

SIMULATING IRON-MELT EQUILIBRIUM FOR SILICATE SYSTEMS

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Last years much attention was given to the experimental studies of metal-silicate equilibria to use that information for analysis of geochemical evolution of planets, meteorites and some igneous rocks. We have systematized the data concerning pure iron-silicate melt equilibrium to develop a generalize model of the metal solubility in molten silicate systems.

Dissolution of iron in multicomponent silicate liquid would be described by the following reaction



so that the equilibrium constant

$$K_T = a(\text{FeO,L})/a(\text{Fe,Met})f_{\text{O}_2}^{1/2} \quad , \quad (2)$$

where $a(\text{FeO,L})$ and $a(\text{Fe,Met})$ are activities of FeO in liquid and iron in metal phase. In the case of pure iron $a(\text{Fe,Met})=1$ and we rearrange (2) to

$$\lg X(\text{FeO}) = 0.5 \lg f_{\text{O}_2} + \lg K_T - \lg \gamma(\text{FeO}) \quad , \quad (3)$$

where $X(\text{FeO})$ and $\gamma(\text{FeO})$ are FeO content and activity coefficient in a melt. The standard state properties of FeO liquid could perhaps be estimated, but as following from the thermodynamic form of Eq. (3) a good approximation for FeO solubility would be also a simple empirical equation

$$\lg X(\text{FeO}) = k \lg f_{\text{O}_2} + h/T + \sum d(i)x(i) \quad , \quad (4)$$

where regression coefficients k , h and $d(i)$ make allowance for influence of oxygen fugacity, absolute temperature and melt composition $x(i)$, mol.%. It is similar to analysis of Fe³⁺/Fe²⁺ equilibrium [1] so that this approach was used for thermodynamic processing data of melting experiments performed in the presence of iron phase. To testify the linear hypothesis we have used a data set including 396 runs conducted in natural and synthetic silicate systems at atmospheric pressure, 1150-1327 C and $\lg f_{\text{O}_2} < -11$ [2-4]. Fe³⁺/FeO ratio in a melt at these conditions doesn't exceed values of 0.01-0.05 [1,5] and iron solubility could be described as total FeO content in the liquid phase.

After calculating $X(\text{FeO})$, mol.% each run liquid composition has been recalculated to iron free matrix and following processing the data was based on the multiple linear regression. The values of the constants in Eq. (4) are given in Table 1 with the standard error for each.

Table 1. Regressed constants for Eq. (4)

Variable	Coefficient	Std.error
1/T(K)	11,500.68	203.24
lg fO ₂	0.513250	0.005469
SiO ₂	0.003014	0.000992
TiO ₂	0.010094	0.001435
Al ₂ O ₃	0.001525	0.001746
MgO	0.001338	0.001035
CaO	-0.003907	0.001414
Na ₂ O	-0.017992	0.003665
K ₂ O	-0.037859	0.002380

Using the regression coefficients and T-fO₂-parameters we calculated equilibrium solubilities of iron for 396 data base experiments. Comparison with the experimental values of $\lg X(\text{FeO})$ indicate average accuracy 0.034. It is equivalent approximately to relative error of 7-8% as compared to total FeO content in silicate melts.

SIMULATING IRON-MELT EQUILIBRIUM: ARISKIN A.A. ET AL.

Using the regressed constants from Table 1 one can transform Eq.(4) to

$$\lg f_{O_2} = -22,446.53/T + 1.948 [\lg X(\text{FeO}) - \sum d(i)x(i)] \quad (5)$$

Providing known temperature and liquid composition Eq.(5) could be used to estimate redox conditions of iron-silicate melt equilibrium. Average accuracy of calculating $\lg f_{O_2}$ values for 396 base experiments [2-4] was found to be 0.066 lg unit.

Eq.(5) could be also modified to

$$T = 11,520.68 / [\lg X(\text{FeO}) - 0.51325 \lg f_{O_2} - \sum d(i)x(i)] \quad (6)$$

so that Eq.(6) enables calculating equilibrium temperatures for silicate melts saturated by metal iron. Testing the expression using data of the of the same 396 base experiments gave average accuracy 7.6 C. Thus, it is no difficult to add Eq.(6) to available systems of mineral-melt geothermometers (e.g. [6-8]) to promote development of current models simulating basalt magma crystallization.

For that purpose we have used the LUNAMAG program designed to simulate mineral-melt equilibria in FeO enriched lunar basalt and eucrite liquids [6]. Testing the new "iron" version of the LUNAMAG model was carried out based on Sioux County eucrite composition [9] investigated experimentally by E.Stolper [10]. Some preliminary modelling results characterizing metal iron stability in the system in terms of temperature and redox conditions are shown in Fig. 1:

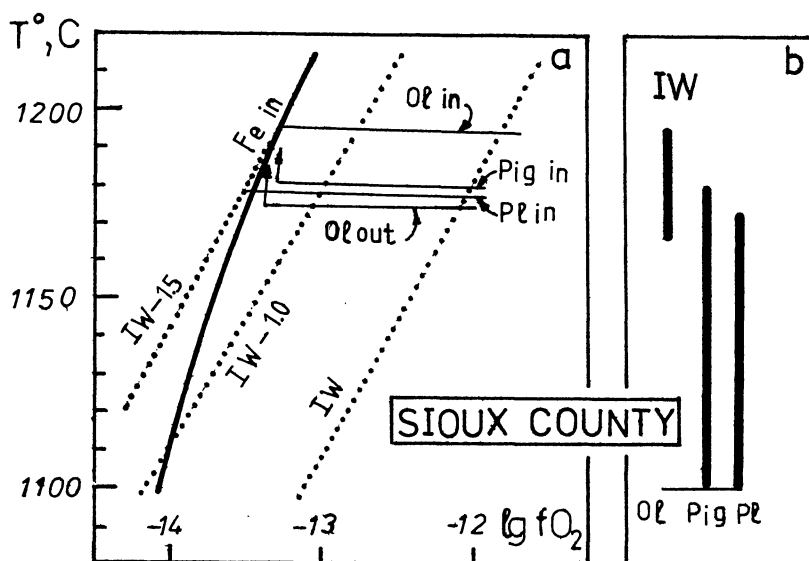


Fig. 1. Phase relations of eucrite composition
a) simulation results using LUNAMAG model [6],
b) experiments [10].

Model calculations have been performed from IW-1.5 up to IW buffer conditions with $\lg f_{O_2}$ increment being 0.1 lg unit. They are in a good agreement with Stolper's data indicating iron precipitation field to be 1 lg below IW oxygen buffer.

- REFERENCES: 1. Sack R.D. et al. *Contrib Mineral Petrol*(1980), 75, P. 369. 2. Roeder P.L. *Earth Planet Sci Lett*(1974), 23, P. 397; 3. Doyle C.D., Naldrett A.J. *Geochim Cosmochim Acta*(1986), 50, P. 435; 4. Doyle C.D. *Geochim Cosmochim Acta*(1988), 52, P. 1827; 5. Borisov A.A., Shapkin A.I. *Geokhimiya* (1989), N 6, P. 892 (in Russian); 6. Ariskin A.A., Barmina G.S., Frenkel M.Ya. *Geokhimiya* (1990), 10, P. 1476 (in Russian); 7. Nielsen R.L. *Computers and Geosciences* (1985), 11, P. 531; 8. Weaver J.S., Langmuir C.H. *Computers and Geosciences* (1990), 16, P.1; 9. Duke M.B., Silver L.T. *Geochim Cosmochim Acta* (1967), 31, P. 1637; 10. Stolper E. *Geochim Cosmochim Acta* (1977), 41, P. 587.