Modeling of the Mn and S Microsegregation During Continuous Casting of Rail Steel

S. Gerasin, D. Kalisz*
* AGH University of Science and Technology, Faculty of Foundry Engineering, Krakow, Poland
ul. Reymonta 23, 30-059 Kraków, Poland
*Kontakt korespondencyjny: e-mail: dak@agh.edu.pl

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Abstract

The aim of this study was to analyze the process of manganese sulfide formation based on thermodynamics calculation. Both experimental and theoretical analysis methods were used in this work. Computer simulation with the use of non-commercial software was used for the calculation of the process of segregation of manganese and sulfur and MnS non-metallic particles precipitates in liquid steel during solidification of ingot. The curves illustrating the inclusion formation process are presented. MnS inclusions are disposed along grain boundaries in thin layers and have a rounded shape.

Key words: MnS precipitates, segregation, computer simulation, rail steel.

1. Introduction

Non-metallic inclusions are one of the factors negatively influencing the strength of rail steel. The Rolling Contact Fatigue (RCF) is an important factor materials used in railways. The manganese sulfide precipitates are formed during steel solidification as a result of segregation processes on the solidification front. The experiments conducted by Liu [1] revealed that non-metallic inclusions do not deform uniformly during rolling.

Pure MnS precipitates are deformed along the direction of rolling. Multi-component precipitates composed of manganese sulfide deform unlike pure MnS. Manganese sulfur can be surrounded by brittle oxidic phases or may constitute a plastic cover of these phases.

Then in the course of plastic processing the precipitations may be flattened or elongated, which may favor cracks formation in the presence of brittle phases.

The participation of elements making up MnS inclusion is established in the process of refining, which precedes the process of casting. The quality of ingots is a result of operation of two factors: structure and presence of non-metallic inclusions [2]. The chemical composition of an ingot after casting is a result of segregation, i.e. enrichment of liquid steel in some components during solidification, which in turn, depends on the value of their interface partition coefficients. The segregation of liquid steel components and MnS precipitations formation at various solidification rates were calculated with a non-commercial computer program, already used in.

MnS inclusions can be formed only when the value of the equilibrium solubility product is exceeded:

\[ Q_{\text{real}} > Q_{\text{equilibrium}} \cdot a_{\text{MnS}} \]

The dependence of solubility product on temperature for manganese sulfide equals to [3]:

\[ \log Q = -8.627/T + 4.745 \]
The analysis of sulphur and manganese microsegregation during solidification and formation of manganese sulfide was conducted for dendritic crystallization in the conditions of directional heat removal. The secondary arms of dendrites were located vertically and heat was discharged towards their axis. The distance between secondary arms of a dendrite is a function of the cooling rate. The diffusion of solid phase components was accounted for in the calculations [5]. It was assumed for liquid phase that the rate of concentration equalization in this area was very high (the process was almost instantaneous).

The calculation of the microsegregation effect and manganese sulfide formation was performed for rail steel having composition as in Table 1.

### Table 1. Chemical composition of rail steel assumed for calculations / %

<table>
<thead>
<tr>
<th>Steel</th>
<th>C</th>
<th>Mn</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.75</td>
<td>0.93</td>
<td>0.32</td>
<td>0.024</td>
<td>0.016</td>
<td>0.0054</td>
</tr>
</tbody>
</table>

The computer simulation was performed for the cooling rate of 100 K/min; the assumed activity of manganese sulfide equaled to: 0.3; 0.6 for MnS being a component of liquid solution, and 1.0 for pure MnS.

### 3. Results of calculations

The results of calculations of sulphur and manganese microsegregation for rail steel at MnS activity equal to 0.3, 0.6 and 1 are presented in figures 3 and 4.

**Fig. 3.** Microsegregation of sulphur during solidification of rail steel at the cooling rate of 100 K/min

Figure 3 illustrates the course of sulphur concentration changes during solidification of rail steel, which increases from the initial value of 0.016%S to 0.095% for $a_{\text{MnS}} = 1$ and 0.58% for $a_{\text{MnS}}=0.6$. It was observed that the breaking of the sulphur segregation curve existed earlier for the lowest activity of manganese sulfide ($a_{\text{MnS}}=0.3$). This means that the precipitation of sulphur being a component of liquid solution took place earlier than for pure MnS ($a_{\text{MnS}}=1$).
Figure 4 illustrates manganese segregation curves during solidification of rail steel for the cooling rate of 100 K/min. A considerable difference can be observed for the sulphur segregation curves.

The cause of it is mainly the value of the interface partition coefficient $k$, which is much higher for manganese than for sulphur. It was observed for the manganese segregation curves that manganese concentration increased from 0.93 to 1.5 in all variants of MnS activity.

Figures 5 to 7 illustrate the course of real and equilibrium values of the solubility product. In all cases the intersection of curves corresponding to the temperature dependence of equilibrium and real solubility product is indicative of the formation of MnS precipitates.

4. Conclusions

Computer simulations and calculations were performed with the use of own computer program «MnS Precipitations». The obtained results revealed that the segregation of sulphur and manganese and MnS precipitates formation take place in the solidification process. The non-metallic phase of MnS is precipitated more readily when being a component of a liquid solution.

MnS precipitates of varying size and shape can be formed during steel solidification, depending on its chemical composition and cooling rate. This will be conditioned by the thermodynamic conditions of their formation. Their chemical composition is especially important as it will decide about the course of plastic processing processes and potential defects on the surface. The chemical composition of the obtained compounds is also very important because on this basis one can determine further course of casting.

The computer calculation procedure assumed for modeling microsegregation and non-metallic precipitates formation in the
course of ingot solidification used in this work can be useful for monitoring processes in real conditions and creating basis for optimizing conditions of non-metallic phase precipitation.

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References


Modelowanie procesu segregacji
Mn i S podczas odlewania stali szynowej

Streszczenie

W pracy analizowano proces powstawania siarczku manganu w oparciu o obliczenia termodynamiczne. Wyniki przedstawiono w odniesieniu do badań eksperymentalnych. Symulacje komputerowe procesu segregacji manganu i siarki oraz powstawania wydzielin MnS podczas krzepnięcia stali zostały wykonane za pomocą nie komercyjnego programu komputerowego. Rezultaty symulacji komputerowej przedstawiono w postaci wykresów prezentujących segregację składników oraz krzywych obrazujących proces powstawania wydzielin. Wtrącenia MnS są rozmieszczone wzdłuż granic ziaren i mają zaokrąglony kształt.