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Formation mechanism of channel segregation in carbon steels by inclusion flotation: X-ray microtomography characterization and multi-phase flow modeling

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ABSTRACT

Recent experimental dissections of steel ingots and multi-scale simulations have led to the discovery of a potential driving force for channel segregation: the flotation of oxide-based inclusion (D. Li et al., Nat. Commun. 5:5572 (2014)). Further experimental analysis and numerical modeling are necessary to clarify this mechanism in detail. In this work, the inclusions in a carbon steel ingot that exhibits severe channel segregations were characterized by the 3D X-ray microtomography, which revealed a significant enrichment and growth of inclusions in the channels. Based on above microtomography characterization, a 2D macrosegregation model encompassing the inclusion flotation was established. In the model, the motions of solid inclusions and liquid were described using the multi-phase flow scheme within the Euler-Lagrange framework. The benchmark simulations showed that sufficient inclusion populations with appropriate sizes are capable of altering the local flow patterns and destabilize the mushy zone, initiating the subsequent channel segregation. The continuous interplay between melt convection, inclusion flotation and solidification eventually causes the formation of macroscale channel. The predicted sizes and volume fraction of inclusions that are able to trigger the channel segregation effectively are consistent with the data obtained via microtomography characterization. The macrosegregation model was then applied to predict the channel segregations in an industrial carbon steel ingot. A rather good agreement of A-segregates was achieved between the simulation and the dissected ingot.

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1. Introduction

As a typical kind of channel segregation, A-segregates are the most prevalent and notorious type of macrosegregation in casting steels and present as one of the main challenges facing the steel-maker at all stages of fabrication. They appear as the linear regions of chemical and even microstructure inhomogeneities, and form along a direction that is roughly antiparallel to gravity during so-lidification [1]. To understand and control their formation during solidification, a large amount of effort has been exerted for decades, including the theoretical analysis using Rayleigh number [2], experimental analysis using model alloys [3,4], numerical simulations based on the continuum model [5], the multi-phase/multi-scale model [6–11], the 3D microscale solidification model [12,13] and so on. With all of these studies, it is generally concluded that

* Corresponding author. E-mail address: chenyun@imr.ac.cn (Y. Chen). the thermosolutal convection induced by the density difference is the origin of channel segregation. In steels, accordingly, it is the sufficient buoyant force of the light interdendritic solute-enriched melt and the hotter liquid at the upper regions of mushy zone that jointly destabilize the mushy zone and cause the formation of A-segregates [2].

Nevertheless, it is frustrating that most of the simulations based on such a mechanism often failed to exactly predict the number, shape and locations of A-segregates in the industrial steel ingots. The failure is normally ascribed to the inputs of complex macrosegregation models, such as the coarsened computing grid, the uncertain material parameters and the simplification of auxiliary models [8,14–16]. However, recent investigations on macrosegregation in steels through a series of dissected steel ingots and multi-scale calculations which were performed by Li et al. [17] and then were highlighted by Plummer [18], have revealed a new mechanism of channel segregation formation. In the widely used steels with a high content of oxygen, they found that the flotation of light oxide-based inclusions is responsible for the formation of

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Nomenclature C_h, C_s, C liquid, solid and mixture concentrations (wt.%) h_s, h_h, H ,solid, liquid and mixture enthalpies (J kg ⁻¹) ΔH latent heat (J kg ⁻¹) $C^{'}$ reference concentration (wt.%) T^{*} reference temperature (K) u_p, v_p particle velocity components in x and y direction	nparticle numbermliquidus slope (K wt.%^{-1}) $T_h T_m$ liquidus of steel and melting point of solvent (K) d_s secondary dendritic arm spacing (μ m)kpartition coefficient f_p area fraction of inclusion β_T thermal expansion coefficient (K^{-1})as (m β_C compositional expansion coefficient (wt.%^{-1})Rerelative Revnolds number
<i>u</i> , <i>v</i> liquid velocity components in <i>x</i> and <i>y</i> direction s^{-1}) <i>ua_p</i> , <i>va_p</i> average particle velocities in <i>x</i> and <i>y</i> directions <i>f</i> _s , <i>f</i> _l fractions of solid and liquid	(m ρ, ρ_p densities of steel and inclusion (kg m ⁻³) P pressure (pa) $n s^{-1}$) d_p particle diameter (m) t time (s)
$ \vec{U} \qquad \text{superficial velocity (m s^{-1})} \\ \vec{U_l} \qquad \text{liquid velocity (m s^{-1})} \\ \lambda \qquad \text{heat conductivity (W m^{-1} K^{-1})} \\ c_p \qquad \text{specific heat (J kg^{-1} K^{-1})} \\ \mu_l \qquad \text{liquid dynamic viscosity (pa s)} \\ \vec{g} \qquad \text{acceleration of gravity (m s^{-2})} $	Subscripts and Superscriptss, lsolid and liquid phasespinclusion particleithe ith inclusion particlesl, plinteraction between liquid and solid or inclusion

channel segregation. The sufficient volume fraction of oxide-based inclusions with appropriate sizes can enhance the local flow, destabilize the mushy zone, and finally dominate the channel segregation formation. Obviously, this mechanism is quite different from the previous recognition of the driving force of channel segregation in solidifying steels.

Therefore, to address the effect of inclusions on channel segregation formation in depth, it is of great significance to establish a macrosegregation model incorporating the flow dynamics of inclusions. The previous multi-phase macrosegregation models that couple the settlement of dendritic or globular crystals are within the Euler–Euler category. Nevertheless, the light inclusion particles are different from these crystals, which are distributed in the melt dispersively and drag the surrounding melt moving together when they are floating upwards. Hence, their moving kinetics should be described within the Lagrange framework to accurately track the motion of each inclusion particle during solidification, as well as the dragging effect [19]. Actually, with the Lagrange approach a wide range of dispersed two-phase flow problems in metallurgy processes were investigated [20-24]. Based on the commonly used dispersed phase model for multiphase flow [20-24], an Euler-Lagrange flow model is incorporated into the conventional macrosegregation model in the current study.

In addition, the detailed examinations of the distributions and features of inclusions in the segregated channels can help further our understanding of the inclusion flotation mechanism in steels, as well as validate the simulation results. Hence, the inclusions in the A-segregate strips are characterized and determined carefully. Here, the three-dimensional X-ray microtomography technique [25,26] is applied to analyze the size, number and volume fraction of inclusions and pores. The theoretical basis of X-ray microtomography is the absorption contrasts between inclusions, pores and matrix. Compared with the conventional destructive metallographic techniques, the microtomography results are considered more reliable [27] because the drawbacks of the grinding and polishing processes during the preparation of samples can be ignored. More importantly, the distribution and morphology of inclusions in three-dimensional space can be visualized.

In this paper, the quantitative characterization of inclusions in carbon steels was first performed using the X-ray microtomography technique. A dispersed phase model that describes the motion of particles was then incorporated into the 2D continuum macrosegregation model. The effect of inclusions on the channel segregation in a benchmark cavity was analyzed in detail based on the developed model. Finally, the model was used to simulate the macrosegregation in a 500-kg 1045 steel ingot, particularly to reproduce the A-segregates that were observed in the dissected section.

2. 3D microtomography characterization of inclusions in the dissected 500-kg 1045 steel ingot

2.1. Experimental procedures

A 500-kg cylinder ingot of 1045 steel was first prepared and synthesized in a sand mould. The chemical compositions (wt.%) of the ingot are: C 0.47, Si 0.26, Mn 0.54, S 0.016, P 0.020, T.O (total oxygen content) 0.0056 and Fe balanced. The ingot dimensions and shape are illustrated in Fig. 1a. An insulation sleeve with a thickness of 40 mm was inserted at the circumference of the hot top sand mould. The top of the riser was covered by a 100 mm thick layer of covering flux. The steel was melted at 1873 K by an induction furnace and poured at 1823 K in the atmosphere after the Aldeoxidation process. The solidified as-cast ingot was cut in half along the longitudinal axis. After being ground and polished, the dissected center surface was etched in 5% aqueous nitric acid solution. Fig. 1b shows the final etched macrostructure of ingot body of which the top riser was cut away. The contrast generated by the etch in the optical microscopy is caused jointly by the contents of carbon, inclusions and even cavities. The darker positions always correspond to higher concentrations of them. With this contrast, severe segregated channels (A-segregates) can be clearly observed on both sides of the ingot body. Evidently, within the zones of Asegregates, besides the obvious positive carbon segregation, inclusions or even cavities can be observed to be converging together [17].

Then, the lab-based Xradia Versa XRM-500 system was used for 3D quantitative characterization of inclusions [28]. The resolution of the system can be as high as 0.7 μ m. Three cylindrical samples with a dimension of Φ 3 mm \times 25 mm were cut from the non-channel zone, the bottom and body of the chosen segregated channel of the sectioned 1045 steel ingot as shown in Fig. 1b. The

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