Phase-field model for crystallization in alkali disilicate glasses: 
Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$

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This study developed phase-field method (PFM) technique in oxide melt system by using a new mobility coefficient ($L$). The crystal growth rates ($v_0$) obtained by the PFM calculation with the constant $L$ were comparable to the thermodynamic driving force in normal growth model. The temperature dependence of the $L$ was determined from the experimental crystal growth rates and the $v_0$. Using the determined $L$, the crystal growth rates ($v$) in alkali disilicate glasses, Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ were simulated. The temperature dependence of the $v$ was qualitatively and quantitatively similar so that the PFM calculation results demonstrated the validity of the $L$. Especially, the $v$ obtained by the PFM calculation appeared the rapid increase just below the thermodynamic melting point ($T_m$) and the steep peak at around $T_m$–100K. Additionally, as the temperature decreased, the $v$ apparently approached zero ms$^{-1}$, which is limited by the $L$ representing the interface jump process. Furthermore, we implemented the PFM calculation for the variation of the parameter $B$ in the $L$. As the $B$ increased from zero to two, the peak of the $v$ became steeper and the peak temperature of the $v$ shifted to the high temperature side. The parameters $A$ and $B$ in the $L$ increased exponentially and decreased linearly as the atomic number of the alkali metal increased due to the ionic potential, respectively. This calculation revealed that the $A$ and $B$ in the $L$ were close and reasonable for each other.

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1. Introduction

The growth of crystals in oxide melts is an important issue for ceramic formation process such as pyrometallurgy, control of the crystal size and development of advanced ceramic materials. The growth rates in most inorganic glasses are sufficiently slow (less than 10$^{-6}$ m/s) so that the thermal effects and the diffusional effects can be neglected. Therefore, it is well known that the crystal growth rates can be determined mainly by the thermodynamic driving force and the interfacial processes. For the interfacial processes on the crystal growth, three phenomenological models which are called as (a) normal growth model, (b) screw dislocation growth model and (c) two dimensions (2D) nucleated growth model were suggested.\textsuperscript{1-3} In alkali disilicate glasses of Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ which are targeted this paper, previous papers\textsuperscript{4-6} analyzed and interpreted the experimental crystal growth rates using the interface-controlled crystal growth models (a–c).

Phase-field method (PFM)\textsuperscript{7-11} is an effective simulation technique that can treat the micro-scaled material evolution such as grain growth, sintering, solidification and phase transformation. The PFM has a significant advantage that it doesn’t need to trace the boundary conditions during the evolution of microstructure by using a diffuse-interface. However, the PFM has been energetically developed for metallic materials, and not been completely extended to oxide systems because the material evolution of the metal is enough speedy for the PFM calculation. However, Heulens et al. developed the multiphase-field method for crystallization growth in the oxide melts, and succeeded the solidification simulation\textsuperscript{12-14} in CaO–Al$_2$O$_3$–SiO$_2$ melts and FeO–SiO$_2$ melts. Also, Xuan et al. calculated the dissolution behavior of alumina particles into molten silicates using a simple and classical PFM.\textsuperscript{15} However, the enough small mesh size for the diffuse interface width and the simulation time scale are restricted less than 0.2 μm × 0.2 μm and less than 0.005 s, respectively. To date, it required a development of the PFM technique for the reasonable prediction in the oxide melt system.

In this study, we modeled the interfacial process to simulate the temperature dependence of crystal growth rates in alkali disilicate glasses of Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ by the simple PFM. Furthermore, the validity of the kinetics simulation on the interfacial process was clarified by comparing the experimental data.
2. Model description

2.1 PFM

In an isothermal system at constant volume and pressure, the classical phase-field equation \(^3\) is derived using the total free energy density \(F\). Here, \(F\) is expressed as sum of the homogeneous and heterogeneous terms: the homogeneous term is obtained by weighted-mean of the solid- and liquid-phase free energy densities \((f^s(T)\) and \(f^l(T)\)) with the classical weighting functions \((h(\phi)\) and \(1 - h(\phi)\)). The heterogeneous term is the excess free-energy due to the overlap of solid and liquid phases, which is expressed by the double-well potential of the phase-field variable \((\phi)\).

\[
F = \int \left\{ h(\phi)f^s(T) + [1 - h(\phi)]f^l(T) + W_g(\phi) + \frac{K}{2} (\nabla\phi)^2 \right\} dV
\]  

(1)

Here, \(h(\phi) = \phi^3(6\phi^2 - 15\phi + 10)\) and \(g(\phi) = \phi^2(1 - \phi^2)\) and the region where \(\phi = 1\) and \(\phi = 0\) correspond to the solid and liquid phases, and the \(\phi\) changes continuously from 0 to 1 at the diffuse-interface of the two phases. The kinetics of the non-conserved phase-field variable \((\phi)\) is described using the time-dependent Ginzburg-Landau equation called as TDGL \((\partial\phi/\partial t = -L^2\delta F/\delta\phi)\):

\[
\frac{\partial\phi}{\partial t} = -L \cdot \left\{ 30\phi^2(1 - \phi^2)[f^s(T) - f^l(T)] + 2W\phi(1 - \phi)(1 - 2\phi) - \frac{K}{2} \nabla^2\phi \right\}
\]  

(2)

Here, \(f^s(T) - f^l(T)\) is difference between free energies of undercooled melt and crystalline phases, which are represented by empirical equations in this paper. \(\phi^s(T)\) shows the empirical equations for \(f^s(T) - f^l(T)\), \(\phi^l(T)\) interfacial energy \((\gamma)\) and viscosity \((\eta)\) in \(\text{Li}_2\text{O}-\text{2SiO}_2\), \(\text{Na}_2\text{O}-\text{2SiO}_2\), and \(\text{K}_2\text{O}-\text{2SiO}_2\). \(\phi^s(T)\) shows \(f^s(T) - f^l(T)\) at supercooling temperature \((-\Delta T = -(T_m - T) = -300 \text{ to } 0 \text{ K})\). The red, blue and green open circles show the experimental data, and the red, blue and green lines show the approximation curves of Table 1. The empirical equations of the \(\gamma\) are given from the experimental data. \(\phi^l(T)\) and \(\phi^s(T)\) in the Eq. (2) are defined by

\[
K = \frac{12\gamma}{b}
\]

(3)

\[
W = \frac{6\gamma b}{\delta}
\]

(4)

Here, the \(\delta\) denotes the interfacial width between crystalline and undercooled melt phases, and the \(b\) equals to \(\sim 2.2\), which is a constant parameter related to the interfacial width.

2.2 Mobility coefficient \((L)\)

According to the normal growth model and the screw dislocation growth model, \(\text{atoms jump over the interface affects strongly crystal growth rates. Especially, the crystal growth rate at large supercooling temperature is limited by the jump. In many cases, the jump frequency factor \((v)\) can be represented through Stokes–Einstein equation:}

\[
v = \frac{k_BT}{3\pi\eta R}
\]

(5)

Here, \(\lambda\) is the jump distance which is usually taken as a molecular diameter, \(\eta\) is viscosity of the undercooled melt phase whose empirical equations are described at Table 1, and \(k_B\) is the Boltzmann constant. Figure 2 shows the \(\eta\) of \(\text{Li}_2\text{O}-\text{2SiO}_2\), \(\text{Na}_2\text{O}-\text{2SiO}_2\) and \(\text{K}_2\text{O}-\text{2SiO}_2\) versus the reciprocal of temperature. Furthermore, the screw dislocation growth model takes the interface as smooth, but imperfect on an atomic scale. The fraction of active sites \((\gamma)\) on the interface where the atoms can be added or removed is given by

\[
r = \frac{\Delta T}{2\pi T_m}
\]

(6)

Here, \(T_m\) is thermodynamic melting point as shown at Table 2. Therefore, temperature dependence of the inter-

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Table 1. Difference between free energy of undercooled melt and crystalline phases \(f^s(T) - f^l(T)\) in \(\text{Li}_2\text{O}-\text{2SiO}_2\), \(\text{Na}_2\text{O}-\text{2SiO}_2\) and \(\text{K}_2\text{O}-\text{2SiO}_2\) at \(-\Delta T = -300 \text{ to } 0 \text{ K}.

| M   | \(f^s(T) - f^l(T)\) \text{[J mol}^{-1}\text{]} \text{T in K} | \(\gamma/\text{J m}^{-2}\text{[J m}^{-2}\text{]} \text{T in K} | \log_{10}\eta/\text{Pa s} \text{T in °C} |
|-----|-----------------------------------------------|-----------------------------------------------|-----------------------------------------------|
| Li  | 53399 - 42.015T + 7.13 \times 10^{-5}T^2 - 4.79 \times 10^{-7}T^3 | 317 + 2.3 \times 10^{-7}T | -2.55 + 3385.5/(T - 218.05) |
| Na  | 30803 - 34.124T + 3.00 \times 10^{-5}T^2 - 2.07 \times 10^{-7}T^3 | 312 - 2.7 \times 10^{-7}T | 22.25 - 3.57 \times 10^{-2}T + 1.56 \times 10^{-3}T |
| K   | 136000 - 360.48T + 3.44 \times 10^{-5}T^2 - 1.13 \times 10^{-7}T^3 | 272 - 4.7 \times 10^{-7}T | -5.00 + 7460.5/(T - 59.52) |
Table 2. Thermodynamic melting point (T_m) and molar volume (V_m) in M_2O–2SiO_2 (M = Li, Na and K).

| M  | T_m/K  | V_m/m^3 mol^{-1} |
|----|--------|------------------|
| Li | 1306.4 | 6.15 x 10^{-5}   |
| Na | 1146.6 | 7.34 x 10^{-5}   |
| K  | 1313.0 | 8.47 x 10^{-5}   |

The simulation procedure consists of 4 steps: in the first step, the classical PFM with the constant mobility coefficient (L = 1) is solved to compare the thermodynamic driving force in the normal growth model. In the second step, the optimal A and B are determined using the ratio of experimental data and the crystal growth rate (v_0) obtained by the calculation in the first step. In the third step, the PFM calculation with the defined L was implemented to obtain the temperature dependence of the crystal growth rate (v). In the fourth step, the PFM calculation for the variation of the B in the L was implemented.

3. Results

3.1 Crystal growth rates at a constant mobility coefficient (L = 1)

The Eq. (2) with the constant mobility coefficient (L = 1) was solved numerically to investigate the thermodynamic driving force for the v_0 of Li_2O–2SiO_2, Na_2O–2SiO_2, and K_2O–2SiO_2. Figure 3 shows the calculation results of the v_0 at wide range of supercooling temperature (ΔT = −300 to 0 K). The v_0 in Fig. 3 changes drastically at around T_m and becomes a gentle slope with −ΔT decreasing. The behavior of the v_0 in Fig. 3 is similar with the past PFM calculation. Furthermore, there are some physical parameters such as the γ, the V_m and the T_m used in this PFM calculation. Nevertheless, the temperature dependence of v_0 is mainly determined by the f^4(T) − f^3(T). In Fig. 1, the f^4(T) − f^3(T) of Li_2O–2SiO_2 is the largest of the three alkali disilicate glasses, and the f^4(T) − f^3(T) decreases with the atomic number of the alkali metal. The v_0 in Fig. 3 decreases with the atomic number of the alkali metal as well as the f^4(T) − f^3(T). Here, ΔT = 0K in Fig. 3 denotes the thermodynamic melting point (T_m) as shown at Table 2. In Fig. 3, the crystallization seems to start at −ΔT ~−10K, which is caused by the thermodynamic error in the f^4(T) − f^3(T) at around T_m. In the PFM, since the thermodynamic driving force is calculated by 15[f^4(T) − f^3(T)]/2W in the Eq. (2), the thermodynamic
error increases at around $T_m$ where $f^L(T) - f^S(T)$ is sufficiently low. The inserted figure shows the PFM calculation results using the much smaller interfacial energy ($\gamma = 0.001 \text{Jm}^{-2}$) which was suggested for Li$_2$O–2SiO$_2$ and Na$_2$O–2SiO$_2$ in the previous paper. The much smaller $\gamma$ improves the start of the crystallization. However, since the interfacial energy is very low and controversial, we use the $\gamma$ in the Table 1 in the PFM calculation.

Figure 4 shows the thermodynamic driving force ($1 - \exp[-(f^L - f^S)/(RT)]$) in the normal growth model.\(^1\)

In Fig. 4, the $1 - \exp[-(f^L - f^S)/(RT)]$ increases smoothly with $-\Delta T$ decreasing. Here, the calculation result of Na$_2$O–2SiO$_2$ is the same as Li$_2$O–2SiO$_2$ in spite of the different $f^L(T) - f^S(T)$ because $T_m$ of Na$_2$O–2SiO$_2$ is 1146.6 K which is lower than that of Li$_2$O–2SiO$_2$. The temperature dependence of the $v_0$ is similar with the $1 - \exp[-(f^L - f^S)/(RT)]$ in the normal growth model so that the $v_0$ can show the thermodynamic driving force in the alkali disilicate glasses.

3.2 Determination of mobility coefficient ($L$)

Figure 5 shows determination of the mobility coefficients ($L$) in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$. The horizontal axis in Fig. 5 represents $T\Delta T/\eta$ of temperature dependence in the Eq. (7). The open circles denote the ratios of the experimental growth rates as referred to the previous papers\(^3\)\(^\text{(11-22)}\) to the $v_0$ as shown in Fig. 3. The solid lines denote the approximation curves in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ with a power function. Because the crystal growth rate in Li$_2$O–2SiO$_2$ shows the 100 times larger than the others in Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$, there are seen relatively large errors of the ratio in Li$_2$O–2SiO$_2$ in Fig. 5. However, they have good agreements with each other so that the mathematical form of the Eq. (7) is considered to be a proper function. Finally, the best approximation curves were determined by:

$\text{Ratio} = 2.7 \times 10^{-9} \left( \frac{T \Delta T}{\eta} \right)^{1.280}$ for Li$_2$O–2SiO$_2$  \(8\)

The Eqs. (8)–(10) can be treated as the $L$ for Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$, respectively. In general, it is well-known that a mobility coefficient depends on the temperature.

3.3 Temperature dependence of crystal growth rates ($v$)

Using the determined mobility coefficient ($L$), the crystal growth rates ($v$) in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ were calculated. Figure 6 shows the comparison between the experiments and the PFM calculation. The black open and red filled circles in Figs. 6(a)–6(c) show the experimental data\(^3\)\(^\text{(11-22)}\) and the $v_0$ obtained by the PFM calculation at each temperature, respectively. The temperature dependence on the $v$ is qualitatively and quantitatively so similar that the Fig. 6 demonstrates the validity of this PFM calculation with the determined $L$. The $v$ appears rapid increase just below the $T_m$ and the steep peak at around $T_m$–100 K. As the temperature decreases, the $v$ apparently approaches zero ms$^{-1}$. In the PFM calculation, the increase of the $v$ just below the $T_m$ is cooperated with both the change of the $f^L(T) - f^S(T)$ as shown in Fig. 3 and the $L$ defined by the Eq. (7). However, the decrease of the $v$ below the peak temperature is almost solely caused by the $L$ because the Fig. 3 shows the $v_0$ becomes the gentle slope in this temperature range. This is the same interpretation as the normal growth model,\(^1\)\(^\text{(3-5)}\) in which the $v$ is limited by the interface jump process at the large supercooling temperature.

Figures 6(d)–6(f) show the calculation results for the variation of the mobility coefficient parameter ($B = 0.0, 0.5, 1.0, 1.5$ and $2.0$). The $v$ in Figs. 6(d)–6(f) is normalized to the maximum value ($v_{\text{max}}$). Here, we focus on the
parameter $B$ because the parameter $A$ means degree of the $L$ and doesn’t affect the temperature dependence of the $v$. As the $B$ increases from zero to two, the peak of the $v$ becomes steeper and the peak temperature shifts to the high temperature side. Because the $B$ is the slope in Fig. 5, the increase of $B$ induces that the $L$ increases exponentially with the temperature. As a result, the $v$ shifts to high temperature side, and the peak of the $v$ becomes steeper with the $B$ increasing. Moreover, Fig. 7 shows the ratio of the maximum $v$ on the basis of the maximum $v$ at $B = 0.5$ ($v_{\text{max}}/v_{\text{max}} (B = 0.5)$). The Fig. 7 shows that the $v_{\text{max}}$ increases exponentially with the $B$ increasing.

4. Discussions

4.1 Parameters $A$ and $B$ of the mobility coefficient ($L$)

Figure 8 shows the best estimated parameters ($A$ and $B$) of the $L$ in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$. The red and blue filled circles in Fig. 8 show the $A$ and the $B$ used in the PFM calculation of Figs. 6(a)–6(c), respectively. As the atomic number of the alkali metal increases, the $A$ increases exponentially and the $B$ decreases linearly, respectively. In the Fig. 1, the $f^2(T) - f^3(T)$ decreases as the atomic number of the alkali metal increases, which
corresponds to tendency of the ionic potential of the alkali metal from the perspective of the heat of fusion. Therefore, the dependence of the atomic number in the $f^d(T) - f^s(T)$ is the same as that of the $B$. According to the past works\textsuperscript{1-3} on the crystal growth model, the crystal growth rate ($v$) just below $T_m$ is proportional to the supercooling temperature ($T_m - T$) since the thermodynamic driving force is approximately proportional to $T_m - T$:

$$v \propto T_m - T \quad (11)$$

Therefore, the $v$ in Li$_2$O–2SiO$_2$ which has the largest $f^d(T) - f^s(T)$ should have the higher temperature peak because the $v$ in Li$_2$O–2SiO$_2$ is more strongly affected by the thermodynamic driving force. As a result, the $B$ in Li$_2$O–2SiO$_2$ is the largest value, and the $B$ values decreases with the atomic number of the alkali metal as well as $f^d(T) - f^s(T)$. On the other hand, the behavior of the $A$ is seemed to be determined by the $B$. As the Fig. 7 shows that the $v_{\text{max}}$ increases exponentially with the $B$ increasing, the degree of the $v$ should change exponentially with the $B$. Because the experimental growth rates are from $10^{-7}$ to $10^{-2}$ ms$^{-1}$, the $A$ increases exponentially to match the experimental data. In Fig. 8, the $A$ increases exponentially with the atomic number of the alkali metal. Therefore, the relationship with the $A$ and the $B$ is very close and reasonable for each other.

4.2 Comparison of the scheme between this PFM and the normal growth model

Figure 9 shows outline of the free energy density in the normal growth model\textsuperscript{1-3} and this PFM which is represented by the Eq. (1). The shapes of the free energy density are almost same as each other. In the PFM, there are the free energy densities of the crystal and the undercooled melt phases, and the double-well potential appears at the diffuse interface. This double-well potential takes part in separating the other phase ($\phi$ and $1 - \phi$) for the crystal and the undercooled melt phases. The degree of the double-well potential ($W$) is related to the interfacial energy ($\gamma$) and the interfacial width ($\delta$) between the crystal and the undercooled melt phases as defined by the Eq. (4). As a result, the PFM simulates the crystal growth rate by the ratio of $15[f^d(T) - f^s(T)]/2W$ in the Eq. (2). To incorporate the atoms jump over an interface and the fraction of active sites in the PFM, the new mobility coefficient ($L$) was defined by the Eq. (7). The $L$ works on the only interface where the phase-field variable changes, and gives the PFM simulation the temperature dependence of the interfacial processes such as the atoms jump and the active sites.

In the screw dislocation model, it is the similar thermodynamic driving force ($f^d(T) - f^s(T)$) with the PFM, but the activation free energy is set for diffusion across the interface between the crystal and the undercooled melt phases, which is calculated by the Stoke-Einstein and/or the Eyring equations as the kinetic process on the interface. The interfacial energy is interpreted as the energy gap for this diffusion process. Because the screw dislocation model treats the diffusional process as the kinetic process, the interpretation in this PFM is totally different from the screw dislocation model. However, the new defined $L$ in this paper enables to calculate the temperature dependence of the $v$ which is equivalent to or higher than the screw dislocation model.

5. Conclusion

In this study, we defined the new mobility coefficient ($L$) and implemented the crystal growth simulation in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ to develop the PFM technique in the oxide melt system.

Firstly, the crystal growth rates ($v_0$) with the constant mobility coefficient were calculated. Using the experimental data and the $v_0$, the temperature dependence of the $L$ was determined. The $v_0$ demonstrates the validity of the PFM simulation, which is consistent with the thermodynamic driving force ($f^d(T) - f^s(T)$). Furthermore, the behavior of the $v_0$ is comparable to the thermodynamic driving force $(1 - \exp[-(f^d - f)/RT])$ in the normal growth model.

Next, the crystal growth rates ($v$) in Li$_2$O–2SiO$_2$, Na$_2$O–2SiO$_2$ and K$_2$O–2SiO$_2$ were calculated using the determined $L$. The temperature dependence of the $v$ is qualitatively and quantitatively so similar that the calculation results demonstrate the validity of the $L$ in the PFM calculation. Especially, the $v$ appears the rapid increase just below the $T_m$ and the steep peak at around $T_m$=100 K. As the temperature decreases, the $v$ apparently approaches zero ms$^{-1}$, which is limited by the interface jump process. Moreover, we implemented the PFM calculation for the variation of the mobility coefficient parameter $B$. As the $B$ increases from zero to two, and the peak of the $v$ became steeper and the peak temperature shifted to the high temperature side. The $A$ increases exponentially and the $B$ decreases linearly as the atomic number of the alkali metal increases, respectively. The PFM calculation revealed that the parameters $A$ and $B$ in the $L$ are very close and reasonable for each other.

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![Fig. 9. Outline of the free energy density between the PFM and the normal growth model.](image-url)
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