CALCULATING METAL-SILICATE EQUILIBRIA IN METEORITIC IGNEOUS SYSTEMS;

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**Abstract**.   2 empirical equations describing the solubilities of Fe and Ni in silicate melts equilibrated with metal [1] have been incorporated into a single program called SILMET. The program calculates crystallization temperatures and compositions of Fe,Ni metal at given $fo_2$'s and compositions of silicate melts.  Results of the test of the SILMET on an achondritic system are reported.

**SILMET program**.  To develop a model simulating crystallization of Ni-Fe alloys from meteoritic melts, the empirical equations describing the Fe and Ni solubilities in silicate melts [1] are necessary to link with the metal stoichiometry ($X_{Ni}+X_{Fe}=1$) and activities of Fe and Ni in the metal. The latters were calculated based on the thermodynamic model of Fe-Ni solid solutions developed in [2]. The solubility equations and the activity-stoichiometry relationships were incorporated into a single algorithm similar to that used earlier [3] to successfully model chromite-melt equilibria.  Based on the algorithm, a special petrological program SILMET has been developed. The program can be applied to a large variety of mafic igneous systems to study the effects of oxygen fugacity (mainly at low $fo_2$ values) and melt composition on the crystallization temperatures and compositions of the Fe,Ni metal equilibrated with silicate melts.

**Testing SILMET**.  To test the SILMET program, we applied this code to two melts produced by the experimental melting of the St. Severin LL chondrite [4]. The experiments have been conducted at 1200 and 1300°C and $log(fo_2)$ = -12.90 and -11.73, respectively.  In both experiments the mineral assemblage stable at 1 atm was Ol+Opx+Metal+Melt. The major element contents of the melts are listed in Table 1.  While the authors of [4] have not analyzed the experimental glasses for Ni, they found 67 and 61 mole % Fe in the metal at 1200 and 1300°C, respectively.

Using the SILMET program we tried to reproduce numerically the experimental results of [4]. A series of isobaric calculations at $log(fo_2)$ = IW-1 was performed for each given melt composition. Since Ni content in the experimental melts is unknown, this parameter was varied in the range of 10 -100 ppm with 5 ppm increment until a satisfactory fit between the calculated and experimental temperature is obtained. In the case of the "1200°C" glass, the melt having 30 ppm Ni is equilibrated with the metal containing 68.47 mole % Fe at 1199.2°C. The "1300°C" melt having 65 ppm Ni is equilibrated with the metal containing 64.56 mole % Fe at 1298.0°C. Comparison of calculated Fe contents in the metal with those obtained in experiments indicate a good reproducibility of the experimental data (Table 1).  Since equations derived in [1] were calibrated on the database which does not include experimental data of [4], such an agreement between calculated and experimental data strongly suggests that the SILMET program can be successfully used in studies of the origin and the evolution of HED parent body(s).

**Genetic implication**.  Based on melting experiments, the authors of [4] have concluded that a direct melting of a volatile-free LL chondritic precursor at $log(fo_2)$ = IW-1 produces partial melts which may be parental for most diogenites.  However, to explain origin of magnesian diogenites, an increase of MgO/FeO ratio in parental melts is necessary. Compositions of metal place additional constraints on the origin of diogenites.

The major difference between the diogenitic metal and that produced by the experimental melting of the St. Severin LL chondrite is their Ni contents.  The metal equilibrated with the chondritic melts produced in the experiments contains as much as 33-44 % Ni, whereas the metal observed in diogenites and howardites [5,6] contains only 2-5% Ni. Extremely high partition coefficients of Ni between the metal and silicate melts calculated here (Table 1) predict that parental diogenitic melts equilibrated with low Ni metal would contain only 2-10 ppm Ni. In principle, the Ni content in both metal and silicate melts may be decreased by reduction of FeO to Fe°, but then the melts equilibrated with low-Ni iron would not be able to crystallize diogenites. Therefore, the depletion of diogenites in Ni could be achieved only by a metal-silicate

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fractionation, nebular or planetary, which predates the formation of diogenitic parental magma(s). Bulk composition of such a fractionated, metal-deficient precursor would be more magnesian and silica enriched as compared to that of LL chondrites. As a result, partial melts formed in MgO- and $SiO_2$-enriched system would be able to crystallize more abundant and more magnesian orthopyroxenes.

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Table 1. Comparison of the calculated temperatures and metal compositions with those obtained in experiments

| Glass, wt% | 1300°C, $\log(fo_2)= -11.73$ | 1200°C, $\log(fo_2)= -12.90$ |
|---|---|---|
| Experiment | | |
| $SiO_2$ | 50.6 | 50.70 |
| $TiO_2$ | 0.29 | 0.47 |
| $Al_2O_3$ | 7.21 | 13.00 |
| FeO | 24.3 | 17.80 |
| MnO | 0.40 | 0.32 |
| MgO | 12.1 | 7.31 |
| CaO | 5.69 | 8.39 |
| $Na_2O$ | 0.01 | 0.69 |
| $Fe_{met}$, mole % | 61 | 67 |
| Calculation | | |
| T, °C | 1198.0 | 1199.2 |
| $Fe_{met}$, mole % | 64.56 | 68.47 |
| $Ni_{melt}$, ppm | 65 | 30 |
| $D_{Ni}$ (met/melt) | 5566 | 10883 |