

A numerical analysis of inverted V-segregation and its dependency on alloy properties

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Abstract. We ran a numerical simulation to investigate the effect of liquidus slope on the formation of inverted V-segregation in laterally solidified ingots of a virtual Fe-based binary-alloy system. The criterion used in this research is based on Suzuki's criterion. Our criterion assumed that inverted V-segregation zones form when the product of the solidification velocity and the cooling rate is below a critical value which depends on the alloy system. We studied the change in the critical value caused by the density and the liquidus slope of added element X. When different elements of varying densities were added, the results were in line with previous experimental results where large density difference causes increased formation of inverted V-segregation. Finally, the effect of the liquidus slope on the formation of the inverted V-segregation was studied. With a decrease in the liquidus slope, the critical value increased and inverted V-segregation tended to form. Furthermore, the streaks formed were more highly concentrated and sharper, and the channel population increased when the solidification temperature range was narrow.

1. Introduction

Thermo-solutal convection during alloy solidification transports concentrated liquid which causes microsegregation in the mushy zone. Subsequently, various types of macrosegregation form in the ingot. Inverted-V segregation is a macrosegregation that can be observed as a string-shaped region where added elements concentrate. Depending on the alloy system, unexpected phases such as intermetallic compound precipitates and fine porosity forms in the inverted-V segregation. It is hard to eliminate local concentration and precipitation of unexpected phases in the segregation region by forging and heat treatment. Hence the segregation region causes a reduction of ingot and product quality. One effectual countermeasure is to solidify the ingot under conditions where the inverted-V segregation doesn't form. To achieve such production, it is important to understand formation conditions of the inverted-V segregation.

Many researchers have investigated the formation conditions or criteria for channel-type segregations such as inverted-V segregation and freckles. One criterion is the mushy zone Rayleigh number [1-4], which is a non-dimensional number based on the kinetics of the interdendritic concentrated liquid. The kinetics-driven force of density difference and flow resistance of the interdendritic region are considered and the model provides industrial applications of prediction using numerical simulation. On the other hand, Suzuki et al. derived the formation conditions by classifying the relationships between the regions where inverted-V segregation forms and the heat transfer condition in actual ingots [5]. Although Suzuki's criterion is an empirical criterion with limited



practical applications, this criterion also can predict inverted-V segregation regions in actual gravity casting ingots and ESR ingots. However, both criteria are not complete in terms of the fact that neither can predict the concentration in the channel segregation, the channel population, or the dimensions of the channels. Also, both criteria don't directly consider important alloy properties, such the liquidus slope, partition coefficient, and so on. Therefore it is necessary to investigate the basic relationship between the alloy properties and the formation of inverted-V segregation, and freckles.

Both criteria focus on density differences between the bulk-liquid and interdendritic concentrated liquid. Density difference is considered as one of parameters in the Rayleigh number and the formation condition changes according to density difference in Suzuki's criterion [6]. It is reasonable to consider density difference in the model of channel segregation because it is a directly driven force of the movement of the concentrated liquid that plays important roll. From the viewpoint of thermodynamics and the fact that channel formation is accompanied with remelting and solidification retardation, the liquidus slope, m , in the phase diagram can be expressed as Eq. (1), which is also important since this strongly affects the solid fraction change.

$$m_i = \frac{\partial T_L}{\partial C_{L,i}} \quad (1)$$

However it is very difficult to experimentally investigate the effect of just the liquidus slope on channel formation, since there are no two elements that have equal density and redistribution coefficients. Thus, when formation conditions in different alloy systems are studied, the change in formation conditions always contains effects of density difference, liquidus slope, and other factors.

In this work, to investigate the effect of liquidus slope on channel formation, numerical simulations were performed in a virtual binary alloy system consisting of Fe and the virtual added element X. The change in the formation conditions of inverted-V segregation in laterally-directionally solidified ingot was studied by varying the liquidus slope of the alloy system.

2. Procedures

2.1. Numerical simulation

The laboratory-scale lateral directional solidification problem was solved as a two-dimensional problem. The height and width of the ingot are 200 mm and 150 mm, respectively. The computational domain and its boundary conditions are shown in Fig. 1. In this simulation, in order to conduct a directional solidification in the numerical simulation, it is assumed that the left wall is at a constant temperature and cool melt, and the other wall is the adiabatic boundary. The properties and parameters of the Fe-X alloy used in this simulation are shown in Table 1. These values were assumed as characteristics of typical low-alloy steels. Numerical simulations are performed with the densities of added element X and liquidus slopes shown in Table 2. Phase diagrams of virtual alloy system are shown in Fig. 2. The values in Table 2 are decided by a preliminary simulation to find the value that forms inverted-V segregation in the computational domain.

The numerical method used in this work is from a previously published model [7]. It was assumed that the melt was an incompressible fluid and that flow in the mushy zone can be expressed by Darcy's law. The thermo-solutal convection of the melt was taken into account with a density variation by temperature and liquid concentration; however, it was assumed that, divergence free, Eq. (3) is satisfied. Solutes in the liquid were moved by the fluid flow and diffusion and redistribution of the solute at the interface between the liquid and the solid was taken into account. Diffusion of the solute was neglected, because it was smaller than the numerical diffusion. The governing equations were as follows:

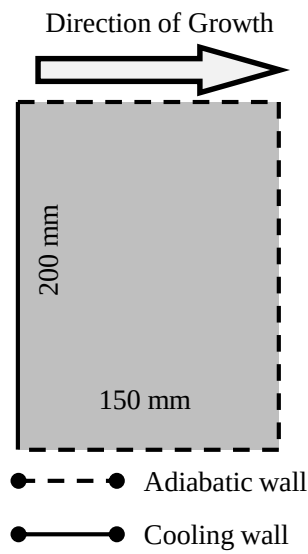


Fig. 1 Computational domain and its boundary conditions

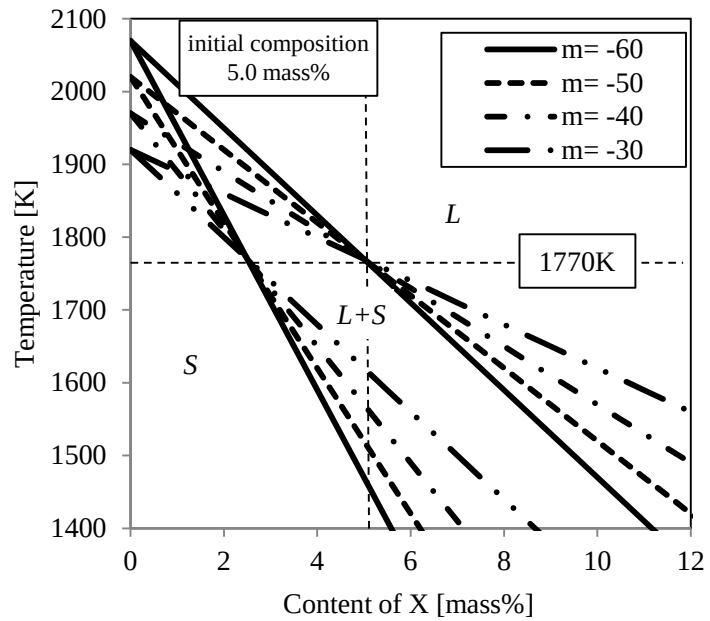


Fig. 2 Phase diagram of virtual alloy system

Table 1 Alloy properties and parameters used in simulation

Properties and parameters	Value	Units
Thermal conductivity	35	W/K/m
Specific heat	680	J/K/kg
Density of Fe	7000	kg/m ³
Latent heat	2.6×10^5	J/kg
Liquidus temperature	1770	K
Initial temperature	1775	K
Added element X content	5	mass%
Redistribution Coefficient	0.5	-
Temperature of cooling wall	300	K
Density of added element	ρ_X	kg/m ³
Liquidus slope	m	K/mass%

Table 2 Density and liquidus slope of virtual alloys

	ρ_X [kg/m ³]	m [K/mass%]
Alloy 1	3500	-60
Alloy 2	3750	-60
Alloy 3	4000	-60
Alloy 4	4250	-60
Alloy 5	3890	-60
Alloy 6	3890	-55
Alloy 7	3890	-50
Alloy 8	3890	-45
Alloy 9	3890	-40
Alloy 10	3890	-35
Alloy 11	3890	-30

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{\nabla p}{\rho} - \frac{\nu}{K} \mathbf{u} + \nu \nabla^2 \mathbf{u} + \mathbf{g} \quad (2)$$

$$\nabla \cdot \mathbf{u}_E = 0 \quad (3)$$

$$\frac{\partial T}{\partial t} + \nabla \cdot T \mathbf{u}_E = \frac{\nabla \cdot \mathbf{q}}{\rho c} + \frac{H}{c} \frac{\partial f_s}{\partial t} \quad (4)$$

$$\frac{\partial C_{L,i}}{\partial t} + \nabla \cdot C_{L,i} \mathbf{u}_E = D_{L,i} \nabla^2 C_{L,i} + \frac{\partial C_{L,i}}{\partial f_s} \frac{\partial f_s}{\partial t} \quad (5)$$

Eqs. (2), (3), (4) and (5) are the momentum equation, the equation of continuity, the energy equation, and the solute conservation equation in liquid, respectively. t is the time, $\mathbf{u}$ is the flow velocity, $\mathbf{u}_E$ is the empty tower velocity, ρ is the density of molten alloy, p is the pressure, ν is the kinetic viscosity, K is the permeability, g is the gravity vector, T is the temperature, c is the specific heat, q is the vector of the heat flux, H is the latent heat in fusion, f_s is the solid fraction, and $C_{L,i}$ and $D_{L,i}$ are the concentration and diffusion coefficients of a i -th solute element in liquid. Following equation was used to calculate density of molten alloy.

$$\rho = \frac{\sum_{i=1}^N M_i X_i}{\sum_{i=1}^N V_i X_i} = \frac{1}{\sum_{i=1}^N \frac{V_i}{M_i} \phi_i} \quad (6)$$

Here V_i , M_i , X_i and ϕ_i are molar volume, molar mass, molar fraction and mass fraction, respectively. The second term on the right hand side in the solute conservation equation, *i.e.* the derivative of the liquid concentration with respect to the solid fraction, shows the micro segregation behavior. Details of the numerical method used in this work can be found in Ref. [7]

2.2. Evaluation of Formation Condition of inverted-V Segregation

Estimation of the formation condition of inverted-V segregation was based on Suzuki's criterion. In Suzuki's criterion, inverted-V segregation forms in the region where Eq. (7) is satisfied.

$$R^{1.1} V < C \quad (7)$$

Where, R , V and C denote the cooling rate [K/s], the solidification velocity [m/s], and the critical value of the inverted-V segregation formation [$K^{1.1}m/s^{2.1}$], respectively. The critical value changes according to the alloy system. As mentioned above, the value strongly depends on the density difference between the bulk liquid and the interdendritic concentrated liquid. In this work, the criterion expressed as Eq. (8) was used to simplify the description of formation conditions.

$$I = RV < S \quad (8)$$

Where, I and S are the segregation index and critical value [Km/s^2] used in this work. The cooling rate and solidification velocity were evaluated at the temperature where the solid fraction reaches 0.3, the "solid fraction" is from the solidification pass of the initial composition and not the physical value defined at each point during the macrosegregation simulation. This segregation index, I , was computed along the centerline at half height of the ingot. Then, the segregation index, I , at the position where the first inverted-V segregation arises was regarded as the critical value, S .

3. Results

3.1. Relationship between segregation formation and density difference

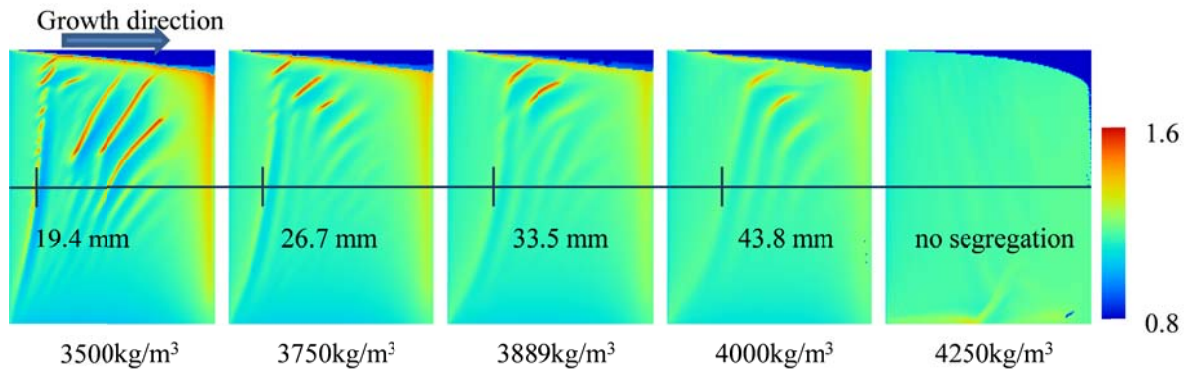


Fig. 3 Distributions of segregation ratio of added element X at fully solidified with various densities

Table 3 Relation between density of added element and critical value

	ρ_X [kg/m ³]	$\Delta\rho$ [kg/m ³]	formation position [mm]	cooling rate [K/s]	solidification velocity [m/s]	critical value [Km/s ²]
Alloy 1	3500	-6.76	19.4	0.718	1.235	0.886
Alloy 2	3750	-5.87	26.7	0.514	1.219	0.627
Alloy 3	3889	-5.42	33.5	0.458	1.212	0.563
Alloy 4	4000	-5.08	43.8	0.394	1.121	0.442

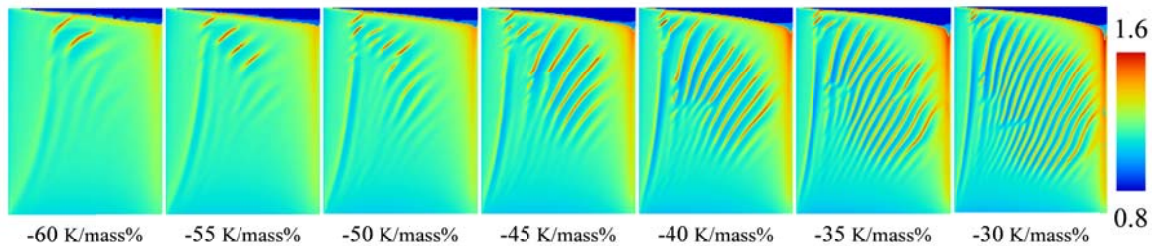


Fig. 4 Distributions of segregation ratio of added element X at fully solidified with various liquidus slopes

Table 4 relation between liquidus slope and critical value

	liquidus slope [K/mass%]	formation position [mm]	cooling rate [K/s]	solidification velocity [m/s]	critical value [Km/s ²]
Alloy 5	-60	33.5	0.458	1.212	0.563
Alloy 6	-55	27.6	0.488	1.198	0.585
Alloy 7	-50	22.4	0.499	1.278	0.638
Alloy 8	-45	19.4	0.564	1.257	0.709
Alloy 9	-40	17.2	0.635	1.177	0.747
Alloy 10	-35	14.7	0.645	1.221	0.788
Alloy 11	-30	13.9	0.633	1.272	0.804

It is known that the critical value in Eq. (7) depends on the density difference between the bulk liquid and the segregated liquid and that the inverted-V segregation is more likely to occur with an increase in the density difference [6]. Numerical analyses with various alloys where the density of the added element is different were performed to validate the simulation model that we used.

The numerical results and the distributions of element X concentration are shown in Fig. 3. The position of the inverted-V segregation at half height moves toward the growth direction side with an increase in the density of the added element and the streak that arises at the bottom of the ingot doesn't

reach half height with the density of 4250 kg/m^3 . This streak shifts to the growth direction side which means the segregation formation occurs at a lower cooling rate position. Thus, the simulation model can replicate the well-known phenomena where the inverted-V segregation formation is inhibited when the density difference between the solvent, Fe, and the added element, X, becomes small. The critical values computed by these simulations are shown in Table 3. In Table 3, ρ_X and $\Delta\rho$ denote the density of the added element, X, and the density difference between the bulk liquid and the segregated liquid at solid fraction 0.3, respectively. In estimation of density difference $\Delta\rho$, Scheil equation was used to compute liquid concentration.

Also, from these critical values we could confirm the tendency that the numerical results used in the present model are consistent with the knowledge that segregation tends to form with larger density differences.

3.2. Relationship between segregation formation and liquidus slope

Fig. 4 and Table 4 show the computed distributions of element X concentration and estimated critical values, respectively. According to Fig. 4 and Table 3, the points at the intersection of the streak with the half-height line shift to the left wall (cold wall) as the absolute value of the liquidus slope decreases, and the critical value of segregation formation also decreases. Furthermore, the distributions show that the alloy with lower liquidus slope forms more channels and more highly concentrated streaks. Thus, the liquidus slope affects not only the formation conditions but also the concentration and numbers of segregation.

To assess the effect of the liquidus slope, the evolution equation of the solid fraction is examined in detail. The evolution equation of the solid fraction in this simulation is expressed as Eq. (9).

$$-\mathbf{u} \cdot \nabla T + \alpha \nabla^2 T + \frac{H}{c} \frac{\partial f_s}{\partial t} = m \left(-\mathbf{u} \cdot \nabla C_L + D_L \nabla^2 C_L + \frac{\partial C_L}{\partial f_s} \frac{\partial f_s}{\partial t} \right) \quad (9)$$

Here, α and m are the thermal diffusivity and the liquidus slope. In binary alloy system, it is assumed that Eq. (10) was satisfied in mushy zone. When it is assumed that the local equilibrium condition is satisfied in the mushy zone, the physical temperature is equal to the liquidus temperature and the liquid concentration can be uniquely determined.

$$T = T_L \rightarrow C_L = \frac{T_L - T_M}{m} \quad (10)$$

Eq. (9) can be rewritten as Eq. (11) by Eq. (10).

$$\frac{\partial f_s}{\partial t} = \frac{(\alpha - D_L) \nabla^2 T}{m \frac{\partial C_L}{\partial f_s} - \frac{H}{c}} \quad (11)$$

Eq. (11) shows that the advection term affects variation of the solid fraction indirectly in mushy zone where local equilibrium is satisfied. Generally, flow direction in the mushy zone with lateral solidification is very close to the isothermal line since a large pressure gradient is necessary to surmount the flow resistance caused by permeability and produce a flow perpendicular to the isothermal line. Hence, the temperature and liquid concentration gradient vector is perpendicular to the flow direction and the advection term that is a dot product of the gradient vector and flow direction does not have a strong effect on the variation of these physical values. According to Eq. (10) and the relation between the gradient vector and the flow direction, the diffusion term in the temperature and

Table 5 critical values and characteristics of Ni-based Alloys

	critical value [K mm/min ²]	density difference [kg/m ³]	liquidus temperature [K]	solidus temperature [K]	solidification temperature range[K]
Alloy A1	2.66	12.9	1673	1589	84
Alloy A2	4.14	13.1	1668	1562	106
Alloy B1	2.88	16.0	1629	1554	75
Alloy B2	5.54	17.6	1662	1625	37
Alloy C1	3.63	22.8	1683	1578	105
Alloy C2	7.17	23.0	1621	1585	36

liquid concentration field is more significant than the advection term as long as stable solidification continues. Even though highly concentrated liquid flows from one region to another in the mushy zone, the temperature of the concentrated liquid is lower than that in the inflow region and the concentrated liquid cannot immediately melt the solid phase in the inflow region. However, the temperature is lower and the liquid concentration is higher in this inflow region than in another region that has an equal solid fraction. With these variations of temperature and concentration, and since the diffusion coefficient of the temperature is much higher than the coefficient of liquid concentration, the temperature variation is reduced by rapid diffusion and the liquidus temperature is kept low. As a result, a difference between the temperature and the liquidus temperature arises due to the difference in the two diffusion coefficients. In other words, the temperature overtakes the liquidus temperature in the region where the concentrated liquid flows. Then, the solid fraction in the region decreases to eliminate the difference between the temperature and the liquidus temperature. By reducing the solid fraction, the liquid concentration and the temperature decrease and the liquidus temperature can be equal to the temperature. It is thought that not only thermodynamic effects of the concentrated liquid but also transportation phenomena on the liquid concentration and temperature are important, in terms of remelting by the concentrated liquid. In the transportation phenomena, the intensity of the flow of concentrated liquid depends on the flow velocity and gradient of temperature. Liquid concentration and the gradients are higher with a narrower mushy zone. The effect of the diffusion cause the difference in temperature and liquidus temperature also becomes higher in a narrower mushy zone. Therefore, the inverted-V segregation tends to form in alloy systems that have lower solidification temperature ranges.

Finally, several critical values of the inverted-V segregation formation of Ni-based alloys are shown in Table 5. These values consist of three pairs. Although these three alloy pairs, Alloys A1 and A2, Alloys B1 and B2, and Alloys C1 and C2, have approximately the same density difference, each alloy has a different critical value. Excepting alloy pair A1 and A2, the critical value of one alloy in each pair has a lower solidification temperature range than that of the other. Although not all the difference in the critical values can be explained by solidification temperature range and liquidus slope, there is the possibility that solidification temperature range strongly affects the critical value and is an important factor that causes a variation in the relation between the density difference and the critical value.

4. Conclusion

The effect of the liquidus slope and density of added element X on the formation condition of inverted-V segregation was investigated by performing numerical simulations of lateral directional solidification with a virtual alloy Fe-X system. A criterion similar to Suzuki's criterion was used to estimate the formation condition. In investigating the effect of the density of element X, numerical simulations replicate well-known results that inverted-V segregation tends to occur when the density difference between Fe and X is larger. On the other hand, numerical simulations performed in this

work suggest that inverted-V segregation also tends to form with a lower liquidus slope. Moreover, the number of inverted-V segregation and the concentration in the streaks increase with a lower liquidus slope. Examining several critical values of an actual Ni-based alloy shows that alloy pairs that have similar density difference present different critical values. Two of the pairs studied show that an alloy with a lower solidification temperature range is apt to form inverted-V segregation. One of the pairs studied did not show this effect. Thus, there is the possibility that the solidification temperature range strongly affects the formation condition of the inverted-V segregation.

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