

FE AND NI SOLUBILITY IN SILICATE MELTS EQUILIBRATED WITH METAL

Alexander Borisov and Alexei Ariskin, Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences, Kosygin St. 19, Moscow 117975, Russia

Abstract. In the scope of our efforts to include the metallic phase into computer models simulating the melting-crystallisation relationships in meteoritic igneous systems [1-2], we present 2 empirical equations which describe the Fe and Ni solubilities in silicate melts at 1 atm as a function of temperature, oxygen fugacity and the melt composition.

Approach. The empirical basis for this study is a library of 1-atm melting experiments that have been carried out in synthetic and natural systems. Data on the equilibrium between the pure iron and silicate melts include 396 runs conducted at 1150-1327°C under controlled oxygen fugacities $-14.5 < \log f_{O_2} < -11.0$ [3-5]. The melt compositions range from "basaltic" to "andesitic", with FeO contents varying from 6 to 60 wt.%. The data set contains systems enriched both in K₂O (up to 13 wt%) and Al₂O₃ (up to 23 wt%); several experiments were conducted on magnesium-free and high-Ti compositions. The data on Ni solubility include 31 experiments on natural melts equilibrated with FeNi alloys (highly enriched in Ni) [6,7] and 22 runs conducted on An-Di eutectic composition equilibrated with the pure Ni metal [8]. These experiments were conducted in the range of temperatures 1122-1437°C and oxygen fugacities $-12.6 < \log f_{O_2} < -8.2$ and cover compositional range as large as ~3 orders of magnitude of Ni contents in the melts.

These data were processed by the least-squares fitting to obtain expressions:

$$\log X_{MeO} (Sil) / a_{Me} (Metal) = 0.5 \log f_{O_2} + h/T(K) + \sum d_i X_i, \quad (1)$$

where MeO is FeO or NiO, $a_{Me} (Metal)$ is the activity of Fe or Ni in the metal [9], and the regression parameters h and d_i account for the effects of temperature and melt composition. The division of FeO_{tot} in melts into Fe³⁺ and Fe²⁺ species was carried out using the Borisov and Shapkin's equation [10]; the X_i values (mol%) were calculated on the iron- and nickel-free basis. The calculated regression parameters with standard deviation for each are listed in Table 1.

Testing the equations. At given parameters of the regression, one can use the equation (1) to calculate FeO or NiO solubility in the experimental melts used to calibrate the equation. Plots in Fig. 1(A,C) compare the calculated values with those obtained in experiments. This fitting is good, and we would specially emphasize an excellent agreement of the calculated and experimental Ni contents at 100-200 ppm level (INAA, synthetic composition [8]) and at 1-2% level (microprobe analyses, natural compositions [6,7]). One can also invert the calculations to reproduce the oxygen fugacity or the temperature of the metal-silicate equilibrium at given FeO or NiO contents in the melts. These data are shown on Fig. 1(B,D) and indicate a high accuracy of 0.1 log units for the log f_{O_2} calculations. The difference between the calculated and experimental temperatures is shown in frequency histograms.

Conclusion. The equations presented above provide a good thermodynamic basis for the development of a numerical model simulating Fe-Ni metal-silicate equilibrium in meteoritic igneous systems [11].

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Table 1. Regression constants h and d_i for the empirical expressions (1) which best describe Fe and Ni solubilities

Variables	"Fe" equation: Constant (1 σ)	"Ni" equation: Constant (1 σ)
1/T,K	11185.7(158.7)	7771.7(909.5)
lgfO2	0.5	0.5
SiO2	0.00357(0.00100)	-0.01223(0.00452)
TiO2	0.01045(0.00149)	0.02683(0.01505)
Al2O3	0.00301(0.00176)	0.02419(0.01146)
MgO	0.00172(0.00107)	0.00275(0.00934)
CaO	-0.00411(0.00147)	-0.00950(0.00586)
Na2O	-0.02027(0.00374)	-0.04076(0.04048)
K2O	-0.03894(0.00247)	-0.05223(0.02598)

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Fig. 1. Comparison of values $\log \text{FeO}$, $\log \text{NiO}$ and $f\text{O}_2$ observed in experiments with those calculated using the parameters given in Table 1 (A, B - "Fe" equation; C, D - "Ni" equation).

