Application of a macroscopic model to predict the band segregation induced by shear deformation of semisolid

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Abstract. Semisolid deformation during solicitation can cause some casting defects such as the band segregation. Since the defect formation originates in nature of semisolid, it is of interest to build a model including the nature and to predict the defect formation. In-situ and time-resolve X-ray imaging has proved that rearrangement of solid grains in semisolid dominantly controls deformation and localization of shear strain leads to the band segregation. On the basis of the observations, a macroscopic model, which explicitly includes the rearrangement, is proposed. The model uses two-phase flow model and introduces hydrostatic stresses to express the rearrangement. The model was applied to simple shear of semisolid to confirm instability against shear. Fluctuation of solid fraction gradually increased and consequently shear deformation was localized. The model is also applied to pseudo 2D deformation in a shear cell, of which dimension was the same as that used in the X-ray imaging. The calculation result qualitatively agreed with the experimental results. It was concluded that the model has a potential to simulate the localization of shear and the band segregation. For further improvement, to measure some physical properties, which are closely related to the rearrangement, is required.

Introduction

It has been known that deformation of semisolid during solidification could cause some casting defects. For example, segregation band observed in centrifugal casting [1] and die casting [2,3], centerline segregation in twin-roll casting [4,5] and even V-type segregation [6] in continuous casting of steel are closely related to semisolid deformation. Semisolids of metallic alloys shows various mechanical phenomena. Thixotropic properties [7,8], agglomeration / disagglomeration [7], deformation of solid globules [9], and dilatancy during solid-grain rearrangement [10-12] have all been reported. It is of interest to know how the semisolid deforms and consequently the band segregation forms during solidification. However, the model that represents the formation of band segregation induced by deformation has not been established well, comparing to the models for predicting macrosegregation induced by melt flow in the mushy region. The aim of this study is to build a model, which explicitly includes nature of semisolid deformation, and to represent the formation of segregation band.
In the semisolid deformation, interactions between solid grains take place and strongly influence dynamics of semisolid [13]. Apparent viscosity depending on shear rate [14], thixotropy [15] and normal stress on the shear plane against shear [16] are typical examples for semisolid. A previous research pointed out that the band segregation formed due to the rearrangement of solid grains during the deformation [10]. Recently, in-situ and time-resolve X-ray imaging has been performed to observe semisolid deformation [12,17-22]. The deformation of semisolid of Al-15mass%Cu alloys with a solid fraction of 48% was characterized [12,18,19]. The rearrangement of solid grains induced dilation where shear deformation occurred and localization of the shear strain was observed in the shear-deformed domain [18]. The qualitative and quantitative data obtained by the observations are useful to build and to validate a semisolid-deformation model. This paper demonstrates a model, which is build on the basis of the observation, and some calculation results. The validity is also discussed, comparing to the observations.

**Macroscopic model**

1.1.2.1 Governing equations

The governing equations were proposed in the previous study [23]. This study slightly modifies the equations to be consistent with the observation. The governing equations of the liquid phase and the solid phase (grains) are given using the Navier-Stokes equations.

\[
\rho \frac{\partial}{\partial t} (f_i u_i) + \rho \frac{\partial}{\partial x_j} (f_i u_i u_j) = -f_i \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij}^{l} - F_{si}^{l}, \tag{1a}
\]

\[
\rho \frac{\partial}{\partial t} (f_s v_i) + \rho \frac{\partial}{\partial x_j} (f_s v_i v_j) = -f_s \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \tau_{ij}^{s} + \frac{\partial}{\partial x_i} (\sigma_s + \sigma_r) + F_{si}^{l}, \tag{1b}
\]

\[
\frac{\partial f_i}{\partial t} + \frac{\partial}{\partial x_i} (f_i u_i) = 0, \quad \frac{\partial f_s}{\partial t} + \frac{\partial}{\partial x_i} (f_s v_i) = 0 \tag{2a, b}
\]

\[
f_i + f_s = 1 \tag{3}
\]

The stresses \(\sigma_s\) and \(\sigma_r\) express the rearrangement of the solid grains. The force of \(F_{si}^{l}\) is an interaction between the liquid and the solid phases. Since the solid particles suspended in the liquid phase are expected to have lower Reynolds number, Stokes’ law is used as the interaction. Thus, the force per unit volume is simply given by

\[
F_{si}^{l} = n_s f_s^{il} = -\frac{18 \mu_s}{d_s^2} f_s (v_i - u_i) \tag{4}
\]

**Figure 1** Example of apparent viscosity \(\mu_s\), stiffnesses \(C_3\) and \(B_1\) as a function of solid fraction.
1.2. Rearrangement of solid grains

In the model [23], the solid phase was treated as a viscoplastic fluid. The in-situ observation showed that collisions and rearrangement of solid particles dilate the liquid-filled spaces during shear [12,17]. As discussed in the previous paper [23], a hydrostatic stress, $\sigma_s$, operating only the solid particles, is introduced to represent the dilation. In addition, another hydrostatic stress, $\sigma_r$, is also introduced. The full stress tensor of the solid phase is given by

$$
\begin{bmatrix}
\sigma_{11}^s & \sigma_{12}^s & \sigma_{13}^s \\
\sigma_{21}^s & \sigma_{22}^s & \sigma_{23}^s \\
\sigma_{31}^s & \sigma_{32}^s & \sigma_{33}^s \\
\end{bmatrix} = 
\begin{bmatrix}
\sigma_s + \tau_{11}^s & \tau_{12}^s & \tau_{13}^s \\
\tau_{21}^s & \sigma_s + \tau_{22}^s & \tau_{23}^s \\
\tau_{31}^s & \tau_{32}^s & \sigma_s + \tau_{33}^s \\
\end{bmatrix} +
\begin{bmatrix}
\sigma_r + \tau_{11}^r & \tau_{12}^r & \tau_{13}^r \\
\tau_{21}^r & \sigma_r + \tau_{22}^r & \tau_{23}^r \\
\tau_{31}^r & \tau_{32}^r & \sigma_r + \tau_{33}^r \\
\end{bmatrix}.
$$

(5)

The deviator stress tensor of the solid phase is simply expressed by the following equation.

$$
\tau_{ij}^s = 2\mu_s \dot{\varepsilon}_{ij}^s
$$

(6)

Here $\mu_s$ is the apparent viscosity of solid particles. Since the viscosity of the liquid phase is much smaller than that of the semisolid at solid fractions more than 0.3, the apparent viscosity of the solid particles should be nearly equal to the apparent viscosity of semisolid. Thus, the apparent viscosity of the solid phase is estimated from the experimentally measured values.

The stress $\sigma_s$ is proportional to normal / shear strain rates.

$$
\sigma_s = -\begin{bmatrix} C_3 \dot{\varepsilon}_{shear}^oct & B_1 \dot{\varepsilon}_{norm}^oct \end{bmatrix}
$$

(7)

Here, $C_3$ is defined as a stiffness to shear strain rate and $B_1$ to normal strain rate. The octahedral shear and normal strain rates are used in this study, because the hydrostatic stresses $\sigma_s$ and $\sigma_r$ should not depend on coordination. Figure 1 shows an example of the apparent viscosity $\mu_s$, the stiffness $C_3$ and the stiffness $B_1$ as a function of solid fraction. The apparent viscosity $\mu_s$ is estimated from the viscosity measured in Sn-Bi semisolid [13]. For simplicity, the stiffness $B_1$ is assumed to be equal to the apparent viscosity. At lower solid fractions, the stiffness $C_3$ is relatively low because solid grains hardly interact each other. Thus, it is considered that $C_3$ is equal to the apparent viscosity $\mu_s$ in the lower solid fractions. At a certain solid fraction, $C_3$ should exhibit a maximum and then decreases due to build-up of solid network. In this study, $C_3$ have a maximum at solid fraction of 0.48. It is note that the solid-fraction-dependence of $C_3$ strongly depends on morphology of solid grains. The value of 0.48
does not have a particular meaning and is set for descriptive purpose.

The stress $\sigma_r$ in eq. (5) is an additional term to express a repulsive force between the solid grains. When the solid fraction exceeds a critical solid fraction $f_{\text{scrit}}$ where the solid grains are closely packed, the solid grains physically contact each other and further increase in solid fraction hardly occurs. Namely, the stress $\sigma_r$ acts like pressure in the fluid flow. In this study, the critical solid fraction $f_{\text{scrit}}$ is set to be 0.6.

**Application of the macroscopic model**

**1.3. Simple shear**

A linear stability analysis in the previous study [23] showed that instability against simple shear appeared in semisolid when the following condition was satisfied.

$$\frac{\partial C_3}{\partial f_s} < 0 \quad (8)$$

However, it is not clear how the shear band is developed. Numerical calculation was performed to confirm the instability and to know how the shear band forms. Figure 2 shows the initial condition of
calculation. The solid fraction between 0.54 and 0.56 is randomly given at each element and average solid fraction in the casting is 0.55. The velocities of the solid and the liquid phases in the x_1 direction are the same at the beginning. The velocities at the bottom (x_2=0mm) and the top (x_2=50mm) are 0 mm/s and 25mm/s, respectively. The initial velocities in the x_2 direction are zero. Calculation domain size, mesh size and boundary condition are listed in Table 1.

Figure 3 shows the distribution of solid fraction (color) and velocity (arrows) of the solid phase after 30s, when the hydrostatic stress \( \sigma_s \) is not introduced (\( C_3=0 \)) in the calculation. It means that the rearrangement of the solid grains is considered. Solid fraction and velocity do not obviously change during the calculation. Even the solid fraction is slightly fluctuated, the semisolid is stable against the shear and nearly steady state is achieved.

In contrast, the shear band forms when the hydrostatic stress \( \sigma_s \) is included in the calculation, as shown in Figure 4. The fluctuation of solid fraction gradually increases at the initial stage as shown in Figure 4(a). Since the apparent viscosity depends on solid fraction, the velocity in the x_1 direction calculation.

Figure 5 Configuration of semisolid deformation observed by the in-situ X-ray imaging.

Figure 6 (a) Radiograph of the semisolid deformation after 3.1d increment of the push plate motion (d: mean grain diameter). (b) Solid displacement rate, (c) shear strain rate, (d) divergence of solid velocity in 0.5d increment of the push plate motion.
fluctuates approximately 10%. The solid fraction has the lowest value at 4.9 mm from the bottom. Localization of shear strain occurs the shear band clearly forms at the position, as shown in Fig. 4(b). Once the shear band forms, the shear strain rates except the localization position are significantly reduced. As a result, the hydrostatic stress $\sigma_s$ becomes sufficiently low to achieve the nearly steady state.

1.4. Deformation in Shear cell
Figure 5 shows the configuration of a shear cell used in the in-situ observation [24]. Alumina plate was inserted into the cell at 2900 $\mu$m/s and the semisolid (mean diameter of grains: 200 $\mu$m) with 200 $\mu$m in thickness was deformed. The localization of shear deformation occurred at the beginning of

**Figure 7** Calculation domain to compare with the in-situ observation.

**Figure 8** Calculated results. (a) Strain rate $\dot{\epsilon}_{12}$ and (b) divergence of solid velocity $\text{div}(\vec{v})$ with flow pattern of solid at 0.128 s. (c) and (d) are enlarged views of (a) and (b), respectively.
deformation. For example, only 3.1d motion of the solid grains was sufficient to cause the localization. Figure 6(a) shows a transmission image of the semisolid during deformation at 0.21s (3.1d). The velocity of solid grains was evaluated by image processing. The green arrows indicate motion of the solid grains. Shear strain rate and divergence of velocity of the solid grains are also shown in Figures 6 (c) and (d). Shear strain rate in the region B’ (within shear band) was 1.92 s\(^{-1}\) while shear strain rate in the region A’ (outside shear band) was 0.19 s\(^{-1}\). The shear strain was clearly localized at the right-top of the alumina plate (region B’). In addition, values of the divergence in the region B’ were mostly positive, indicating decrease in solid fraction. It should also be noted that the values of the divergence fluctuated from time to time even though time-average values were positive.

A model calculation for the shear cell is done to verify validity of the model. Figure 7 shows the configuration of calculation. The solid and the liquid phases are inserted into the cell from the inlet (left-bottom) and are ejected from the outlet (left-top) at 2900 μm/s. At the beginning, velocities of the solid and the liquid phases are zero. Physical properties used in the calculation are the same as those used in the simple shear.

Figure 8(a) shows the distribution of shear strain rate and the flow pattern of the solid phase at 0.128s. As indicated by the blue color, the shear strain is localized at the right-top of inlet. When the calculation is done for Newtonian fluid, the localization is much weak. Namely, the introduction of the hydrostatic stress causes the localization. As shown in Fig. 8(b), values of the divergence are positive, although they fluctuate significantly. The position of the localization obtained by the calculation coincides with that observed in the experiments. Thus, the proposed model qualitatively simulates the coupling of the shear deformation and the decrease in solid fraction.

There is still quantitative discrepancy between the observation and the calculation. Shear strain rates in the regions A’ and B’ are 0.29 s\(^{-1}\) and 0.59 s\(^{-1}\), respectively. The localization in the calculation is relatively weak, comparing to the observation. Several possibilities to cause the discrepancy are considered. One is the accuracy of stiffnesses C\(_3\) and B\(_1\), and the other is looseness of the semisolid at the beginning.

The stiffness C\(_3\) and B\(_1\) should depend on not only solid fraction but also morphology of solid grain. We assumed that the value of C\(_3\) is equal to the apparent viscosity \(\mu\) at low solid fraction, because a water-model experiment shows that C\(_3\) is in the same order of \(\mu\) [24]. However, no experimental data for the stiffnesses are available for metallic systems. Stiffness C\(_3\) can influence degree of the localization. To measure the physical properties of the semisolid qualitatively is required for further development of the macroscopic model.

The looseness of solid grains is not included in the present model. In the semisolid before deformation, the solid grains are isolated by the liquid phase and most of them do not physically contact each other. Namely, the liquid phase can exist in the gap between the solid grains. Thus, the external force is not transmitted by contact of the solidi grain at the beginning. The force starts to be transmitted between the solid grains after the solid grains physically contact. This looseness can enhance the localization at the beginning. To include the looseness is a problem to be solved in the next step.

Summary

The macroscopic model, which includes the rearrangement of the solid grains during deformation, is examined.

1. In the 1D simple shear of semisolid, the model well reproduces the localization of shear strain and the decrease in solid fraction. Consequently the band segregation is reproduced in the calculation.
2. Semisolid deformation in the shear shell used in the in-situ observation is calculated. The calculated result qualitatively agrees with the observation results. The agreement indicates that the proposed model has potential to predict the shear band and consequently the band segregation.
3. There are still quantitative discrepancies between the calculation and the observation. Further understanding of some physical properties such as the stiffnesses C\(_3\) and B\(_1\) is needed. In addition, the looseness of the semisolid is also included in the model to simulate the initial stage of deformation.
Symbols

- $u_i$: flow velocity of liquid. $i$ is direction
- $v_i$: flow velocity of solid particles
- $f_s$: fraction of solid
- $e_{s,l}^{ij}$: Strain rate tensor of solid (s) / liquid (l)
- $\sigma_{s,l}^{ij}$: Full stress tensor of solid (s) / liquid (l), including the hydrostatic stress
- $\tau_{s,l}^{ij}$: Deviator stress tensor of solid (s) / liquid (l)
- $\sigma_{s,r}$: Normal stress induced by collisions/rearrangement of solid particles
- $P$: Pressure in liquid phase
- $F_{sl}^i$: Interaction between liquid and solid particles
- $\mu_s$: Apparent viscosity of solid particles

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References

[1] Kang I, Ohnaka I, 1997 J Japan Foundry Engineering Society 69 240
[2] Gourlay C M, Laukli H I, Dahle A K, Metall 2007 Mater Trans A 38 1833
[3] Otarawanna S, Gourlay C M, Laukli H I, Dahle A K 2009 Mater Charact 60 1432
[4] Yun M, Lockyer S A, Hunt J D 2000 Mater Sci Eng A 280 116
[5] Lockyer S A, Yun M, Hunt J D, Edmonds V D 1996 Mater Charact 37 301
[6] Suzuki K, Miyamoto T 1974 ISIJ international 14 296
[7] Young KP, Riek R G, Flemings M C 1979 Metals Technology 6 130
[8] Flemings M C 1991 Metall Trans 22A 957
[9] Tzimas E, Zavaliangos A 1999 Acta Materialia 47 517
[10] Gourlay C M, Dahle A K 2007 Nature 445 70
[11] Gourlay C M, Meylan B, Dahle A K 2008 Acta Mater 56 3403
[12] Gourlay C M, Dahle A K, Nagira T, Nakatsuka N, Nogita K, Uesugi K and Yasuda H 2011 Acta Mater 59 4933
[13] Flemings M C 1991 Metall Trans B, 22B 269
[14] McLelland A R A, Hendraerson H V, Atkinson H V, Kirkwood D H 1997 Mater Sci Eng A, A232 110
[15] Modigell M, Koke J 2001 J Mat Proc Technol 111 53
[16] Hunt M L, Zenit R, Campbell C S, Brennen C E 2002 J Fluid Mech 442 1
[17] Nagira T, Gourlay C M, Sugiyama A, Uesugi M, Kanazawa Y, Yoshiya M, Uesugi K, Umetani K and Yasuda H 2011 Scripita Mater 64 1129
[18] Nagira T, Yokota H, Morita S, Yasuda H, Yoshiya M, Gourlay C M, Sugiyama A, Uesugi K and Umetani K 2013 ISIJ International 53 1195
[19] Fonseca J, O’Sullivan C, Nagira T, Yasuda H and Gourlay C M 2013 Acta Mater 61 4169
[20] Nagira T and Yasuda H 2014 In-situ Studies with Photons, Neutrons and Electrons Scattering II, (Switzerland: Springer) p 231
[21] Gourlay M, O’Sullivan C, Fonseca J, Yuan L, Kareh K M, Nagira T and Yasuda H 2014 JOM 66 1415
[22] Nagira T, Morita S, Yokota H, Yasuda H, Gourlay C M, Yoshiya M, Sugiyama A, Uesugi K, Takeuchi A and Suzuki Y 2014 Metall Mater Trans A 45 5613
[23] Morita S, Yasuda H, Nagira T, Gourlay C M, Yoshiya M, Sugiyama A 2012 IOP Conf Ser: Mater Sci Eng 33 012053
[24] Nagira T, Morita S, Yokota H, Yasuda H, Gourlay C M, Yoshiya M, Sugiyama A, in preparation.