Molecular dynamics (MD) simulation has been widely used as a very useful method for the calculation of thermodynamic, structural and transport properties for the molten slags and fluxes at high temperatures. In this study, MD simulation using the Born-Mayer-Huggins type pairwise potential with partial ionic charges has been used to calculate the thermodynamic, structural and transport properties for the FeO–SiO$_2$ system. The calculated structural properties such as pair distribution functions and fractions of bonding types of oxygen (bridging, non-bridging and free oxygen) with silicon atoms in FeO–SiO$_2$ melts were in good agreement with previously measured and estimated results, and also the self-diffusion coefficients of iron, silicon and oxygen have been calculated at various temperatures and compositions. The enthalpy, entropy and Gibbs energy of mixing for the FeO–SiO$_2$ system were calculated based on the thermodynamic and structural parameters obtained from MD calculation. The phase diagram for the FeO–SiO$_2$ system estimated by calculated Gibbs energy of mixing shows good agreement with observed result in the range from pure iron to fayalite, and the liquid–liquid immiscibility region in the FeO–SiO$_2$ system has also been assessed by MD calculation.

Keywords: molecular dynamics, simulation, iron silicate, molten silicate structure, thermodynamics, phase diagram

1. Introduction

In recent years, the thermodynamic properties for the multiphase molten slags and fluxes are generally calculated from the computational thermodynamics by using computer-based software packages such as FactSage$^{1,2}$ and Thermo-Calc.$^3$ These calculation methods require the experimentally measured databases for the calculation of thermodynamic properties of multiphase systems. Therefore, the application of these methods can be limited. On the other hand, molecular dynamics (MD) simulation is to calculate the various physicochemical properties based on the dynamic quantities of individual particles in the solid and fluid simulation cells with optimized potential models and calculation algorithms without any basic database. Therefore, the thermodynamic, structural and transport properties at high temperatures, which are difficult to measure by experimental methods can be effectively estimated.

The MD calculations for silicate systems have been performed by several researchers using various potential models for the estimation of realistic structural and thermodynamic properties at high temperatures. Belashchenko$^4$ reported the various structural properties of non-crystalline oxide systems by the MD calculation, and these results of calculation are in good agreement with experimentally measured results. Belonoshko et al.$^5,6$ have successfully assessed the thermodynamic and structural properties for silica and magnesium silicates at various temperatures and pressures by using transferable pairwise interatomic potential model. Kiffer et al.$^7$ have calculated the structural incompatibilities and liquid–liquid phase separation in molten binary silicates with the rigid ion model. Takei et al.$^8$ have calculated the metastable immiscibility region in the Al$_2$O$_3$–SiO$_2$ system from the thermodynamic and structural data obtained by the MD simulation. In the previous work, we also successfully assessed the structural, transport and thermodynamic properties for BaO, CaO and CaF$_2$ binary systems$^9$ and CaO–SiO$_2$ system$^{10}$ by the MD calculation, and the phase diagrams for these systems were calculated based on the thermodynamic and structural parameters obtained by the MD calculation. These results of calculation show that the MD simulation is a useful method for the calculation of various physicochemical properties for the oxide and halide systems at high temperature.

In the present study, the effective potential model for the FeO–SiO$_2$ system with optimized parameters was determined. The thermodynamic, structural and transport properties for FeO, Fe$_2$SiO$_4$ and FeO–SiO$_2$ melts were calculated by optimized potential model, which were compared with observed results. The phase diagram for the FeO–SiO$_2$ system, especially the liquid–liquid immiscibility region in the SiO$_2$-rich region was estimated by the thermodynamic and structural parameters obtained from the MD calculation.

2. Molecular Dynamics Calculation

2.1 Interatomic potential

For the calculation of various physicochemical properties by using MD simulation, the interatomic potential is required to evaluate the total force on particles in system, and it is most important to obtain the exact calculation results. In this study, the interatomic potential energy was calculated by the summation of pairwise interactions between ions $i$ and $j$ that was the Busing approximation of Born-Mayer-Huggins form of eq. (1).

$$\phi_i(r) = \frac{q_iq_je^2}{r_{ij}} + f_0(b_i + b_j)\exp\left(\frac{a_i + a_j - r_{ij}}{b_i + b_j}\right) - \frac{c_je_j}{r_{ij}^6}$$

where $r_{ij}$ is the interatomic distance between ions $i$ and $j$, $q_i$ is the valence of the ion $i$, $e$ is the electron charge, $f_0$ is the
standard force of 41.84 kJ nm\(^{-1}\) mol\(^{-1}\), \(a_i\) and \(b_i\) are repulsive radius and softness parameter of the ion \(i\), \(c_i\) is the van der Waals interaction parameter of the ion \(i\), respectively. The interatomic potential terms of eq. (1) represent the Coulomb, short-range repulsion and van der Waals interactions, respectively. Three-body, high order interactions and angle-dependence terms are neglected in this study.

The interatomic potential parameters of SiO\(_2\) for the FeO–SiO\(_2\) system in this study were taken from potential model by Tsuneyuki et al.\(^\text{11}\) that has been derived by the ab initio Hertree–Fock self-consistent-field calculations for model clusters of silica. The effective charges for Si and O ions have been represented 2.4 and \(-1.2\), respectively. The potential model reported by Tsuneyuki et al. has successfully reproduced the structural and dynamical properties for various silica polymorphs, glasses and molten SiO\(_2\).\(^\text{11–17}\) and the thermodynamic properties such as phase transition of quartz.\(^\text{18}\)

The interatomic potential parameters for Fe–Fe and Fe–O pairs in the FeO–SiO\(_2\) system were calculated by fitting the experimentally measured structural, transport and thermodynamic properties of FeO, Fe\(_2\)SiO\(_4\) and FeO–SiO\(_2\) melts by fixing the interatomic potential parameters of Si and O pairs for SiO\(_2\) by Tsuneyuki et al. In this study, the effective charge of Fe ions for the FeO–SiO\(_2\) system was determined to be 1.2, in order to maintain electroneutrality in the simulation system. The interatomic potential parameters used in this study are listed in Table 1.

### 2.2 Methods for calculation

The MD simulations were carried out using the isobaric and isothermal (\(N\cdot p\cdot T\)) ensemble. Temperature is controlled by velocity scaling method. Pressure is controlled by Parrinello and Rahman method at atmospheric pressure. The periodic boundary conditions were employed for each simulation system. The long-range Coulomb interactions have been summated by Ewald method. The equations of motion were integrated by fifth-order Gear’s predictor-corrector algorithm using a time step of \(1 \times 10^{-15}\) s. The atomic configurations of initial cells for solid phases were taken from the respective unit cell structures. The FeO crystal structure was composed of 1000 (Fe 500 and O 500) atoms according to an array of \(5 \times 5 \times 5\) unit cells of rocksalt structure (cubic, Fm\(\overline{3}\)m).\(^\text{19}\) The Fe\(_2\)SiO\(_4\) crystal structure was composed of 672 (Fe 192, Si 96 and O 384) atoms according to an array of \(4 \times 2 \times 3\) unit cells of Fe\(_2\)SiO\(_4\) (orthorhombic, \(Pbnm\)).\(^\text{20}\) The interatomic configurations for liquid phases were set to be random in the cubic cell. The total number of atoms was taken to be from 1000 to 1500. The densities of initial liquid cells were adopted to be 2200 to 2700 kg/m\(^3\) for liquid phases were set to be random in the cubic cell. The total number of atoms was taken to be from 1000 to 1500.

### 3. Results and Discussion

#### 3.1 Structural property

The structural stability of solid FeO and Fe\(_2\)SiO\(_4\) with potential model used in this study was assessed by calculation of structural parameters such as lattice constants, molar volumes and nearest-neighbor distances between ions at 300 K. The calculated structural parameters of solid FeO and Fe\(_2\)SiO\(_4\) at 300 K are reasonably well reproduced within negligible deviation with measured results\(^\text{9,20}\) as shown in Table 2.

Table 3 shows the structural parameters estimated from the pair distribution functions and running coordination numbers between ions in solid FeO just below melting point of 1650 K and molten FeO at 1700 K with measured results.\(^\text{21,22}\) The pair distribution function, \(g_{ij}(r)\), and running coordination number, \(N_{ij}(R)\), of the simulated system can be calculated by eqs. (2) and (3).

\[
g_{ij}(r) = \frac{V}{N_i N_j} \sum_j \frac{\langle n_i(r - \Delta r/2, r + \Delta r/2) \rangle}{4\pi r^2 \Delta r}
\]

\[
N_{ij}(R) = 4\pi \rho_i \int_0^R r^2 g_{ij}(r)dr
\]

where \(\langle n_i(r - \Delta r/2, r + \Delta r/2) \rangle\) is the average number of ion \(j\) surrounding ion \(i\) in a spherical shell within \(r \pm \Delta r/2\), \(N_i\) and \(N_j\) are the total number of ions \(i\) and \(j\), \(V\) is the volume of the system, \(\rho_i\) is the partial number density of ion \(i\) and \(R\) is the distance of the first minimum of \(g_{ij}(r)\). The calculated nearest-neighbor distances and coordination numbers between ions for solid FeO are in good agreement with measured results by Waseda et al.\(^\text{21,22}\) In the case of molten FeO, Waseda et al. reported that the octahedral site is realistic with respect to the position of Fe\(^{2+}\) ions based on the coordination number of Fe–O pairs, which was \(n_{Fe\cdotO} = 5.7\) atoms at \(T_{Fe\cdotO} = 0.205\) nm. However, the calculated nearest-neighbor distance and coordination number of Fe–O pairs show a difference with measured results as shown in Table 3.
These differences are considered due to the kinetic effect by high heating rate in this study. Nevertheless, MD calculation has successfully represented the nearest-neighbor distances and coordination numbers between ions in solid FeO just below melting point and molten FeO.

Figure 1 shows the calculated pair distribution functions of Si–Si, Si–O, Fe–O and O–O in molten Fe$_2$SiO$_4$ at 1600 K with observed results.$^{21}$ The positions of first peak of calculated pair distribution functions are $r_{\text{Si-Si}} = 0.32$ nm, $r_{\text{Fe-O}} = 0.19$ nm, $r_{\text{Si-O}} = 0.16$ nm and $r_{\text{O-O}} = 0.265$ nm, which show good agreement with the nearest-neighbor distances of ion pairs measured by Waseda et al.$^{21}$

The degrees of polymerization in FeO–SiO$_2$ melts are assessed by the fractions of oxygen species such as bridging (O$^\circ$), non-bridging (O$^\sim$) and free (O$^2-$) oxygen calculated as a function of composition. The cut-off distance between Si and O ions for the calculation of oxygen species was determined by minimum position of first peak in silicon–oxygen pair distribution function, $g_{\text{Si-O}}(r)$. Figure 2 shows the silicon–oxygen pair distribution functions calculated as a function of composition at 1873 and 3000 K. These results represent that the silicon–oxygen pair distribution functions do not have special composition and temperature depend-

### Table 2 Observed and calculated structural parameters for FeO and Fe$_2$SiO$_4$ at 300 K.

<table>
<thead>
<tr>
<th></th>
<th>FeO [Space Group: Fm$ar{3}$m]</th>
<th>Fe$_2$SiO$_4$ [Space Group: Pbnm]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Observed$^{[29]}$</td>
<td>Calculated</td>
</tr>
<tr>
<td>$a$ (nm)</td>
<td>0.431</td>
<td>0.442</td>
</tr>
<tr>
<td>$b$ (nm)</td>
<td>0.431</td>
<td>0.442</td>
</tr>
<tr>
<td>$c$ (nm)</td>
<td>0.431</td>
<td>0.442</td>
</tr>
<tr>
<td>$V$ ($10^{-6}$m$^3$/mol)</td>
<td>12.06</td>
<td>12.99</td>
</tr>
<tr>
<td>Fe–O (nm)</td>
<td></td>
<td>0.218</td>
</tr>
<tr>
<td>Si–O (nm)</td>
<td></td>
<td>0.163</td>
</tr>
<tr>
<td>O–O (nm)</td>
<td></td>
<td>0.266</td>
</tr>
</tbody>
</table>

### Table 3 Structural parameters estimated by pair distribution functions, $g_{ij}(r)$, and running coordination numbers, $N_{ij}(R)$, of solid and molten FeO with experimentally measured results. ($r_{ij}$: first peak positions of pair distribution functions, $n_{ij}$: coordination numbers)

<table>
<thead>
<tr>
<th></th>
<th>Fe–Fe</th>
<th>Fe–O</th>
<th>O–O</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$r_{ij}$, nm</td>
<td>$n_{ij}$, atoms</td>
<td>$r_{ij}$, nm</td>
</tr>
<tr>
<td>Solid state just below melting point</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Present work $^{[1650K]}$</td>
<td>0.315 13</td>
<td></td>
<td>0.200 6</td>
</tr>
<tr>
<td>Waseda et al.$^{[21,22]}$</td>
<td>0.311 12</td>
<td></td>
<td>0.216 5</td>
</tr>
<tr>
<td>Molten state</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Present work $^{[1700K]}$</td>
<td>0.320 12.5</td>
<td>0.185 4.2</td>
<td>0.320 12.0</td>
</tr>
<tr>
<td>Waseda et al.$^{[1673K]}$</td>
<td>0.320 11.4</td>
<td>0.206 5.5</td>
<td>0.320 11.4</td>
</tr>
<tr>
<td>$^{[1693K]}$</td>
<td>0.315 11.8</td>
<td>0.205 5.7</td>
<td>0.320 12.2</td>
</tr>
</tbody>
</table>

Fig. 1 Calculated and observed pair distribution functions in molten Fe$_2$SiO$_4$ at 1600 K.

Fig. 2 Calculated pair distribution functions of Si–O, $g_{\text{Si-O}}(r)$, on the composition of the FeO–SiO$_2$ system at 1873 and 3000 K.
Thermodynamic modeling

The maximum value at about 40 mol% SiO$_2$ content, and the fraction of non-bridging oxygen represents
differences in FeO–SiO$_2$ melts. Therefore, in this study, the cut-off
distance between silicon and oxygen was determined to be 0.235 nm. Figure 3 shows the fractions of oxygen species
(bridging, non-bridging and free oxygen) calculated as a function of composition at 1873 and 3000 K with the
thermodynamic modeling result calculated from the equilibrium constant, eq. (5), of oxygen equilibrium reaction,
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The coefficient of iron calculated in this study is in good agreement with estimated results by electrical conductivity for Fe$_2$SiO$_4$ of Wejnarth, and the apparent activation energy for diffusion of iron estimated from calculated self-diffusion coefficients, about 50 kJ/mol, is also in good agreement with results by Agarwal et al. and Wejnarth of 73 ± 10 kJ/mol and about 35 kJ/mol. Figure 6 shows the self-diffusion coefficients of Fe–SiO$_2$ melts at 1600 K. The calculated self-diffusion coefficients of each ion show the relationship of $D_{Fe} > D_{O} > D_{Si}$ and decrease with increasing SiO$_2$ content in FeO–SiO$_2$ melts. These results represent reasonably well the structural properties of FeO–SiO$_2$ melts, which restrict the diffusion of silicon and oxygen by the formation of silica network structure in melts.

### 3.3 Thermodynamic property

#### 3.3.1 Enthalpy of pure FeO and Fe$_2$SiO$_4$

The enthalpies of solid and liquid FeO and Fe$_2$SiO$_4$ were calculated as a function of temperature. The enthalpy of simulated system can be directly calculated from the internal energy, pressure and volume obtained by MD simulation. The calculated enthalpies are compared with observed results at the sufficiently high reference temperature above the Debye temperature to neglect the quantum correction terms in this study. The Debye temperature for oxides and silicates is typically from 800 to 1200 K. The enthalpy of simulated system, $H_T$, can be calculated by eq. (8). The internal energy, $U_T$, which is given by eq. (9), is obtained as the sum of kinetic and potential energies calculated by the MD simulation. The heat capacity at constant pressure, $C_p$, can be calculated from the temperature dependence of enthalpy according to eq. (10).

$$H_T = U_T + PV_T$$  \hfill (8)

$$U_T = \sum_{i<j} \sum_{n} \phi_n(r) + \frac{3}{2} N k_B T$$  \hfill (9)

$$C_p = \left( \frac{\partial H}{\partial T} \right)_p$$  \hfill (10)

where $N$ is the number of ions of system, $k_B$ is the Boltzmann constant and $T$ is the absolute temperature.

Figure 7 shows the calculated enthalpies of solid and liquid FeO with observed results at reference temperature of 1000 K. The calculated melting temperature and enthalpy of fusion for FeO are 1670 ± 20 K and 25 kJ/mol, which show good agreement with observed results of 1650 K and 24 kJ/mol. Figure 8 shows the enthalpies of solid and liquid Fe$_2$SiO$_4$ calculated as a function of temperature at reference temperature of 1000 K. The calculated melting temperature and enthalpy of fusion for Fe$_2$SiO$_4$ are to be 1450 ± 20 K and 36 kJ/mol. The calculated melting temperature is in good agreement with measured result of 1490 K. However, the calculated enthalpy of fusion is lower than measured results of 92 kJ/mol. This difference is considered due to the several reasons such as the overestimation of Coulombic energy on the ion charges, polarization of the ions, crystalline field effect of iron ions and the kinetic effect by the high heating rate. However, it is not clear yet. Nevertheless, the MD calculation has successfully represented the temperature dependence of enthalpies of solid and liquid phases, in spite
of the perfect crystal cells without defects such as vacancy and dislocation. Therefore, the potential model used in this study is reasonable to calculate the thermodynamic properties of FeO–SiO$_2$ system. The calculated thermodynamic properties of FeO and Fe$_2$SiO$_4$ are summarized in Table 4.

### 3.3.2 Enthalpy of mixing for the FeO–SiO$_2$ system

The enthalpy of mixing for the FeO–SiO$_2$ system can be directly calculated by MD simulation at various compositions and temperatures. The enthalpy of mixing was calculated as a difference between the enthalpy of solution at certain composition and the sum of the enthalpies of pure components according to eq. (11).

\[
\Delta H^M = H_{A-B} - (X_A H_A^M + X_B H_B^M)
\]  

where $H_{A-B}$ is the molar enthalpy of A and B binary solution, $H_A^M$ and $H_B^M$ are the standard molar enthalpies of component A and B, $X_A$ and $X_B$ are the mole fractions of component A and B, respectively.

Figure 9 shows the enthalpy of mixing for the FeO–SiO$_2$ system calculated as a function of composition at various temperatures. The enthalpy of mixing was calculated by using a quasi-lattice model suggested by Lin et al.\textsuperscript{29} and Rey.\textsuperscript{31} The calculated enthalpy of mixing below 2000 K shows almost the same values within calculation error range of 2 kJ/mol in this study. However, the calculated enthalpy of mixing shows an abrupt positive variation in the silica-rich region from 2000 to 2700 K, and then decreases with increasing temperature. Figure 10 shows the enthalpies of mixing for the FeO–SiO$_2$ and CaO–SiO$_2$ systems calculated by MD simulation compared with thermodynamic modeling results estimated by previous researchers.\textsuperscript{29,30} These MD calculation results are in good agreement with thermodynamic modeling results. These results show that the MD calculation is a useful method for the calculation of enthalpies of mixing for the MO–SiO$_2$ systems, where $M$ = Ca, Mn, Fe, Pb and so forth.

### 3.3.3 Entropy of mixing for the FeO–SiO$_2$ system

For the calculation of entropy of mixing for the FeO–SiO$_2$ system, we assumed that each Si atom in FeO–SiO$_2$ melts is associated with four oxygen ions, and Si and O atoms are randomly distributed in the tetrahedral quasi-lattice site. The entropy of mixing has been calculated by using a quasi-lattice model suggested by Lin et al.\textsuperscript{29} This model is expressed by multiplicity for the random distribution of O$^2-$ ions and Si atoms on the lattice site ($\Omega_1$ in eq. (12)) and that of bridging oxygen ions over neighboring Si–Si pair positions ($\Omega_2$ in eq. (12)). The entropy of mixing according to $\Omega_1$ and $\Omega_2$ can be expressed as eq. (14).

\[
\Omega_1 = \frac{(N^O(X_{SiO_2} + N_{O:-}))!}{(N^O(X_{SiO_2}))!(N^O N_{O:-})!}
\]

\[
\Omega_2 = \frac{(N^O(N_{Si-Si}))!}{(N^O N_{O:-})!(N^O N_{Si-Si} - N^O N_{O:-})!}
\]  

![Fig. 9](image1.png)  
Fig. 9 Calculated enthalpy of mixing as a function of composition for the FeO–SiO$_2$ system at various temperatures.

![Fig. 10](image2.png)  
Fig. 10 Calculated enthalpies of mixing as a function of composition for the FeO–SiO$_2$ and CaO–SiO$_2$ systems at various temperatures with thermodynamic modeling results.
The calculated entropy of mixing for the FeO–SiO$_2$ system with thermodynamic modeling results.

$$N_{SI-SI} = \frac{4X_{SiO}}{2} \left( \frac{X_{SiO}}{X_{SiO} + N_{O'}} \right)$$

$$\Delta S^M = k \ln(\Omega_1/\Omega_2) = -R \left[ X_{SiO} \ln \left( \frac{X_{SiO}}{X_{SiO} + N_{O'}} \right) \right.$$  

$$+ N_{O'} \ln \left( \frac{N_{O'}}{X_{SiO} + N_{O'}} \right) + N_{O'} \ln \left( \frac{N_{O'}}{N_{Si-Si}} \right)$$

$$\left. + \left( N_{Si-Si} - N_{O'} \right) \ln \left( \frac{N_{Si-Si} - N_{O'}}{N_{Si-Si}} \right) \right]$$

where $N^0$ is Avogadro’s number, $X_A$ is a mole fraction of component $A$ in the A–B binary system, $N_{O'}$, $N_{O}$ and $N_{O'}$ are the number of moles of various oxygen species per mole of solution and $N_{SI-SI}$ is the number of moles of neighboring Si–Si pair per mole of solution.

Figure 11 shows the calculated entropy of mixing for the FeO–SiO$_2$ system at 1873 K based on the fractions of oxygen species at each composition obtained by the MD simulation as shown in Fig. 3 with the results calculated by equilibrium constant ($K_{1873K} = 0.17$) of oxygen equilibrium reaction reported by Toop et al. and thermodynamic modeling by Lin et al.

The calculated entropy of mixing for the FeO–SiO$_2$ system is in good agreement with thermodynamic modeling results reported by previous researchers. The entropy of mixing has been successfully assessed by the fractions of oxygen species calculated from the MD simulation.

3.3.4 Gibbs energy of mixing for the FeO–SiO$_2$ system

The Gibbs energy of mixing for the FeO–SiO$_2$ system was calculated from the enthalpy and entropy of mixing obtained by MD simulation. Figure 12 shows the calculated Gibbs energy of mixing as a function of composition at various temperatures for the FeO–SiO$_2$ system.

$$\Delta G^\theta_{1450K} = -8.7 \text{kJ/mol}$$

$$\Delta G^\theta = -10100 + 0.93T1/\text{mol}$$

Figure 13 shows the calculated standard Gibbs energy of formation of solid Fe$_3$SiO$_4$ from liquid FeO and SiO$_2$, eq. (15), as a function of temperature. This calculation result is in good relationship with estimated and observed results within the allowable error range for the calculation of thermodynamic properties.

Figure 14 shows the phase diagram for the FeO–SiO$_2$ system estimated by MD calculation with observed result. In this study, the solid–liquid phase equilibrium in the SiO$_2$-rich region for the FeO–SiO$_2$ system has been clearly calculated. Because the potential model of Tsuneyuki et al. adopted for the calculation of SiO$_2$ in this study has not exactly reproduced the thermodynamic properties such as solid phase transitions and fusion data of cristobalite. However, the calculated phase diagram is in good agreement with observed result in the range from pure iron to fayalite.
4. Conclusions

The thermodynamic, structural and transport properties for the FeO–SiO$_2$ system were calculated by MD simulation using Born-Mayer-Huggins type potential model. The calculated thermodynamic and structural properties of FeO and Fe$_2$SiO$_4$ successfully assessed the measured results. The calculated pair distribution functions and the fractions of oxygen species with silicon atoms were in good agreement with previously measured and estimated results. The self-diffusion coefficients of Fe, Si and O ions in the Fe$_2$SiO$_4$ and FeO–SiO$_2$ melts at various temperatures and compositions have been estimated from MD calculation. The enthalpy and entropy of mixing for the FeO–SiO$_2$ system can be calculated by the thermodynamic parameters obtained from MD calculation and quasi-lattice model based on the calculated fraction of oxygen species. The calculated phase diagram for the FeO–SiO$_2$ system shows good agreement with observed result in the range from pure iron to fayalite, and the liquid–liquid immiscibility region in the FeO–SiO$_2$ system has also been assessed. These calculation results show that the MD simulation can be used for the calculation of structural, transport and thermodynamic properties and the estimation of phase diagrams for the silicate systems at high temperature.

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