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THERMODYNAMIC PROPERTIES OF IRON, ALUMINUM, BORON, AND PHOSPHORUS IN DILUTE SILICON SOLUTIONS BY MOLECULAR INTERACTION VOLUME MODEL

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Abstract

The thermodynamic properties of impurity components in silicon solutions play an important role in the chemical removal process to the metallurgical route. In this paper, the component activity coefficients and interaction parameters of dilute silicon solutions were estimated by the molecular interaction volume model (MIVM). The activity coefficients (γ_i) of component *i* in dilute binary S*i*-i and ternary S*i*-*i*-*j* solutions at 1687-1873 K were firstly calculated. The concentration dependences of the interaction parameter and activity coefficient were also obtained. The self-interaction parameters (ε_i^I) for S*i*-*i* system were obtained as $\varepsilon_B^B = -2.728 - 362.031/T$, $\varepsilon_{AII}^{AI} = 2.157 - 1876.776/T$, $\varepsilon_{Fe}^F = -4.842 + 14445.926/T$ and $\varepsilon_P^P = -2.543 + 13767.036/T$. At the same time, the interaction parameters among components B, Al, and Fe in dilute ternary S*i*-*i* solutions were also derived as $\varepsilon_B^{Fe} = -1.2758 - 2946.306/T$, $\varepsilon_{AII}^{BI} = 0.7467 - 9765.9298/T$ and $\varepsilon_{AII}^F = -1.39677 + 3319.6803/T$. Most important of all, the temperature dependences of the interaction parameters and activity coefficients in dilute S*i*-*i* and S*i*-*i* solutions with a certain *i* or *j* concentration were deduced. The results show that the predicted self-interaction parameters of B, Al, Fe, and P in binary silicon solutions reasonably agree with the experimental data. This further shows that MIVM is of reliability and can be expanded to a multi-component dilute silicon solution.

Keywords: Molecular interaction volume model; Activity coefficient; Interaction parameter; Silicon solution

1. Introduction

With the increase of energy consumption in the wo rld, renewable resources become fewer. Solar energy is an important renewable energy source that is considered to be promising in the future. However, the process of producing solar energy materials is complicated, resulting in the high cost of solar cells production [1, 2]. An expensive semiconductor grade silicon (SEG-Si, >99.999999%) yielded from the chemical method is used as a solar cell to convert solar energy to electric power. However, SEG-Si for solar cell supply is restricted and extravagant. We have to develop an innovative process for the production of solar grade silicon (SoG-Si, >99.9999%) with low energy consumption in order to spread solar cell system widely [3].

The typical impurity elements such as boron, phosphorus, aluminum, calcium, and iron play an important role in silicon materials and simultaneously

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exert a pronounced and negative influence upon the photoelectric properties of SoG-Si [4, 5]. Many researchers focused on impurity removal from silicon solutions using the metallurgical route. The thermodynamic parameters of these impurity components in silicon solutions are crucial to study the reactions between impurity elements and oxidizing mediums. In order to supply help to the removal of impurity elements in MG-Si solution, Miki et al. [6, 7] measured the activity and interaction coefficients of some impurity components in silicon. However, not enough experimental and computational data have been collected and used for the research of impurity removal so far. Therefore, a unique economic and effective method to estimate the thermodynamic parameters of silicon solutions depending on less experimental data by a computational module is required. Safarian et al. [8] calculated the activities of elements such as Al, Ca, and Mg in silicon solutions through a quasi-regular



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solution model. There is a good correlation between the calculated activities and the reported activity data in the literature. However, the component activity coefficients of dilute Si-Me solutions were just calculated at 1687 K (the melting point of silicon) and the interaction parameters were not calculated and mentioned. Matsumiya et al. [9] predicted the activity coefficients and the interaction parameters of the solute components in infinite dilute Si solutions by the use of first-principles calculations based on the density functional theory (DFT). The calculated activity coefficients and interaction parameters of Al, Fe, Ti, and Pb in Si solutions are roughly in agreement with the results of the experiments but there are some quantitative discrepancies from the experimental results.

Due to the complexity of high-temperature experiments and the limitations of experimental accuracy, it is difficult to obtain thermodynamic data by experimental means under certain conditions. In addition, the reproducibility of the measurement results is also poor. The differences between the results of different researchers are also very large and even the signs are the opposite. In addition, there are many binary and ternary alloy systems, and it is impossible to rely on experiments to fill this huge data gap. Therefore, many scientific researchers try to use the thermodynamic model to predict the activity coefficient of the component. For example, Wilson [10] proposed Wilson's equation in 1964; Lupis et al. [11] proposed a quasinormal solution theoretical model in 1967; Zhou [12] proposed a new generation of geometric models in 1997. However, these models are only applicable to a specific system and a specific concentration range. The MIVM model [13] has a clear physical basis and can predict the thermodynamic properties of different types of universal multi-alloy systems. Moreover, the model is inclusive and can be reverted to the well-known Wilson equation, Flory-Huggins equation and NRTL equation under certain conditions, and the thermodynamic consistency and diffusion stability satisfy the Gibbs-Duhem equation. The MIVM that was invented by Tao [14-16] was derived from the statistical thermodynamics and was of better and reliability stability to predict the thermodynamic parameters of binary and multicomponent alloy solutions. Tao derived a new expression of the regular partition function of liquids and their mixtures based on statistical thermodynamics. The concept and expression of the local coordination number of liquid mixtures were proposed, and the molecular interaction volume model was deduced.

In the present work, the component activity coefficients and some meaningful interaction

parameters in dilute binary and ternary silicon solutions at 1687-1873 K have been calculated by the MIVM. The results will be significant to guide and optimize the purification techniques of silicon for metallurgical route. Furthermore, this work supplies an important method in the theoretical research of silicon material and many thermodynamic parameters of silicon solutions will be calculated.

2. Thermodynamic background

According to the definition of molecular interaction volume model by Tao [10], the molar excess Gibbs energy G_m^E of mixed solution i-j is expressed as Eq. (1).

$$\frac{G_{m}^{E}}{RT} = x_{i} \ln \left(\frac{V_{mi}}{x_{i}V_{mi} + x_{j}V_{mj}B_{ji}} \right) + x_{j} \ln \left(\frac{V_{mj}}{x_{j}V_{mj} + x_{i}V_{mi}B_{ij}} \right) -$$
(1)
$$\frac{x_{i}x_{j}}{2} \left(\frac{Z_{i}B_{ji} \ln B_{ji}}{x_{i} + x_{j}B_{ji}} + \frac{Z_{j}B_{ij} \ln B_{ij}}{x_{j} + x_{i}B_{ij}} \right)$$

where x_i and x_j are the molar fractions of components i and j, V_{mi} and V_{mj} the molar volumes, Z_i and Z_j the nearest molecules that construct a molecular cell or first coordination shell surrounding a center molecule i and j. B_{ij} and B_{ji} the pair-potential parameters for the i-j binary system and are defined as Eq. (2).

$$B_{ji} = \exp[-(\varepsilon_{ji} - \varepsilon_{ii}) / kT], B_{ij} = \exp[-(\varepsilon_{ij} - \varepsilon_{jj}) / kT] \quad (2)$$

where ε_{ii} , ε_{jj} and ε_{ij} are the pair-potential energies of i-i, j-j and i-j, respectively. $\varepsilon_{ij} = \varepsilon_{ji}$. k is the Boltzmann constant. The expressions of activity coefficient for component i and component j (γ_i , γ_j) are listed as Eqs. (3) and (4, as well).

$$\ln \gamma_{i} = \ln \left(\frac{V_{mi}}{x_{i}V_{mi} + x_{j}V_{mj}B_{ji}} \right) + x_{j} \left(\frac{V_{mj}B_{ji}}{x_{i}V_{mi} + x_{j}V_{mj}B_{ji}} - \frac{V_{mi}B_{ij}}{x_{j}V_{mj} + x_{i}V_{mi}B_{ij}} \right) - (3)$$

$$\frac{x_{j}^{2}}{2} \left(\frac{Z_{i}B_{ji}^{2} \ln B_{ji}}{(x_{i} + x_{j}B_{ji})^{2}} + \frac{Z_{j}B_{ij} \ln B_{ij}}{(x_{j} + x_{i}B_{ij})^{2}} \right)$$

$$\ln \gamma_{j} = \ln \left(\frac{V_{mj}}{x_{j}V_{mj} + x_{i}V_{mi}B_{ij}} \right) - x_{i} \left(\frac{V_{mj}B_{ji}}{x_{i}V_{mi} + x_{j}V_{mj}B_{ji}} - \frac{V_{mi}B_{ij}}{(x_{j} + x_{i}B_{ij})^{2}} \right) - (4)$$

$$x_{i}^{2} \left(Z_{i}B_{ii}^{2} \ln B_{ij} - Z_{i}B_{ij} \ln B_{ij} \right)$$

 $\frac{1}{2} \left(\frac{j \cdot j}{(x_j + x_i B_{ij})^2} + \frac{j \cdot j}{(x_i + x_j B_{ji})^2} \right)$ Expanding Eq. (1) to a multi-component silicon solution i-j-k, the molar excess Gibbs energy can be expressed as Eq. (5).



$$\frac{G_m^E}{RT} = \sum_{i=1}^n x_i \ln\left(\frac{V_{mi}}{\sum_{j=1}^n x_j V_{mj} B_{ji}}\right) - \frac{1}{2} \sum_{i=1}^n Z_i x_i \left(\frac{\sum_{j=1}^n x_j B_{ji} \ln B_{ji}}{\sum_{k=1}^n x_k B_{ki}}\right)$$
(5)

The activity coefficient of component i in solution is expressed as Eq. (6).

$$\ln \gamma_{i} = 1 + \ln \left(\frac{V_{mi}}{\sum_{j=1}^{n} x_{j} V_{mj} B_{ji}} \right) - \sum_{k=1}^{n} \left(\frac{x_{k} V_{mi} B_{ik}}{\sum_{j=1}^{n} x_{j} V_{mj} B_{jk}} \right)$$
$$- \frac{1}{2} \left(\frac{Z_{i} \sum_{j=1}^{n} x_{j} B_{ji} \ln B_{ji}}{\sum_{k=1}^{n} x_{k} B_{ki}} + \sum_{j=1}^{n} \left(\frac{Z_{j} x_{j} B_{ij}}{\sum_{k=1}^{n} x_{k} B_{kj}} \right) \left(\ln B_{ij} - \frac{\sum_{k=1}^{n} x_{k} B_{ij}}{\sum_{k=1}^{n} x_{k} B_{kj}} \right) \right)^{(6)}$$

For the binary system i-j, the infinite dilution activity coefficients are evolved and shown in Eqs. (7) and (8).

$$\ln \gamma_{i}^{\infty} = 1 - \ln \left(V_{mj} B_{ji} / V_{mi} \right) - V_{mi} B_{ij} V_{mj} - \frac{1}{2} \left(Z_{i} \ln B_{ji} + Z_{j} B_{ij} \ln B_{ij} \right)$$

$$\ln \gamma_{j}^{\infty} = 1 - \ln \left(V_{mi} B_{ij} / V_{mj} \right) - V_{mj} B_{ji} V_{mi} - \frac{1}{2} \left(Z_{i} \ln B_{ij} + Z_{i} B_{ji} \ln B_{ji} \right)$$
(8)

Based on the infinite dilution activity coefficients γ_i^{∞} , γ_j^{∞} of the binary alloy solutions and the value of the related parameters of their pure components in Table 1 [17-19], the required binary parameters B_{ij} and B_{ji} can be obtained by Eqs. (7) and (8) by using the Newton-Raphson methodology [13]. The coordination number Z_i of liquid components was available in document [20].

Meanwhile, B_{ij} and B_{ji} at other temperature can be obtained from Eq. (2), in which the pair-potential energy interaction parameters– $(\varepsilon_{ji}-\varepsilon_{ij})/k$ and – $(\varepsilon_{ij}-\varepsilon_{jj})/k$ is assumed to be independent of temperature when the values of B_{ij} and B_{ji} at a given temperature are known. Substituting the parameters B_{ij} and B_{ji} into Eqs. (2) and (3), the component activities of binary Si-Al, Si-Fe and Si-P solutions can be obtained. The required binary parameters B_{ij} and B_{ji} and the infinite dilution activity coefficients of the binary alloy solutions are shown in Table 2, respectively [21-24].

3. Results and discussion

The MIVM was derived from the statistical thermodynamics, which is of better stability and reliability to predict the activity coefficients of binary, ternary, and even multi-component alloy solutions at the whole composition range. In our previous work, the binary Si-Al and Si-Fe solutions

were selected as examples for verifying effectiveness of MIVM at the whole composition range [25, 26]. Then, the binary Si-B and Si-P solutions could also be worked out. The calculations were employed at the same temperature as experiments for the binary Si-B, Si-Al, Si-Fe and Si-P systems by Eqs. (2-4). The activity values calculated by the MIVM model were compared with the experimental values reported in the literature [23] as shown in Fig. 1. It was found that the activities of components Si, P, Fe in the binary Si-P and Si-Fe solutions calculated by MIVM were completely in accord with the determined experimental results at the whole composition range of solutions. In spite of some differences in a high P concentration range, they were still accordant in a low P concentration range for the Si-P solution. Considering all these, it was confirmed that the prediction to the component activities in binary Si-Fe and Si-P solutions by MIVM were basically reasonable and reliable. At the same time, this model was also the base of the component interaction parameters in the solutions.



Figure 1. Calculated activities of related binary solutions by MIVM (lines) and by experimental data (points) (a) Si-Fe at 1873 K; (b) Si-P at 1700 K



i	$V_{\rm c}$ (cm ³ /mol)	AH (kJ/mol)	σ _i	d _{covi}
	· mi (********)		$(\times 10^{-8} \text{ cm})$	$(\times 10^{-8} \text{ cm})$
Si[17]	11.1[1+1.4×10-4(T-1687)]	50.63	2.64	2.25
Fe[17, 18]	7.94[1+1.3×10-4(T-1808.15)]	13.77	2.55	2.34
Al[19]	11.3[1+1.5×10-4(T-933.52)]	10.46	2.86	2.36
B[19]	4.64	22	1.96	1.76
P[17]	16.9	0.63	2.21	1.89

Table 1. Related parameters of components in Si-based solutions

Table 2. Values of γ_i^{∞} and γ_j^{∞} , B_{ij} and B_{ij} , Z_i and in relevant solutions *i*-*j*

i-j	T /K	γ_i^{∞}	γ_j^{∞}	\mathbf{B}_{ij}	B_{ji}	Z _i	Z_{j}		
Si-Fe[21, 22]	1873	0.00132	0.0162	2.5204	0.189	7.5543	10.2351		
Si-Al[23]	1700	0.416	0.495	1.2793	0.8827	7.9532	8.2782		
Si-B[23]	1873	4.199ª	3.835 ^b	0.8271	0.8266	7.5543	8.3723		
Si-P[23]	1700	0.765	0.125	1.2916	1.2254	7.9532	3.0417		
Fe-B[23]	1873	0.0118	0.0119	1.317	1.4315	10.2351	8.3723		
Al-B[23]	1873	_	—	1.4865	0.4964	8.0439	8.3723		
Fe-Al[23]	1900	0.054	0.034	1.2611	1.3008	9.4477	7.8875		
a The value of γ_{si}^{∞} is estimated from Ref. [22]									
b The value of $\gamma_{\rm B}^{\infty}$ is obtained from Ref. [24]									

It is too rough to get the activities of components Fe and P in binary solutions at the whole composition range. The mass concentration (w_i , ppmw) of impurity component i in MG-Si is usually very low. The activities of these components in dilute silicon solutions with a mass concentration range of 1-2000 ppmw were calculated by MIVM and shown in Fig. 2. It was found that the activity of component i with the same mass concentration in the dilute binary silicon



Figure 2. Calculated activities of B, Al, Fe and P in dilute binary silicon solutions at a concentration range of 1 ~ 2000 ppmw at 1693 K

solution was $a_B > a_{Al} > a_P > a_{Fe}$. They even had the difference of one or several orders of magnitude.

The Wagner's equation [27] for the component interaction parameter in solution is frequently used to represent the thermodynamic parameters of dilute solutions, particularly for the iron-based alloys. It is often used to calculate the component activity coefficients in at finite solutes using the first or the second order interaction parameters. In this paper, the second and the higher-order interaction parameters are neglected. The Wagner's equation for dilute binary solution can be defined as Eq. (9).

$$\ln \gamma_i = \ln \gamma_i^\infty + x_i \varepsilon_i^i \tag{9}$$

The concentration (x_i) dependence of component activity coefficients (γ_i) at 1873 K was estimated and the relation between $\ln \gamma_i$ and x_i are shown in Fig. 3.

The effectiveness of MIVM has been verified in Ref. [13-16] and the predicted activity coefficients are in good agreement with both the experimental results and the calculated ones by the Wagner's equation. Therefore, the interaction parameters can be indirectly acquired by Eq. (9) based on the calculated results of MIVM. Then, the self-interaction parameters can be estimated by the logarithm fitting of the activity coefficient as a function of solute concentrations





Figure 3. Activity coefficient of component i with different concentration in binary Si-i solutions at 1873 K

based on the results of MIVM. In order to remove impurities B, P, Al, and Fe from silicon, we will calculate their self-interaction coefficients for diluted silicon solutions at 1687-1873 K. The activities of solutes B, Al, Fe and P in dilute Si-B, Si-Al, Si-Fe and Si-P solutions with a certain concentration range at the temperature range of 1693-1873 K can be calculated by the MIVM. The slope and the intercept of fitting straight line represent the self-interaction parameter (ε_i^i) and the infinite dilution activity coefficient γ_i^{∞} of Si-i dilute solution at a certain temperature. The temperature dependence of self-interaction parameter can be expressed as Eq. (10).

$$\varepsilon_i^i = A + B / T \tag{10}$$

where A and B are constant. Using the least-squares method and taking ε_i^i and 1/T as the ordinate and the abscissa, A and B can be derived from Y axis and the slope, respectively.

The temperature dependences of self-interaction parameter (ε_i^i) and activity coefficient (γ_i) with a component i mass concentration of 50 ppmw at 1693-1873 K are shown in Fig. 4, which displays a reasonable agreement with the results by literatures [6, 7, 9, 22, 28-30]. The self-interaction coefficients of boron calculated using MIVM agree with those determined by Tang in Fig. 4(a). ε_{AI}^{AI} shows a good agreement with the results by Matsumiya and Tao in Fig. 4(b). However, there is a large deviation between this study and Miki et al. [6]. The main reason is that the experimental method they used for Si-AI system was at a high Al concentration. There is a good correlation between the calculated ε_{Fe}^{Fe} and the reported

data by Miki and Tao in Fig. 4(c). However, there is a large deviation from the results of the first-principles calculation method based on density functional theory by Matsumiya [9], which may be caused by the limitations of the density functional theory. The predicted value of $\varepsilon_{\rm p}^{\rm P}$ is between the experimental values of Tang, shimpo and Chen in Fig. 4(d). The self-interaction coefficient of P obtained indirectly by the MIVM model deviates from the results obtained by Shimpo [30] and Chen [29], but the results are within the same order of magnitude. This may be the poor agreement between the activity data of Si-P binary system calculated using the MIVM model and the experimental data reported in the literature, resulting in the self-interaction coefficient of P under low P concentrations having some deviation from other researchers' results. There is a certain deviation from the results of others. This result is inconsistent with the sign of that of Dalaker [28]. The reason may be that the method to obtain the self-interaction coefficient of P by FACT thermodynamic calculation software was not accurate enough. It was confirmed that a linear functional relationship between selfinteraction parameter (ε_i^i) and 1/T was obeyed by the fitting of results and Eqs. (11) - (14) can be gotten.

$$\varepsilon_{\rm B}^{\rm B} = -2.728 - 362.031/T \tag{11}$$

$$\varepsilon_{\rm Al}^{\rm Al} = 2.157 - 1876.776 / T \tag{12}$$

$$\varepsilon_{\rm Fe}^{\rm Fe} = -4.842 + 14445.926 / T \tag{13}$$

$$\varepsilon_{\rm p}^{\rm P} = -2.543 + 13767.036 / T \tag{14}$$

Although there are no related reports to the interaction parameter (ε_i^j) for the dilute ternary silicon solution, similarly with the binary solution, the Wagner's equation for the dilute ternary solution can be defined as Eq. (15).

$$\ln \gamma_i = \ln \gamma_i^{\infty} + x_i \varepsilon_i^i + x_j \varepsilon_i^j \tag{15}$$

Then, a linear functional relation between logarithm of activity coefficient $(\ln \gamma_i)$ and concentration (x_i) can be gotten as Eq. (16).

$$\ln \gamma_i - x_i \varepsilon_i^i = \ln \gamma_i^\infty + x_i \varepsilon_i^j \tag{16}$$

The concentration (x_j) dependence of component activity coefficients (γ_i) at 1873K was estimated and the relation between $\ln \gamma_i - x_i \varepsilon_i^i$ and x_j are shown in Fig. 5. For the dilute ternary SiB-Fe, SiB-Al, and Si-Al-Fe solutions, the temperature dependences of the interaction parameter (ε_i^j) and $\ln \gamma_i - x_i \varepsilon_i^i$ at 1693-1873 K are shown in Fig. 6. With the increase of temperature, the interaction parameters ε_B^{Fe} and ε_B^{Al} of the ternary dilute Si-B-Fe and Si-B-Al solutions also





Figure 4. Temperature dependences of the self-interaction parameter (ε_i^i) and the activity coefficient (γ_i) with the component i mass concentration of 50 ppmw at 1693-1873 K (a) Si-B solution; (b) Si-Al solution; (c) Si-Fe solution; (d) Si-P solution



Figure 5. Activity coefficient of component i with different j concentration of in ternary Si-i-j solutions at 1873 K



Figure 6. Temperature dependences of interaction parameter $(\varepsilon_i^{\ j})$ and $\ln \gamma_i - x_i \varepsilon_i^i$ in dilute ternary Si-i-j solution with a component j concentration of 1500 ppmw (a) Si-B-Fe solution; (b) Si-B-Al solution; (c) Si-Al-Fe solution



increase. And it is the opposite to ε_{AI}^{Fe} in the Si-Al-Fe solutions. It was confirmed that a good linear functional relationship between interaction parameter (ε_i^j) and 1/T was obeyed by the fitting of results and Eqs. (17) - (19) can be gotten.

 $\varepsilon_{\rm B}^{\rm Fe} = -1.2758 - 2946.306 / T \tag{17}$

 $\varepsilon_{\rm p}^{\rm AI} = 0.7467 - 9765.9298 / T \tag{18}$

$$\varepsilon_{\rm Al}^{\rm Fe} = -1.39677 + 3319.6803 / T \tag{19}$$

4. Conclusions

The reliability of prediction by MIVM depends on the data of the activities or the infinite dilute activity coefficient in binary silicon solutions. In this paper, the activity coefficients and self-interaction parameters of B, Al, Fe, and P in dilute binary Si-B, Si-Al, Si-Fe, and Si-P solutions were calculated and then contrasted with the results in the existing literature. They are consistent with the results in the literature. It was proved that the prediction of the component activity coefficients and the interaction parameters of silicon solutions by MIVM was credible. By comparison, the predicted results showed good agreement with the ones in the literatures. The model calculation was also applied to the ternary silicon solutions. The activity coefficients of components B, Al, and Fe in dilute ternary Si-B-Fe, Si-B-Al, and Si-Al-Fe solutions and the corresponding interaction parameters among B, Al, and Fe were obtained. The concentration dependences of the interaction parameter and the activity coefficient of dilute binary Si-i and ternary Si-i-j solutions were derived. The temperature dependences of interaction and the activity coefficients parameter were deduced and obtained by a linear fitting.

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TERMODINAMIČKE OSOBINE ŽELEZA, ALUMINIJUMA, BORA I FOSFORA U RAZREĐENIM RASTVORIMA SILICIJUMA PO MODELU JAČINE MOLEKULARNE INTERAKCIJE

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Apstrakt

Termodinamičke osobine primesa u rastvoru silicijuma imaju važnu ulogu u procesu hemijskog uklanjanja metalurškim putem. U ovom radu su procenjeni koeficijenti aktivnosti komponente i parametri interakcije razređenog rastvora silicijuma modelom jačine molekularne interakcije (MIVM). Prvo su izračunati koeficijenti aktivnosti (γ_i) komponente i u razređenom dvojnom Si-i i trojnom Si-i-j rastvoru na temperaturi od 1687-1873 K. Takođe je dobijena koncentracijska zavisnost interakcionih parametara i koeficijenata aktivnosti. Parametri samo-interakcije (\mathcal{E}'_i) za Si-i sistem dobijeni su kao $\mathcal{E}^{\rm B}_{\rm B} = -2.728 - 362.031/T$, $\mathcal{E}^{\rm AI}_{\rm AI} = 2.157 - 1876.776/T$, $\mathcal{E}^{\rm Fe}_{\rm Fe} = -4.842 + 14445.926/T$ i $\mathcal{E}^{\rm P}_{\rm P} = -2.543 + 13767.036/T$. U isto vreme, izvedeni su interakcioni parametri među komponentama B, Al i Fe u razređenom trojnom Si-i-j rastvoru kao $\mathcal{E}^{\rm Be}_{\rm Fe} = -1.2758 - 2946.306/T$, $\mathcal{E}^{\rm AI}_{\rm AI} = 0.7467 - 9765.9298/T$ i $\mathcal{E}^{\rm Fe}_{\rm AI} = -1.39677 + 3319.6803/T$. Najvažnije od svega je da su utvrđene temperaturne zavisnosti interakcionih parametara i koeficijenata i koeficijenata i soeficijenata aktivnosti u razređenim Si-i j rastvoru kao $\mathcal{E}^{\rm Fe}_{\rm AI} = 0.7467 - 9765.9298/T$ i $\mathcal{E}^{\rm Fe}_{\rm AI} = -1.39677 + 3319.6803/T$. Najvažnije od svega je da su utvrđene temperaturne zavisnosti interakcionih parametara i koeficijenata aktivnosti u razređenim Si-i j rastvorima sa određenom i ili j koncentracijom. Rezultati pokazuju da su predviđeni samo-interakcijski parametri B, Al, Fe i P u dvojnim rastvorima silicijuma u skladu sa eksperimentalnim podacima. Ovo dalje pokazuje da je MIVM pouzdan i da se može proširiti na višekomponentne razređene rastvore silicijuma.

Ključne reči: Model jačine molekularne interakcije; Koeficijent aktivnosti; Interakcioni parameter; Rastvori silicijuma.

