Proceedings

10th International Conference on **Trends in Welding Research**

& 9th International Welding Symposium of Japan Welding Society (9WS)



October 11 - 14, 2016

Hitotsubashi Hall, National Center of Sciences Building Tokyo, Japan

Organizing Society American Welding Society (AWS) Japan Welding Society (JWS)



http://trends2016.org

Numerical simulation of Pearlite formation during welding of rails

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Abstract

In this work, a thermo-metallurgical coupled simulation model of welding of R350HT pearlitic rail steel was realized to estimate the mechanical properties in the HAZ. The applied approach was to estimate the hardness of pearlitic phase fractions by calculating the interlamellar spacing. This was realized in a methodology of multiple calculation steps. Therein, MATLAB®-routines are used to calculate parameters for a metallurgical model to be used in SYSWELD®, based on a simulated TTT-diagram from JMatPro® and an experimentally determined welding- CCT-diagram of R350HT rail steel. This so established metallurgical model was verified by a simulation of dilatometry tests in SYSWELD® and subsequent quantitative comparison to experimental results. In a final step three more MATLAB®-routines are used to calculate phase fractions, interlamellar spacing and hardness for a practical example. Therefore, measured temperature curves from instrumented flash-butt welding (FBW) experiments of standard rails were used as input. The results of the simulation are compared to real welds' phase fractions and hardness values in the HAZ and showed very good agreement.

Introduction

Due to various reasons – such as increased traffic, higher market shares of high speed trains, a general increase in traveling speeds and axle loads, but also increased safety regulations – the requirements for railways have increased in recent decades [1] und thus have tightened the cost situation. Consequently, the intention of rail operators to extent maintenance intervals and overall lifetime of tracks in order to cut down operation cost is more vital as ever. In answer to this development manufacturers seek to provide rails with improved properties against wear and rolling contact fatigue (RCF) [2], [3]. However, when welding modern rail steel grades undesirable microstructures are formed within the HAZ, which deteriorates the designed properties locally [4], [5]. As a countermeasure in today's common rail welding processes thermal cycles are adjusted to reduce the dimension of this so called soft zone. However with further increasing mechanical properties of newly development rail steel grades also requirement for correspondingly optimized welding processes is given.

Interlamellar spacing is an informative aspect in order to characterize the mechanical properties of pearlitic steels such as strength, hardness and thus wear-resistance [6]–[8]. The pearlitic phase transformation is influenced beside others by the thermal history of the material [9]. Thus, by adapting the thermal cycle during welding also the properties of the weld joint can be controlled.

steel grade		main a	HBW				
acc. to [10]	С	Si	Mn	P max.	S max.	Cr	on running surface
R350HT	0,72- 0,80	0,15- 0,58	0,70- 1,20	0,020	0,025	≤0,15	350- 390

Table 1: Chemical composition and Brinell hardness at running surface of investigated pearlitic rail steel [10].

Work content

The objective of this work was to have a tool to estimate the influence of microstructure changes in the HAZ of R350HT rail steel – s. *Table 1* – on the mechanical properties as a function of the thermal history due to welding. Therefore a simulation model was developed which consists of numerical calculations, but also uses experimental methods for data gathering and validation. It calculates pearlitic phase fractions and the interlamellar spacing, as well as the hardness.

Approach

The thermo-metallurgical numerical simulation was realized by using MATLAB® routines in combination with SYSWELD®. The general approach is schematically depicted in a flow chart in *Fig. 1* and calculation steps are correspondingly described in the following passages.

In the first preparatory step (i) required material and process data are gathered. This is done with the help of:

- Simulation of a TTT-diagram of R350HT rail steel in JMatPro®, based on measured chemical composition and austenitization conditions comparable to welding.
- A welding-CCT-diagram of R350HT rail steel, obtained by dilatometry experiments.
- Instrumented flash-butt welding experiments to capture T(t)-curves (T_{ij}) in the HAZ at the rail head at different distances (points of measurement P_{ii}) from the weld centerline (WCL).

These so retrieved data are than preprocessed to the corresponding format and provided for further deployment.

In the subsequent calculation step (ii) MATLAB®-routine (a) is used in order to determine parameters of the metallurgical model of the type SYSWELD® uses, s. [11]. Johnson-Mehl-Avrami-Kolmogorov (JMAK) type kinetics model for diffusion controlled but non-isothermal transformations, as also described in [12], is used. For martensitic transformations Koistinen-Marburger type model is used [13]. For both, the routine initially calculates parameters based on the data from the simulated TTT-diagram and experimental welding CCT-diagram. Subsequently an iterative algorithm, based on additivity rule, as also described in [14], calculates the final phase fractions P_f of Martensite, Bainite and Pearlite for each cooling rate T_1 . In order to optimize the results the parameter $F(T_1)$ is determined by comparing numerical and experimental results and recomputing P_f at every repetition cycle until sufficient agreement is reached. Finally, all determined parameters are put together to establish the metallurgical database file for SYSWELD®.

In the next step (iii) the accuracy of the model is verified. Therefore, the beforehand conducted dilatometry experiments are simulated using the thermo-metallurgical coupled calculation option of SYSWELD®. Simplified sample geometry and artificially adapted cooling parameters are used. The cooling curves from the experimental welding CCT diagram are accurately reproduced. Phase fractions of Martensite, Bainite and Pearlite are quantitatively compared to the experimental results in order to verify the established metallurgical model.



Fig. 1 Schematic flow chart of the used calculation approach.

In step (iv) the calculation is finalized by using three more MATLAB® routines. First, routine (b) is fed with two T(t)-curves measured in the HAZ during welding, gathered during experiments in a recently published work [15]. Based on these so defined thermal cycles the metallurgical model established in step (ii) is used to calculate the phase fractions of Martensite, Bainite and Pearlite in distinct points. Subsequently, MATLAB®-routine (c) calculates the interlamellar spacing S of the computed pearlitic phase fraction and corresponding $T_{(t)}$ -curve, respectively the corresponding cooling rate. The calculation of S is based on an empirical expression proposed in [16] and depicted in *Equation 1*. Thereafter the interlamellar spacing in eutectoid steel can be predicted for isothermal transformation as a function of specific alloying elements' content, the temperature T, at which pearlite

formation happens, and the eutectoid temperature T_E . In order to take into consideration the non-isothermal formation of the Pearlite during welding, a weighted average of the interlamellar spacing is calculated subsequently for each cooling rate $\overline{S}(T_1)$ based on *Equation 2* subsequently. It integrates the interlamellar spacing S(T) over the derivatives of formed phase fractions dP at the corresponding calculation step for a given cooling rate and finally sets it in relation to the final phase fraction P_f. Finally MATLAB®-routine (d) calculates the hardness based on an empirically determined equation proposed in literature [6], s. *Equation 3*.

Equation 1 [16]:

$$\log(S) = -2.2358 + 0.09863 \times Mn - 0.05427 \times Cr + 0.03367 \times Ni - \log\left(\frac{T_{\rm E} - T}{T_{\rm E}}\right)$$

Equation 2:
$$\overline{S} = \frac{1}{P_{\rm f}} \int_{0}^{P_{\rm f}} S(T) dP$$

Equation 3 [6]:

Results

rate.

First of all the results of step (iii) from the dilatometry simulation in SYSWELD® are compared in *Fig. 2* to experimental results from the welding CCT-diagram of R350HT. It can be derived that the simulation shows very good agreement to the experimental data for all three relevant phases and in all investigated cooling rate ranges. The calculation of formed phase fractions based on the new metallurigcal model of this work and two experimental T(t)-curves in step (iv) show fully pearlitic transformation in the HAZ. This is in very good agreement with metallography data provided by rail steel manufactrurers [17]. *Table 2* shows the final result for computed interlamellar spacing at two distinct points in the HAZ – represented by their distances from WCL–together with computed hardness. Accordingly, the interlamellar spacing inside the HAZ of FBW rail decreases with increasing distance from the WCL resulting in an increased hardness. This can be understood as a result of the higher cooling rate. For comparison reasons the computed values are converted and compared to values from a literature source [4]. The computed hardness values are in very good agreement to experimental results. Thus, the model is able to very accurately calculate the hardness based on interlamellar spacing as a function of the cooling



Fig. 2. Calculated vs.measured phase fractions as a functions of cooling rates for R350HT rail steel.

 Table 2: Calculated interlamellar spacing and corresponding calculated hardness for 2 exemplary thermal cycles in the HAZ for R350HT 60E1 rail and comparison to experimental values.

distance from weld centerline (WCL) in mm	average cooling rate from 800°C to 500°C	peak temperature in °C	calculated average interlamellar spacing §(Ť) in μm	calculated hardness HV10	HV10 converted to HRC acc. to [18]	experimental HRC of FBW of rails acc. to [4]
1	-0,9321	1355	0,1078	357	36,6	38,5
10	-1,1565	854	0,0809	388	39,5	39

Conclusions

A methodology of combining MATLAB® routines, SYSWELD® and JMatPro®, as well as data from experimental work was developed to implement a multistep thermo-metallurgical simulation of phase transformations in the HAZ during welding of pearlitic rail steel R350HT. With the help of the determined metallurgical model phase fractions and interlamellar spacing was calculated as well as the hardness was calculated for different distances from the WCL in the HAZ at the rail head for a practical example. The comparison of calculated and experimental results showed that very good agreement was obtained. Thus, it was shown that the proposed approach to estimate the hardness in the HAZ by calculating the interlamellar spacing as a function of thermal history in a numerical welding simulation is a very practicable method.

Outlook

In a next step the model will be further extended in order to estimate the softening in the annealed zone of the weld. Therefore additional metallurgical phenomena which are believed to also have influence on the softening in the HAZ of pearlitic rail steel will be studied. Furthermore, additional T(t)-curves at the corresponding locations in the HAZ and proper material parameters are needed. Based on this, an extended approach will be developed and implemented to further enhance the here presented simulation model.

Acknowledgments

K-Project Network of Excellence for Metal JOINing is fostered in the frame of COMET - Competence Centers for Excellent Technologies by BMWFW, BMVIT, FFG, Land Oberösterreich, Land Steiermark, Land Tirol and SFG. The programme COMET is handled by FFG.

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