

Supplementary Material to: Predictive Modeling of the Bainite Start Temperature using Bayesian Inference

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1. Heat treatment parameter for the production and the characterization of model alloys

Table 1 lists the normalization temperature T_N , the heating rate \dot{T}_{heat} , austenitization temperature T_{Aus} , austenitization time t_{Aus} and the cooling rate \dot{T}_{cool} of the experiments.

Table 1: Austenitization parameters

Nr	T_N / °C	\dot{T}_{heat} / °C/s	T_{Aus} / °C	t_{Aus} / s	\dot{T}_{cool} / °C/s
T1	960	2	960	1800	50
T2	960	2	960	1800	50
T3	960	2	960	1800	50
T4	960	2	960	1800	50
T5	960	2	960	1800	50
T6	880	2	960	1800	25
T7	1100	2	1100	1200	25
T8	1010	2	1010	1800	25
T9	880	2	950	900	25

2. Determination of the bainite start temperature for the model alloys

The bainite start temperatures (B_S) for the model alloy are determined using a combination of dilatometry and light optical microscopy (LOM), as demonstrated for model alloy T1. Figure 1 a) shows the LOM image of the purely martensitic microstructure of model alloy T1 after quenching from austenitization to room temperature. Comparing this microstructure with those formed under various isothermal holding temperatures T_{iso} (Fig. 1 b–e) followed by quenching the samples to room temperature, the greatest similarity is observed in Fig. 1 b). Dilatometry measurements during isothermal holding

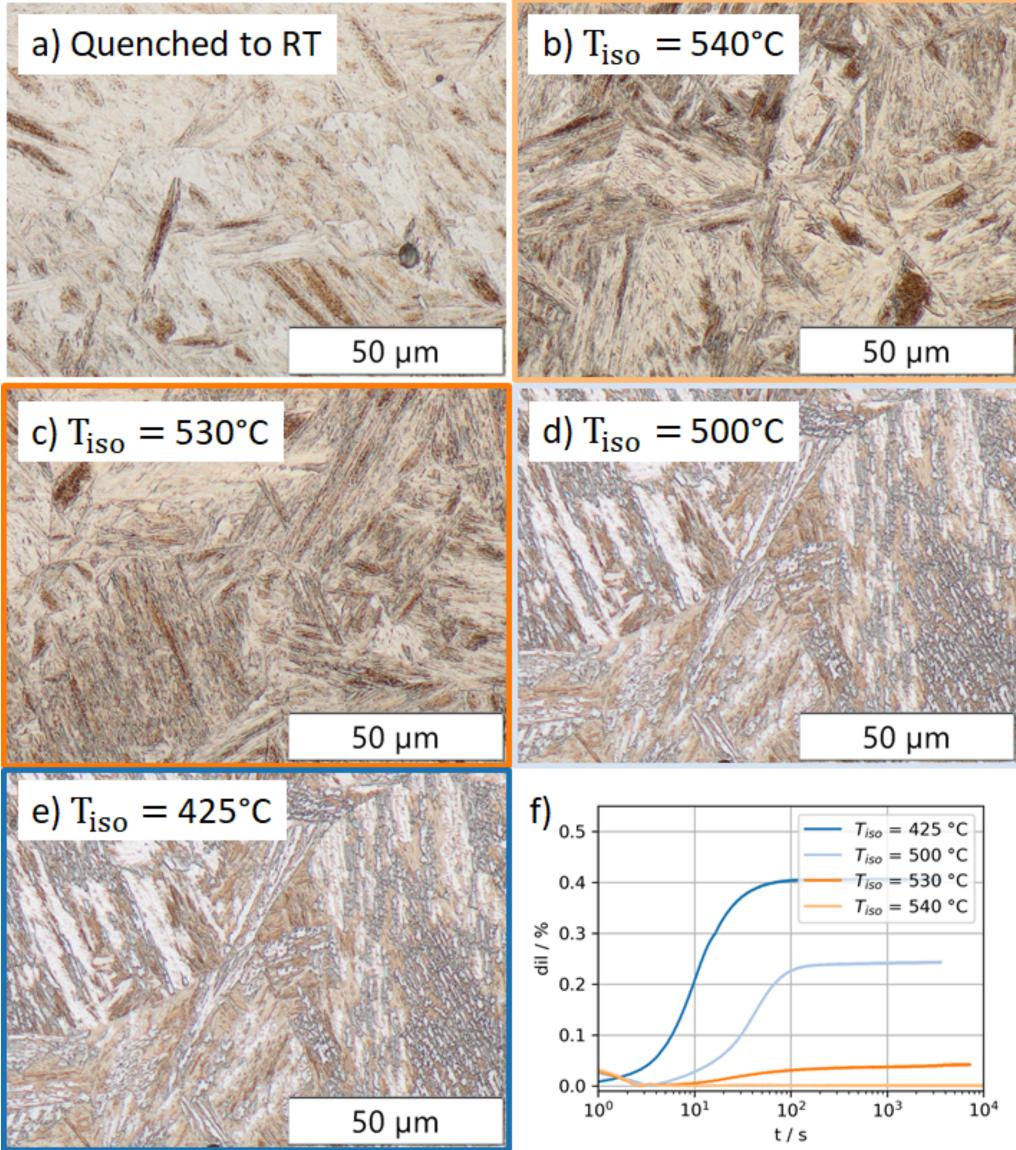


Figure 1: LOM images of model alloy T1 microstructure after a) quenching from austenitization temperature to room temperature to obtain a purely martensitic microstructure and b) – e) quenching from austenitization temperature to an isothermal holding temperature T_{iso} ranging between 540°C and 425°C, respectively, and holding times from 3600s to 10800s to obtain the Bs by comparing the evolving microstructures with the corresponding dilatation data f). After isothermal holding, all samples were quenched to room temperature.

at 540°C reveal no significant dilatation, indicating the absence of bainitic ferrite formation at this temperature, which is visible in Fig. 1 f). When the isothermal holding temperature is lowered to 530°C, subtle changes in the microstructure become apparent,

with some areas appearing grainy (compare Fig. 1 b) and c)). Additionally, a slight increase in dilatation is observed beyond 10 seconds (Fig. 1 f), suggesting the onset of bainitic ferrite transformation at 530°C. The dilation changes in the first seconds are interpreted to stem from the experimental setup. This combined analysis of LOM images and dilatometry data identifies the B_S for model alloy T1 as $535 \pm 15^\circ\text{C}$, lying between 540°C and 530°C. The error of $\pm 15^\circ\text{C}$ reflects the uncertainty due to the combined resolution of dilatometry measurements, the subjective interpretation of microstructural changes in LOM images and a safety margin. The bainite start temperatures for other model alloys are determined using the same methodology.

3. Literature dataset

The literature dataset can be found as "data_Bs.csv".

4. Inference results

The posterior distribution of the model parameters shows correlations among the parameters. Samples of this distribution can be found in the files "[Modelname]_[Database].csv". If a respective model for B_S is evaluated once for each sample, the resulting distribution for B_S gives an uncertainty prediction. If these correlations are not considered, like in the case of Tab. 2 and Tab. 3, the resulting uncertainty will be overestimated.

The mean and standard deviation of the parameters of the posterior samples for the "mc_fe_bainite" database can be found in Tab. 2.

Table 2: Parameter values for the different models when using the "mc_fe_bainite" database (mean value $\pm \sigma$ value).

Par	Unit	Dis1	Dis2	Dis3	Dis4	Diff
e_t	kJ			7 ± 5		
b_0	J/mol		-1172 ± 11	-1172 ± 11		
b_1	J/(mol K)		1.57 ± 0.27	1.56 ± 0.27		
a_0	J/mol	708 ± 12	343 ± 59	480 ± 110	16 ± 57	28 ± 25
a_{Al}	J/(mol a%)				-104 ± 40	-140 ± 54
a_C					-150 ± 15	156 ± 14
a_{Co}					236 ± 75	388 ± 88
a_{Cr}					294 ± 15	286 ± 14
a_{Mn}					305 ± 25	306 ± 23
a_{Mo}					509 ± 31	479 ± 20
a_{Ni}					80 ± 11	82 ± 10
a_{Si}					64 ± 12	68 ± 13
a_V					416 ± 194	493 ± 197

The mean and standard deviation of the parameter of the posterior samples for the "TCFE12" database can be found in Tab. 3.

Table 3: Parameter values for the different models when using the "TCFE12" database (mean value $\pm \sigma$ value).

Par	Unit	Dis1	Dis2	Dis3	Dis4	Diff
et	kJ			9 ± 5		
b_0	J/mol		-1114 ± 11	-1113 ± 11		
b_1	J/(mol K)		1.12 ± 0.28	1.10 ± 0.29		
a_0	J/mol	632 ± 11	193 ± 60	388 ± 140	72 ± 55	30 ± 25
a_{Al}	J/(mol a%)				-56 ± 41	-90 ± 53
a_C					-174 ± 15	163 ± 15
a_{Co}					241 ± 70	378 ± 89
a_{Cr}					266 ± 15	259 ± 14
a_{Mn}					271 ± 24	288 ± 22
a_{Mo}					476 ± 30	467 ± 21
a_{Ni}					59 ± 10	69 ± 10
a_{Si}					55 ± 11	59 ± 12
a_V					412 ± 180	511 ± 195

5. Transformation between driving forces

The Parameter for the transformation energy G_{Trans}

$$G_{\text{Trans}} = a + b \cdot x_C + c \cdot x_C \cdot (T - 273.15) \quad (1)$$

for the other database are:

- mc_fc_bainite: $a = 15.6 \text{ J} \cdot \text{mol}^{-1}$, $b = 597 \text{ J} \cdot (\text{mol at\%})^{-1}$, and $c = -0.403 \text{ J} \cdot (\text{mol at\% K})^{-1}$ with an MAE of 13.83 J/mol.
- TCFE12: $a = 10.6 \text{ J} \cdot \text{mol}^{-1}$, $b = 532 \text{ J} \cdot (\text{mol at\%})^{-1}$, and $c = -0.435 \text{ J} \cdot (\text{mol at\% K})^{-1}$ with an MAE of 16.11 J/mol.

6. Influence of database

When comparing the model parameters from different databases, while there are some differences, all coefficients have significant overlap. The trend stays the same, but one has to be cautious with the interpretation of absolute numbers. Another check was done by comparing the T_0 temperatures for the dataset, which is shown in Fig. 2.

The databases "mc_fe" and "TCFE12" give very similar values, while there is temperature dependent deviation for "mc_fe_bainite" for lower temperatures. Regardless, it can be said that the thermodynamic databases give similar results, which can be explained because of their partly shared data-basis and models.

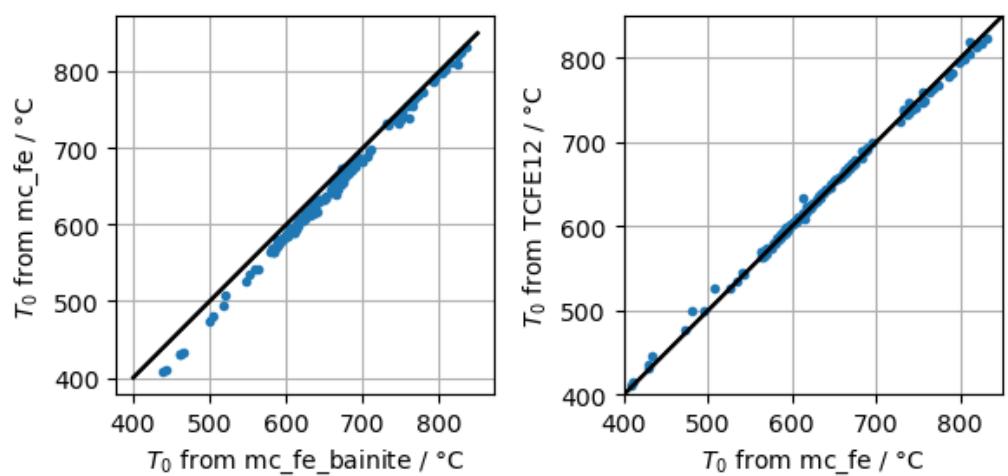


Figure 2: Comparison of T_0 temperature for the different databases.