Kinetic model on manganese sulfide formation during solidification of steel

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During solidification of steel, the enrichments of sulfur and manganese in the residual liquid melt lead to the formation of manganese sulfide. The formation of manganese sulfide influences both casting process and final product quality, such as enhancing the hot ductility and promoting the acicular ferrite formation. In this work, a coupling model of manganese sulfide formation kinetics and microsegregation in steel is proposed. The model is capable to describe the nucleation and growth of manganese sulfide based on the classical nucleation and growth theory. The size and number evolution of the particles are described using the Particle Size Distribution (PSD) and Particle Size Grouping (PSG) methods. For considering collisions of particles, an adjustable parameter was introduced and calibrated using experimental results. With the calibrated parameters, manganese sulfide formation in the samples with different sulfur contents and cooling rates are simulated. Compared with the experimental results, the size distributions of manganese sulfide are well predicted. It shows that the formation of manganese sulfide considerably reduces the sulfur and manganese segregation. Strengthening cooling condition and decreasing the sulfur content are in favor to obtain the fine dispersed particles.

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Preferred Contribution: Poster/Oral

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Introduction

Model description

Experiments

Table 1. Chemical compositions of analyzed steels (wt. %).

<table>
<thead>
<tr>
<th>Samples</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>S</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>0.22</td>
<td>0.03</td>
<td>1.40</td>
<td>0.0060</td>
<td>0.0055</td>
</tr>
<tr>
<td>S2</td>
<td>0.21</td>
<td>0.04</td>
<td>1.50</td>
<td>0.0021</td>
<td>0.0036</td>
</tr>
</tbody>
</table>

Calibration

<table>
<thead>
<tr>
<th>Sources</th>
<th>Collision factor (f)</th>
<th>Mean diameter (µm)</th>
<th>Number (mm⁻³)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.48</td>
<td>2.12×10⁶</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.49</td>
<td>1.83×10⁶</td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>0.60</td>
<td>9.67×10⁵</td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>0.67</td>
<td>6.78×10⁵</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>0.71</td>
<td>5.34×10⁵</td>
<td></td>
</tr>
<tr>
<td>Experiment</td>
<td>0.54-0.65</td>
<td>5.05-6.22×10⁵</td>
<td></td>
</tr>
</tbody>
</table>
Simulated and experimental results

**Number density (mm$^{-3}$)**

- **Diameter (µm)**: 0.0 0.5 1.0 1.5 2.0 2.5
- **Number density**: 0.0 5.0x10$^4$ 1.0x10$^5$ 1.5x10$^5$ 2.0x10$^5$ 2.5x10$^5$ 3.0x10$^5$
- **Number density (mm$^{-3}$)**

**Measured**

**Calculated**

**Diameter (µm)**

- **Diameter (µm)**: 0.0 0.5 1.0 1.5 2.0 2.5
- **Number density**: 0.0 5.0x10$^4$ 1.0x10$^5$ 1.5x10$^5$ 2.0x10$^5$ 2.5x10$^5$ 3.0x10$^5$
- **Number density (mm$^{-3}$)**

**Measured**

**Calculated**

**B: 13.5**

**A: 25.4**

**S1: Cooling rate (K$s^{-1}$)**

**Measured**

**Calculated**

**S2(C): 20**

**S1(A): 60**

**Concentrations in liquid (%)**

**Solid fraction**

**A: 25.4**

**B: 13.5**

**Mn**

**S**

**MnS**

**Concentrations in liquid (%)**

**Solid fraction**

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**B: 13.5**

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**S**

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