GROWTH MODEL OF BI-COMPONENT OXIDE NONMETALLIC INCLUSIONS IN LIQUID STEEL

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Abstract

Modeling the growth of nonmetallic inclusions can be realized in a number of ways. Authors worked out their own mathematical model for calculating the increase of nonmetallic phase in liquid steel. The spherical shape of the particle and independent increase of inclusions were assumed; the participation of the diffusion of the component dissolved in the liquid phase was ignored. The mixing of metallic bath with the neutral gas of high intensity was assumed as the initial state. The simulations were performed both for the increase of a precipitate composed of two oxides: Al_2O_3 and Y_2O_3. Assumption was made that each of the oxides grows in the precipitate area of the precipitate of the same chemical composition. It was assumed that in a metallic bath there are 1 000 000 nuclei, each 5 µm. The calculations were performed for the initial oxygen concentration in steel of 0.05 % assuming two variants of aluminum and yttrium contents in the metallic bath: 0.06 % Al, 0.09 % Y - variant 1 and 0.09 % Al and 0.06 % Y - variant 2. The obtained results were presented in the form of plots of oxides increase in a function of time and change of O, Y and Al content in liquid bath in the precipitation process.

Keywords: Nonmetallic inclusions, precipitations growth, Al_2O_3, Y_2O_3, numerical modelling

INTRODUCTION

Nonmetallic inclusions generated in the process of refining liquid metallic bath are nonhomogeneous; they are a mixture of two oxides or oxides and sulfides. These compounds are a result of introducing metals and iron alloys as complex deoxidants, as a consequence of which liquid or liquid/solid nonmetallic phase is formed. Silicon, manganese and aluminum usually play the role of deoxidants in steel, therefore a liquid phase containing their oxides, and also iron oxide, can be formed. Upon adding yttrium to steel, Y - O, Y - S compounds are generated, with stable Y_2O_3 and Y_2S_3 Y_2O_2S inclusions can be also formed [1,2]. Information about the whole population of inclusions can be hardly verified and its chemical composition and physical form depend on the phase of the refining process. When the oxygen considerably exceeds the deoxidant and simultaneously the concentration of this component in the metallurgical reactor is nonhomogeneous, complex nuclei are very likely to be generated. This will be also favored by locally nonuniform concentration of the deoxidant. The particle growth can be modeled in a number of ways. In all cases the particles are assumed to have a spherical shape, stationary diffusion and independent growth of the inclusions [3-10]. The problem of growth of multicomponent nuclei has been already analyzed in many works [11-15], where the growth of single- and two-component deoxidization products were analyzed with the use of the population balance model [5,12,15].

1. GROWTH MODEL FOR TWO-COMPONENT OXIDE NONMETALLIC INCLUSIONS

Authors of this paper present their own concept of growth of two-component oxide inclusions, concentrating on the generation of this phase after introducing aluminum and yttrium to steel. Refining processes are associated with the use of high mixing energies, therefore the role of diffusion of reagents to the reaction zone was neglected. It was assumed that the system is ideally homogeneous as far as its chemical composition goes, and that each inclusion grows on its own surface, i.e. yttrium oxide only grows on the surface of Y_2O_3, and aluminum oxide only on the surface of Al_2O_3. In this case it was established that the growth rate of a particle solely depends on the concentration of all three components, i.e. Y, Al and O. The nucleus was assumed to consist of *n1* mole oxide 1 and *n2* mole of oxide 2. Coefficient *Aij* (1) depends on the value of oversaturation defined as a difference between actual and equilibrium concentration of oxygen in steel and reaction rate constant *kij*. It was assumed that *Aij > 0*, i.e. deficiency of any of the components terminates the growth of a given inclusion without leading to its dissolving. This means that the end of the growth is determined by the oxygen concentration.

$$A_{ij} = k_{ij} : \quad S_i^{\alpha_i} = k_{ij}\left(c_{[0]}(t) - c_{[0]}^{(i)}\right)^{\alpha_i} \tag{1}$$

where: A_{ij} - coefficient (depends on oxygen concentration), S_i - oversaturation, β - mass penetration parameter (assumed β = 1), α - order of reaction (assumed α=1), k_{ij} - velocity constant, depends on the type of oxide „i" and surface „j".

Hence the increase of amount of oxide 1 and oxide 2 in the two-component nucleus totals to [4, 6]:

$$dn_i / dt = \left(A_{i1} \cdot n_1 + A_{i2} \cdot n_2\right) / r^{\beta} \tag{2}$$

where: i = 1, 2; β is assumed to be equal 1.

Under those assumptions following set of Ordinary Differential Equation is obtained:

$$\frac{dn_1}{dt} = \frac{A_{11} n_1 + A_{12} n_2}{r} \tag{3}$$

$$\frac{dn_2}{dt} = \frac{A_{21} \cdot n_1 + A_{22} \cdot n_2}{r} \tag{4}$$

where: n_1- number of moles in oxide 1, n_2- number of moles in oxide 2, A_{i1}- coefficient depending on oxygen concentration (for oxide 1), A_{i2}- coefficient depending on oxygen concentration (for oxide 2).

Radius of growing nucleus can be calculated with equation:

$$\frac{4}{3} \cdot \pi \cdot r^3 = \sum_{i=1}^{2} \nu_i \cdot n_i \tag{5}$$

where: r- radius of nucleus [cm], v- molar volume [cm^3/mole].

Hence:

$$r = \sqrt[3]{\frac{\frac{3}{4} \cdot \frac{1}{\pi} \cdot \left(\upsilon_1 \cdot n_1 + \upsilon_2 \cdot n_2\right)}{z}} \tag{6}$$

where: v_1- molar volume of oxide 1 [cm^3/mole],

v_2- molar volume of oxide 2 [cm^3/mole].

The growth of a nucleus results in a change of chemical composition expressed with a molar fraction of oxide 1 - x1.

$$x_1 = \frac{n_1}{n_1 + n_2} \tag{7}$$

During nucleation decrease of Al, O and Y solutes mass in liquid is calculated and it influence the growing oxide mass.

2. RESULTS OF GROWTH CALCULATION FOR TWO-COMPONENT INCLUSIONS AL_2O_3 - Y_2O_3

The results of calculations of growth of two-component nonmetallic inclusions were realized with a mathematical model and computer program prepared for a nucleus composed of oxides: Al_2O_3 and Y_2O_3. The following assumptions were made for the calculations:

2.1. Variant 1

Number of nuclei in 1 cm^3 steel: 10^6, aluminum and yttrium content in steel: Al = 0.06 %, Y = 0.09 %, oxygen content: O = 500 ppm, equilibrium concentration of oxygen O = 0.009 %, coefficient β = 1. Aluminum and yttrium are introduced at the end of the process of steel refining, when the oxygen content was low. The initial oxygen content in steel was purposefully overestimated in calculations (500 ppm), to highlight the results. **Figures 1 - 3** illustrate the results of calculation of growth of two-component nuclei Al_2O_3 - Y_2O_3 of initial radius 5 μm.

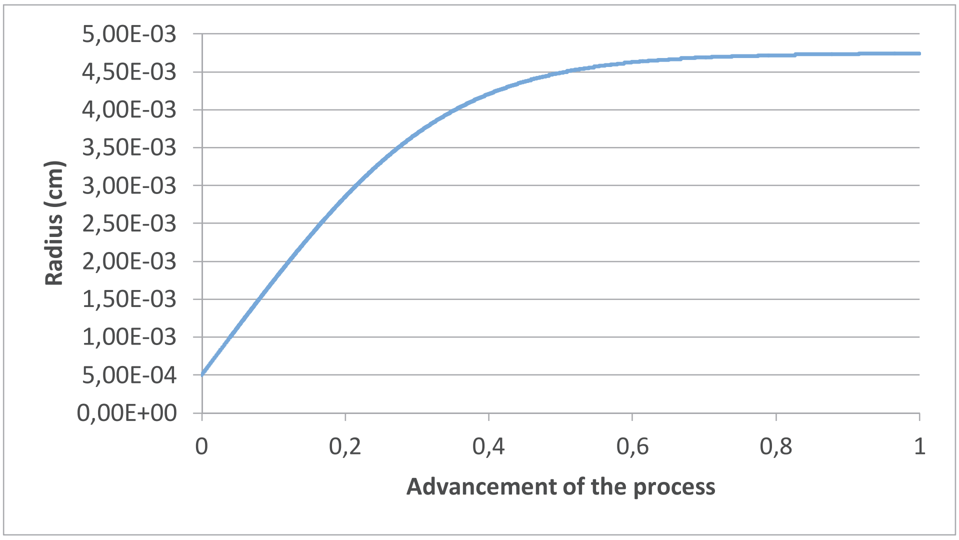

Figure 1 Increase of radius of nucleus (initial radius r_0 = 5 μm)

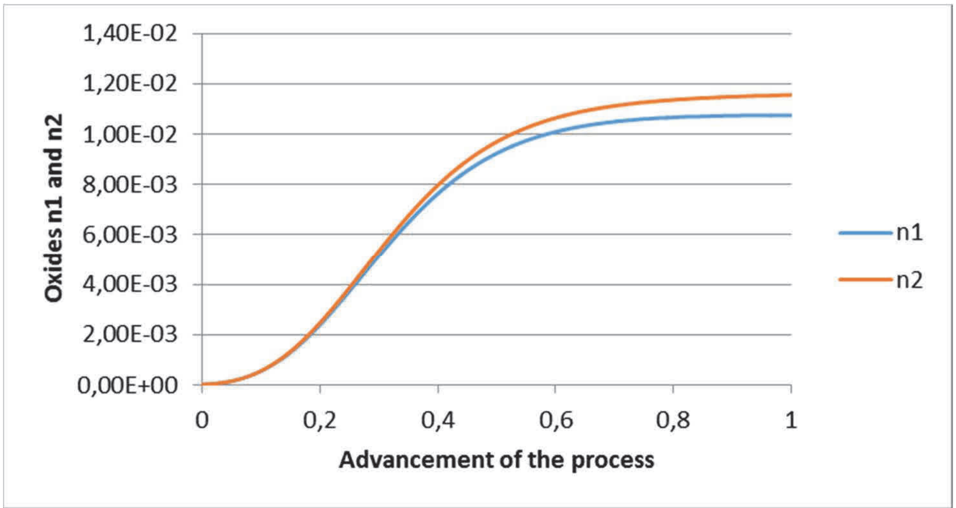

Figure 2 Increase of two-component nuclei of oxides n1 (Al_2O_3) [mole] and n2 (Y_2O_3) [mole] (for r_0 = 5 μm)

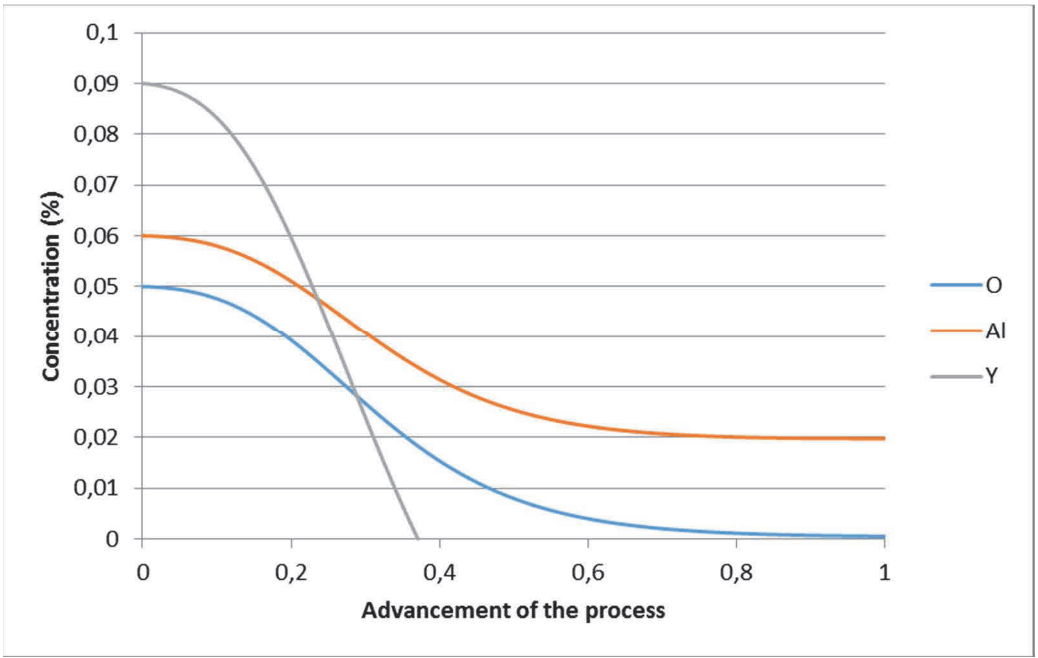

Figure 3 Change of concentration of components in the course of growth of two-component nucleus Al_2O_3 Y_2O_3 (for r_0 = 5 μm) concentration

2.2. Variant 2

Number of nuclei in 1 cm^3 steel: 10^6, aluminum and yttrium content in steel: Al = 0.09 %, Y = 0.06 %, oxygen content: O = 500 ppm, equilibrium concentration of oxygen O = 0.009 %, coefficient β = 1.

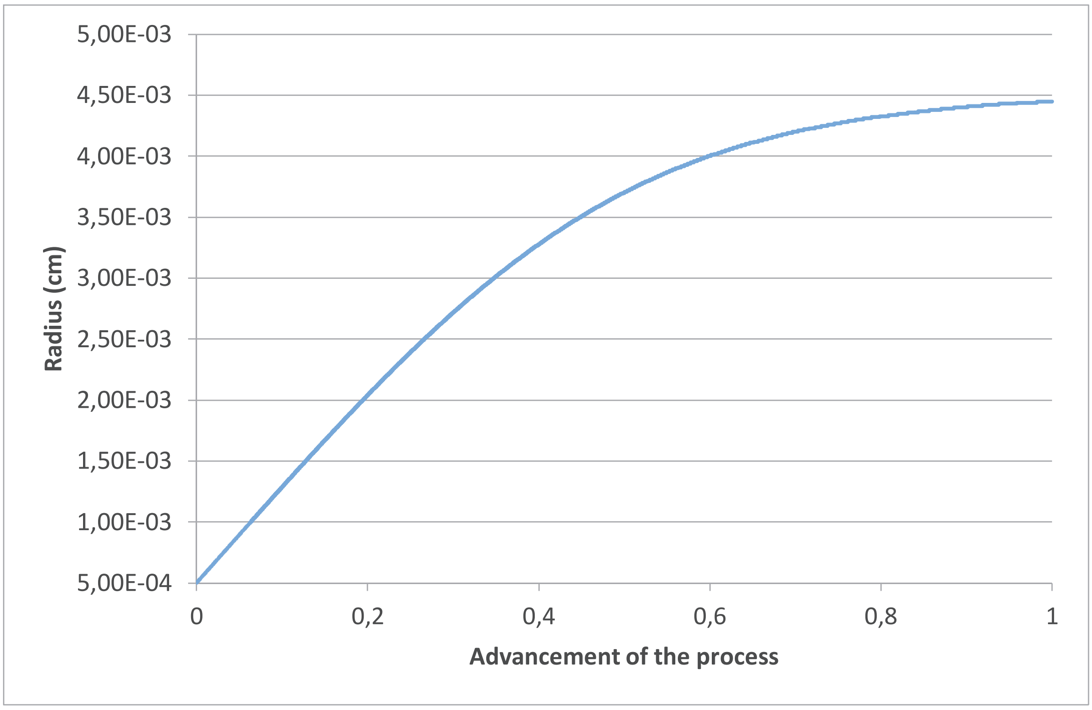

Figure 4 Increase of radius of nucleus (initial radius r_0 = 5 μm)

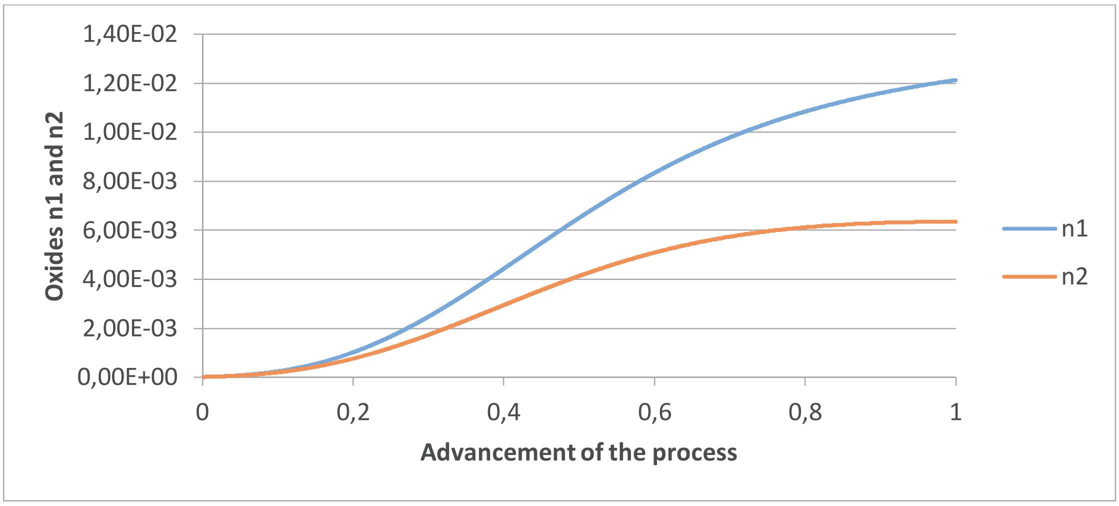

Figure 5 Increase of two-component nuclei of oxides n1(Al_2O_3) [mole] and n2 (Y_2O_3) [mole] (for r_0 = 5 μm)

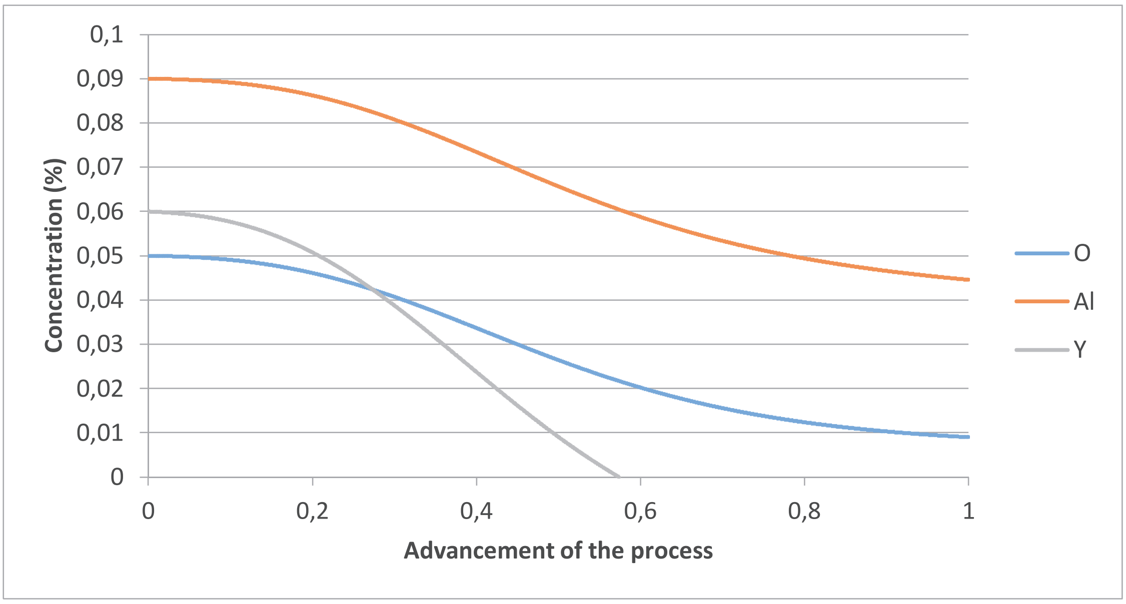

Figure 6 Change of concentration of components in the course of growth of two-component nucleus Al_2O_3 Y_2O_3 (for r_0 = 5 μm)

In the first variant yttrium is the deficient element. The Al content in liquid steel changes from the initial value of 0.06 % to 0.02 % for nucleus of initial radius 5 micrometer. At about 0.35 stage of the process, yttrium content is close to the equilibrium oxygen content (**Figure 3**). The double oxide inclusion content most rapidly increases to about half of the process; in this phase the increase of Al_2O_3 content is almost identical as the increase of Y_2O_3, as illustrated by the coinciding lines n1 and n2 [mole] (**Figure 2**). Further in the process the oxides' increase is rather small.

In variant 2 it is also yttrium which is deficient. The Al content in liquid steel changes from 0.09 % to about 0.055 %. The increase of inclusion growth is mainly associated with the production of aluminum oxide. The increase plots of oxides n1 and n2 (**Figure 5**) slightly differ. At about 0.7 stage of the process the Y_2O_3 in mole increase is minimum, while the Al_2O_3 in mole increase is observed over the entire process, till its end. As compared to variant 1 there is also obtained a considerably higher final oxygen content in steel, which is a result of deficiency of a stronger deoxidant (Y).

3. CONCLUSION

The chemical composition of a double inclusion Al_2O_3 - Y_2O_3 of radius 5 µm depends on the oxide and deoxidants content in liquid steel. Yttrium belongs to strong deoxidants and its deoxidizing ability is much stronger than that of aluminum, therefore yttrium content will mainly condition the character of the growth of the inclusion, its chemical composition and final oxygen content in the metal bath. In variant 1 the growth of the nucleus generates an inclusion which molar composition is about 50 % of Al_2O_3 and 50 % of Y_2O_3. In conditions corresponding to variant 2 the Al_2O_3 mole content in the inclusion exceeds the amount of produced Y_2O_3

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