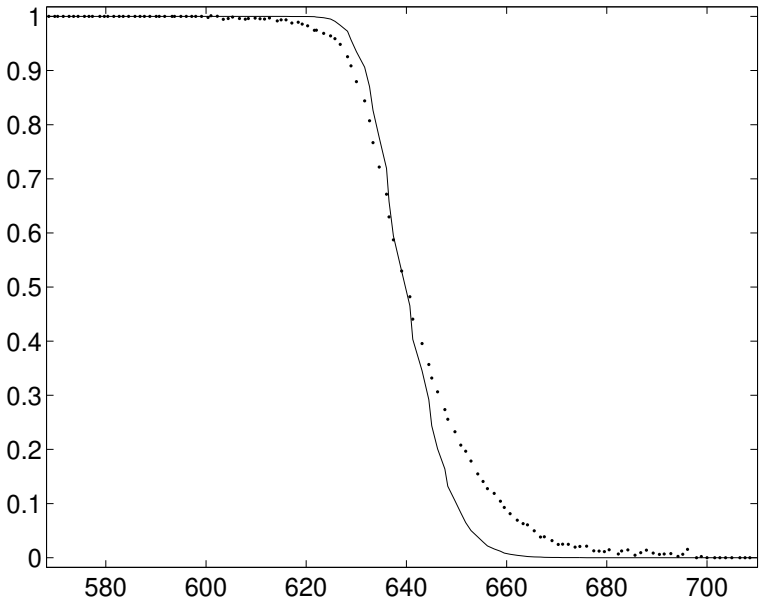

Figure 5: $t_{850/500} = 500s$ - the dotted line represents the experiment, the solid line corresponds to the simulation (Vertical is the volume fraction of pearlite, horizontal is the temperature in $^\circ C$).

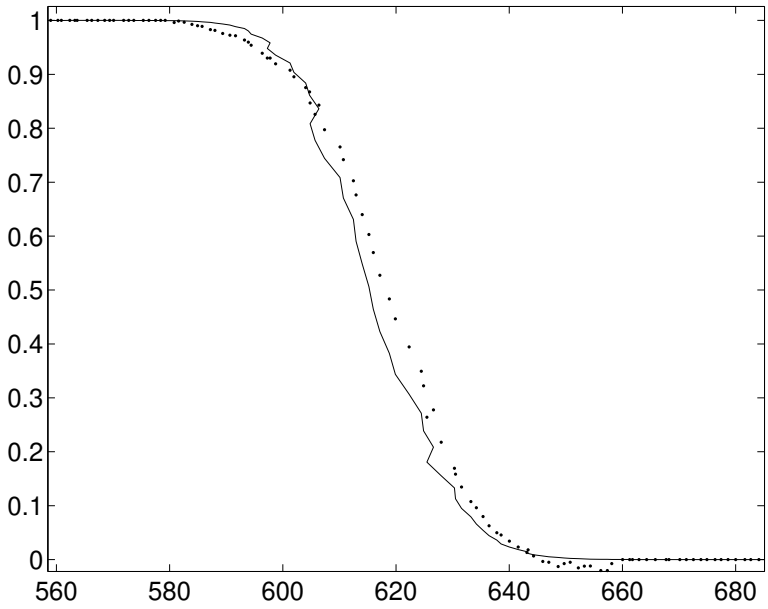

Figure 4: $t_{850/500} = 300s$ - the dotted line represents the experiment, the solid line corresponds to the simulation (Vertical is the volume fraction of pearlite, horizontal is the temperature in K).

achieve the desired accuracy in simulation. However one has to change the obtained model drastically in case of a different variation of temperature or in case of some changes in composition of material. That is why we believe that some new approaches for the kinetic modeling are still needed.

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