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Modeling of Precipitate Oxide and Sulfide Inclusions Formation in Liquid Steel

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Abstract

The behaviour of non-metallic inclusions MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O3,Y_2S_3 in liquid steel were modelled in commercial software FactSage. It allowed for calculating and designing diagrams of dependence of inclusions formation from the concentration of yttrium in determined limits of aluminium and oxygen. As a result, the influence of the increasing yttrium concentration on the precipitations of oxide and sulfide inclusions is observed. The behavior of precipitation the another analyzed oxides and sulfides is also observed in liquid steel, giving a full composition in non-metallic inclusions, formatted in specified conditions.The amounts of mass fractions of Y_2O_3 and Y_2S_3 are increasing at the growing Y in liquid steel, which shows the active formation of these inclusions.

Keywords: Yttrium; Non-metallic inclusions; Oxides; Sulfides; FactSage.

1. Introduction

Nowadays the qualitative requirements of construction materials have considerably raised, therefore modern metallurgists focus not only on the content of sulfur, phosphorus and gases in steel, but also on the content, form, distribution and size of non-metallic inclusions. The nonmetallic inclusions can be divided into sulphidic, oxidic and oxisulfidic. The latter are formed by dissolution of the remaining components and are a result of refining processes taking place beyond the furnace, i.e. mainly deoxidization and supplementation of the chemical composition. Such inclusions have a negative impact as they lower the strength and resistance to corrosion. Nonmetallic inclusions behave differently in local processes, significantly influence the origin of the centers of crystallization and formation of grains in steel. The perspective direction of modifying nonmetallic inclusions is the use of rare-earth metals and their combinations.

In this context authors of this paper carried out the modelling and further calculation of interaction of oxygen and sulfur with yttrium in metal. Yttrium actively reacts, firstly with oxygen and sulfur, forming complex oxide of type Y_2O_3 and Y_2S_3 sulfides of globular form.

The calculation of non-metallic inclusions in liquid steel was executed with the use of commercial software FACTSAGE [1]. Attention was also paid to the next formations of non-metallic inclusions in liquid steel: MnS, MnO, Al_2O_3, SiO_2, FeS.

For determining the parameters of interaction of inclusions with oxygen and sulfur it is necessary to know a constant of balance of deoxidization in metal [2-6].

The constant of balance for MnS inclusion in solid phase:

$$Mn+S=MnS \quad (1)$$

$$logK= -8627/T+4.745(s) \quad (2)$$

The constant of balance for MnO in liquid phase:

$$Mn+O=MnO \quad (3)$$

$$logK= 16820/T-7.79(l) \quad (4)$$

The constant of balance for Al_2O_3 in liquid phase:

$$2Al+3O=Al_2O_3 \quad (5)$$

$logK= 64000/T-20.57(l)$ (6)

The constant of balance for SiO_2 inclusion in liquid and solid phases:

$Si+2O=SiO_2$ (7)

$logK= -30000/T+11.40(s)$ (8)

$logK= 30720/T-11.78(l)$ (9)

The constant of balance for FeS in liquid and solid phases:

$Fe+S=FeS$ (10)

$logK= 339/T+2.57(l)$ (11)

$logK= -1376/T+3.74(s)$ (12)

The constant of balance for Y_2O_3 inclusion in liquid and solid phases:

$2Y+3O= Y_2O_3$ (13)

$lgK= -67028/T+20.19(l)$ (14)

$lgK= -71400/T+21.81(s)$ (15)

The constant of balance for Y_2S_3:

$2Y+3S=Y_2S_3$ (16)

$lgK= -61190/T+23.10(s)$ (17)

2. Modelling and calculation

For modelling the behavior of non-metallic inclusions we used another chemical composition of steel:

Table 1. The chemical composition of applied steel

C	Mn	Si	P	Cr	Ni	N	S
0.054	0.05	0.23	0.007	0.05	0.03	0.005	0.01

We were also interested in the use of components at the following limits: Y= 0.02(0.01, 0.005) %, O= 0.03(0.0005) % and Al= 0.02(0.015, 0.01, and 0.005) %.

Data that we got as a result of modelling allowed for the calculation and designing figures of dependence (Fig.1-8)

Fig.1-4. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y in steel with high concentration of oxygen.

Fig.5-8. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y in steel with low concentration of oxygen.

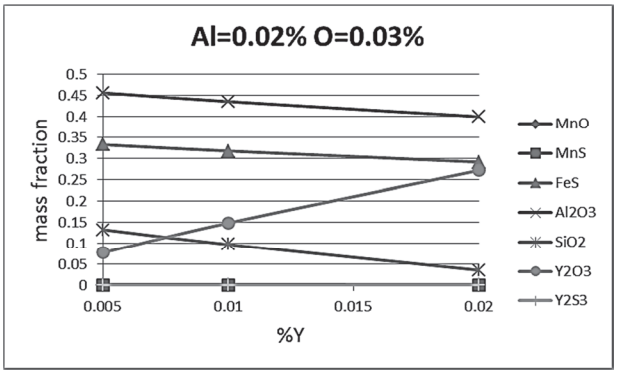

Fig. 1. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.02% and O= 0.03%

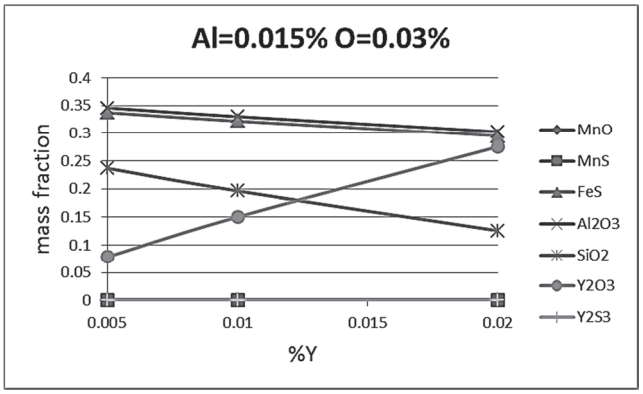

Fig. 2. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.015% and O= 0.03%

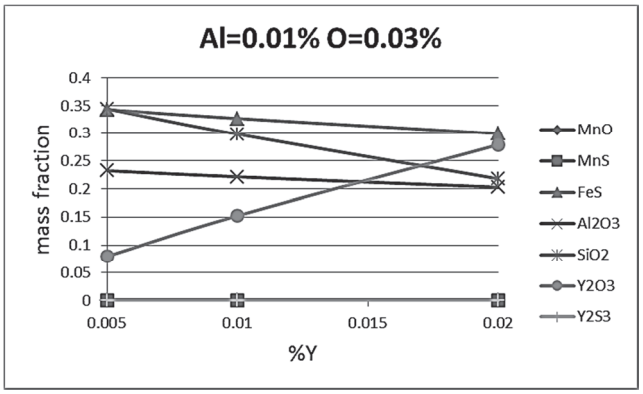

Fig. 3. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.01% and O= 0.03%

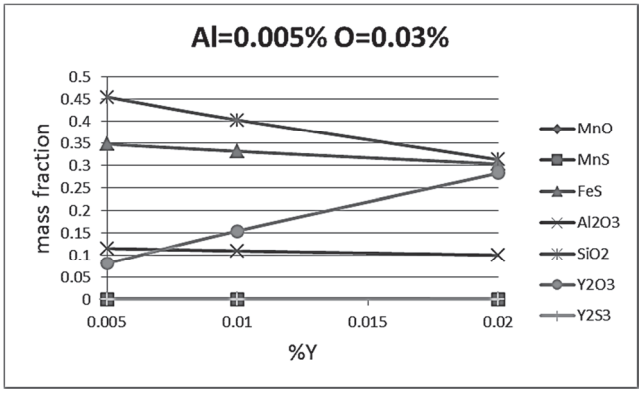

Fig. 4. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.005% and O= 0.03%

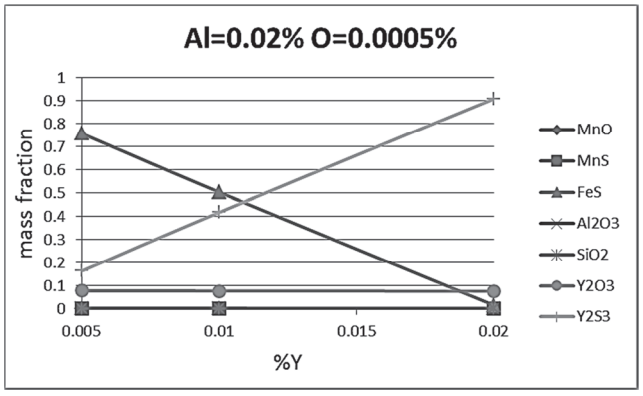

Fig. 5. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.02% and O= 0.0005%

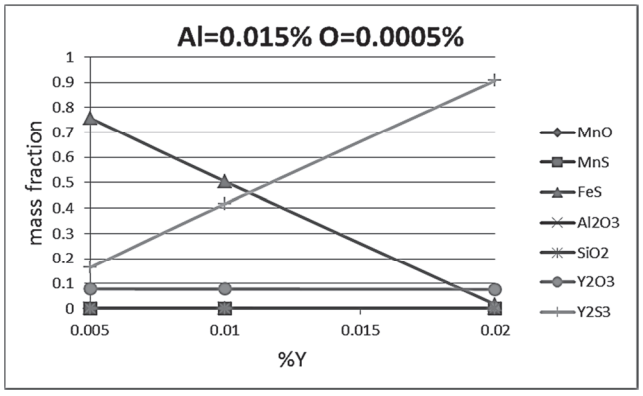

Fig. 6. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.015% and O= 0.0005%

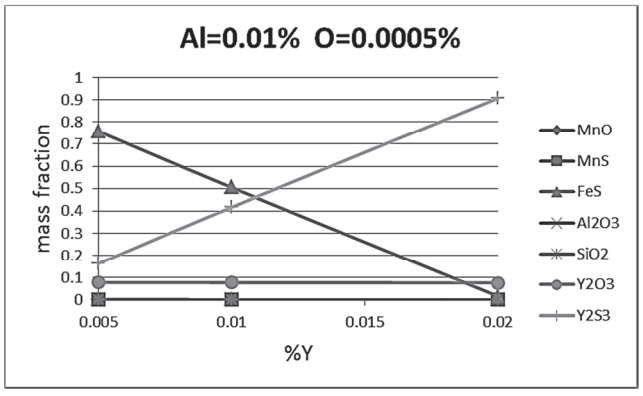

Fig. 7. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.01% and O= 0.0005%

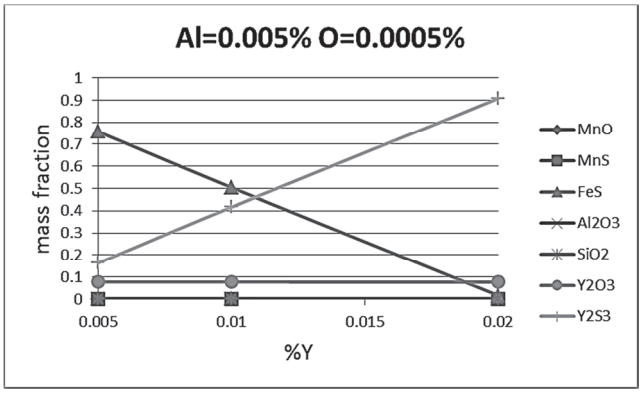

Fig. 8. Diagrams of dependence of non-metallic inclusions (MnO, MnS, FeS, Al_2O_3, SiO_2, Y_2O_3,Y_2S_3) formation from %Y with Al= 0.005% and O= 0.0005%

3. Results and discussion

For determining the precipitation of oxide and sulphide inclusions in liquid steel, the received data were modelled and calculated. The results of research are plots of non-metallic inclusions formation in a function of yttrium concentration. Therefore, we can observe the formation of inclusion for a different percent concentration of aluminium and oxygen in liquid steel. In figures 1-4 the O= 0.03%, and Al changes from 0.005% to 0.02%.

The analysis of the first diagram reveals that with the increasing yttrium concentration to 0.02% the mass fraction of Y_2O_3 actively formats. The diagram of Y_2O_3 is increasing from 0.07 mass fraction at Y= 0.005% to 0.3 at 0.02% of attached yttrium. The concentration of FeS is decreasing from 0.33 mass fraction at Y= 0.005% to 0.29 at Y= 0.02%.The Al_2O_3 inclusion is decreasing from 0.45 to 0.4.The SiO_2 diagram is decreasing from 0.15 at Y= 0.05% to 0.04 mass fraction.

On the fourth figure another situation is observed, i.e. with the decreasing concentration of aluminum from 0.02% to 0.005% the Al_2O_3 is equal to 0.012 at Y= 0.05% and 0.01 at Y= 0.02%.At the same time, the diagram of SiO_2 is equal to 0.45 at Y= 0.05% and 0.3 mass fraction at Y= 0.02%.

In figures 5-8 the concentration of oxygen is equal to 0.0005%, and aluminum limit are the same from 0.005% to 0.02%. In this case another behavior is observed.

First of all, the diagram of Y_2S_3 is increasing from 0.15 at Y= 0.005% to 0.9 at Y= 0.02%. The inclusion FeS is decreasing from 0.75 at Y= 0.005% to 0.0 mass fraction at 0.02% of yttrium. Concentration of Y_2O_3 is equal to 0.1 and does not change during increasing %Y. There are not formatting following oxide and sulfide inclusions: MnO, MnS, Al_2O_3, SiO_2.

4. Conclusions

The amount of mass fraction of Y_2O_3 is increasing at the increasing %Y in liquid steel which shows the active formation of

this oxide. On the other hand, the amount of other oxides (Al_2O_3, SiO_2) in the analyzed steel is decreasing.
Also, the aluminum level has an influence on the formation of Al_2O_3, SiO_2 inclusions, and when the concentration of Al is equal to 0.02% the mass fraction of Al_2O_3 stays in the range of 0.45-0.40. But when the concentration of Al is equal to 0.005% the mass fraction of SiO_2 is in the range of 0.45-0.35.

From the diagrams we can see that yttrium actively reacts with oxygen, because it has high deoxidization ability. And only then it reacts with sulphur, formatting the Y_2S_3 inclusion.

When the %O in liquid steel is low and consists of 0.0005% the mass fraction of yttrium is actively increasing from 0.18 to 0.9, instead of it the mass fraction of FeS is decreasing and at Y= 0.02% is equal to 0. This shows us the high desulfurizing ability of yttrium in specified conditions of aluminium, oxygen and yttrium concentrations in liquid steel.

Acknowledgements

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