

## THE IMPACT OF SILICA TO A $\text{SiO}_2\text{-MgO-FeO}_x$ SLAG

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### Abstract

The sensitivity of silica concentration in  $\text{SiO}_2\text{-MgO-FeO}_x$  nickel smelting slags is studied at three different Fe/MgO ratios using calculated phase equilibria in slag cleaning conditions in an electric furnace. According to the constructed phase diagrams, when the silica concentration exceeds 40 wt-%  $\text{SiO}_2$  the liquidus temperature increases rapidly. This study uses the thermodynamic software MTDATA and the slag database of MIRO "MTOX" for covering the liquidus surface of the oxide system of Fe-O-MgO- $\text{SiO}_2$  with modifying additions of CaO and  $\text{Al}_2\text{O}_3$ . In the results the precipitating phases from the liquid and the liquidus temperatures at silica concentrations ranging from 20 wt-% to 50 wt-%  $\text{SiO}_2$  will be discussed and compared at three Fe/MgO ratios, typical to sulphidic nickel concentrates.

## INTRODUCTION

When treating nickel slag from primary matte smelting in an electrical furnace (EF) the silica concentration varies. It consists typically of the basic system  $\text{FeO}_x\text{-MgO-SiO}_2$ . Modifying additions of  $\text{Al}_2\text{O}_3$  and  $\text{CaO}$  may occur. Usually the level of silica is between 20 and 30 wt-%, but sometimes it can reach 40 wt-%  $\text{SiO}_2$ . It is known that when the silica in the slag exceeds 40 wt-% the liquidus surface will increase rapidly because of the precipitation of tridymite ( $\text{SiO}_2$ ), see figure 1. The aim in this work is to evaluate the impact of silica on the liquidus and phase precipitation temperatures. The temperature area will be studied from 1100 °C to 1600 °C.

The calculations will be performed using NPL's software MTDATA which is developed for advanced thermodynamic calculations /2/. The data used will be retrieved from the database MTOX /3/. The database has been developed in collaboration between different parties coordinated by MIRO. A part of the database covers the thermodynamic data for the system  $\text{FeO}_x\text{-MgO-SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$ .

## COMPOSITIONS

The chosen slag system to describe the EF slag is  $\text{FeO}_x\text{-MgO-SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$ . The calculations will be done for three Fe/MgO ratios 4, 5 and 6. The silica concentration will be changed from 20 to 50 wt-% using a 2.5 wt-% step. The temperature range will be from 1100 °C to 1600 °C using a step of 10 °C. The ratio between  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  will be determined indirectly, by the partial oxygen pressure set to  $10^{-9}$  bar. The  $\text{CaO}$  and the  $\text{Al}_2\text{O}_3$  additions will be 5 and 10 wt-%. The composition for each case will be normalised to 100 wt-%. As an example of the compositions some of the original calculated input balances are reproduced in tables 1 (Fe/MgO = 4), 2 (Fe/MgO = 4 + CaO) and 3 (Fe/MgO = 4 +  $\text{Al}_2\text{O}_3$ ).

The solid and liquid substances and solution phases were taken from the mtox database and the gaseous substances from an additional pure substance (mtoxgas) database. Three different data files were created, the first one for the system Fe-O-SiO<sub>2</sub>-MgO, the second one for the system Fe-O-SiO<sub>2</sub>-MgO-CaO and the third one for the system Fe-O-SiO<sub>2</sub>-MgO-Al<sub>2</sub>O<sub>3</sub>. The phases and substances chosen for these calculations are the known stable ones. When defining the system Fe-O-SiO<sub>2</sub>-MgO 28 phases and 71 species were retrieved from the databases. In the system Fe-O-SiO<sub>2</sub>-MgO-CaO 44 phases and 105 species were retrieved from the databases. When defining the system Fe-O-SiO<sub>2</sub>-MgO-Al<sub>2</sub>O<sub>3</sub> 31 phases and 86 species were retrieved from the databases.

## CALCULATIONS

The calculations were performed using the NPL software MTDATA /2/ and the database for oxide systems MTOX developed for MIRO /3/.

The calculations were done at three different ratios of Fe/MgO = 4, 5 and 6. The silica concentration was calculated using a step of 2.5 wt-% from 20 to 50 wt-%. The temperature was changed using a step of 10 °C from 1100 to 1600 °C. The addition of  $\text{CaO}$  (5 or 10 wt-%) or  $\text{Al}_2\text{O}_3$  (5 or 10 wt-%) increased the calculation sets to a total 15. The constant partial oxygen pressure of  $10^{-9}$  bar was defined by setting the total gas pressure to  $10^{-9}$  bar and was maintained with only oxygen in the gas phase. A total of 195 diagrams were calculated including 9945 equilibrium points. The final results shown have been post processed by a spreadsheet program.

The phases considered in the slag system can be seen in tables 4, 5 and 6. In case 1 (table 4) seven potential solid phases were considered, in case 2 (+ CaO, table 5) eight and in case 3 (+ Al<sub>2</sub>O<sub>3</sub>, table 6) seven. Wollastonite was stable in some cases when the addition of CaO (table 5) was used. In some cases when the addition of Al<sub>2</sub>O<sub>3</sub> (table 6) was used cordierite stabilised, but halite did not as in the two earlier cases. The gas phase was stable in all calculations.

## RESULTS

### PRIMARY SMELTING

Primary smelting of nickel sulphide concentrates uses iron silicate slags for fluxing the iron as oxidised iron from the charge. For mineralogical reasons the slag also contains magnesia which enhances its melting properties already at low concentrations /4/, and at magnesia concentrations in excess of 10 wt-% MgO viscosity is too high for tapping. Therefore, the slag chemistry is different as compared to copper smelting.

Figure 1 shows the impact of silica concentration on the phase equilibria of a nickel smelting slag with Fe/MgO = 5 at constant oxygen pressure of  $P_{O_2} = 5.5 \cdot 10^{-7}$  bar corresponding to a high-grade nickel matte containing 4 wt-% {Fe} /4/. One can easily observe that the liquidus temperature of the slag is lowered from 1430 °C to 1300 °C when the silica concentration is increased from 20 – 22 wt-% SiO<sub>2</sub> to 37 – 38 wt-% SiO<sub>2</sub>. The primary crystallising phase is over the concentration range mostly olivine, but the cooling and tapping character of the slag may be much different at low silica concentrations as compared to slags at high silica concentrations as the smelting interval decreases from about  $T_{liq-sol} = 150$  °C to 30 °C.

Figure 2 shows the calculated phase equilibria during slag cleaning when the prevailing oxygen partial pressure gradually is lowered in an electric furnace from the primary smelting range to  $P_{O_2} = 10^{-9..-10}$  bar. The end point of slag cleaning is not directly controlled but it depends on the iron concentration of the EF-matte produced. Phase equilibrium calculated for an industrial slag with Fe/MgO = 5.3 and 33 wt-% SiO<sub>2</sub> show that the liquidus contour pushes slightly to higher temperatures by 30 °C to 40 °C. No dramatic effects are found and the melting range increases from about 70 °C to 160 °C in maximum at  $P_{O_2} = 2 \cdot 10^{-8}$  bar. The primary crystallising phase during the whole reduction step is olivine.

### EF-SLAGS

The results show that the increase of silica from 20 wt-% to 50 wt-% SiO<sub>2</sub> at the three different Fe/MgO ratios 4, 5 and 6 influences the liquidus temperature of the slag, especially when the silica concentration exceeds 40 wt-%. All the results presented here are shown in isopleths, as a function of the silica concentration in the slag.

Figures 4, 5, 6, 7 and 8 show the calculated liquidus temperatures. In figure 4, the liquidus contours for the case of Fe/MgO = 4, 5 and 6 without addition of CaO or Al<sub>2</sub>O<sub>3</sub> are displayed. In figures 5 and 6 are the corresponding results for the cases with an addition of 5 and 10 wt-% CaO, and in figures 7 and 8 are the result for the cases with 5 and 10 wt-% Al<sub>2</sub>O<sub>3</sub>, respectively.

The cases of precipitating phases for Fe/MgO = 5 as well as Fe/MgO = 4 + 5wt-% CaO and Fe/MgO = 4 + 5 wt-% Al<sub>2</sub>O<sub>3</sub> are displayed in figures 9, 10, and 11, respectively.

In figure 4 can be seen that when the silica level increases from 20 wt-%  $\text{SiO}_2$  the liquidus temperature rises at all three Fe/MgO ratios. The local maximum for the liquidus temperature is reached at 27.5 wt-% of silica. The liquidus temperature starts to decrease and reaches a local minimum at 40 to 42.5 wt-% of silica. When exceeding this point in silica concentration the liquidus level increases rapidly. The ratio Fe/MgO = 6 gives the lowest liquidus temperature when the silica concentration is lower than 40 wt-%  $\text{SiO}_2$ , but when exceeding this point a higher ratio of Fe/MgO results in a higher liquidus temperature. The solidus temperatures vary for the ratios Fe/MgO = 4, 5 and 6 between 1210 °C to 1280 °C, respectively.

In figure 5 can be seen that at 5 wt-% CaO when the silica level increases from 20 wt-% the liquidus temperatures rise at all three ratios of Fe/MgO. A local maximum for the liquidus temperature is reached at 30 wt-% of silica. The liquidus temperatures start to decrease and reach a local minimum at 42.5 to 45 wt-% of silica. When exceeding this point in silica concentration the liquidus increases rapidly. The ratio Fe/MgO = 6 gives the lowest liquidus temperature when the silica concentration is lower than 42.5 wt-%, but when exceeding this point a higher Fe/MgO ratio gives a higher liquidus temperature. When the silica concentration increases from 20 wt-%, the solidus temperatures decrease 100 - 130 °C and stabilise to a temperature range of 1100 to 1120 °C at a silica concentration of 32.5 wt-%.

In figure 6 can be seen that at 10 wt-% CaO when the silica level increases from 20 wt-% to 22.5 wt-% the liquidus temperature decreases slightly and then it increases and reaches a local maximum at the silica concentration 32.5 wt-%. The liquidus temperature starts to decrease and reaches a local minimum at 45 to 47.5 wt-% of silica and then the liquidus level increases. Higher ratios of Fe/MgO give lower liquidus temperature when the silica concentration is less than 45 wt-%, but above this point the higher ratio Fe/MgO gives a higher liquidus temperature. When the silica concentration increases from 20 wt-%, the solidus temperatures decrease 90 °C to 130 °C and stabilise to a temperature range of 1110 °C to 1140 °C at the silica concentration of 32.5 wt-% and above.

Figure 7 shows that at 5 wt-%  $\text{Al}_2\text{O}_3$  when the silica level increases from 20 wt-%  $\text{SiO}_2$  the liquidus temperature rises for all three ratios of Fe/MgO. A local maximum for the liquidus temperature is reached at 27.5 wt-% of silica. The liquidus temperatures start to decrease and reach local minima at 42.5 to 45 wt-% of silica. When exceeding this point in silica concentration the liquidus increases rapidly. The influence of the ratio of Fe/MgO gives a lower liquidus temperature for the higher ratio when the silica concentration is lower than 42.5 wt-%, but when exceeding this point the higher ratio of Fe/MgO gives a higher liquidus temperature. First when the silica concentration increases the solidus temperatures decrease, but on the level of 25 wt-%  $\text{SiO}_2$  the solidus temperature stabilises between 1110 °C and 1120 °C.

Figure 8 shows the results of the highest alumina concentration studied. One can see that when the silica level increases beyond 20 wt-% the liquidus temperatures rise for the ratios 4 and 5 of Fe/MgO and reach local maxima at 25 wt-% of silica. The liquidus temperatures start then to decrease and reach local minima at 42.5 to 45 wt-% of silica. When exceeding this point in silica concentration the liquidus level increases rapidly. The influence of the Fe/MgO ratio gives a lower liquidus temperature for the higher ratio when the silica concentration is lower than 42.5 wt-%, but when exceeding this point the higher ratio of Fe/MgO gives a higher liquidus temperature. First when the silica concentration increases the solidus temperatures decrease, but at the concentration of 22.5 wt-%  $\text{SiO}_2$  the solidus temperature stabilises between 1100 °C and 1120 °C.

Figure 9 shows the precipitating phases in the case  $\text{Fe/MgO} = 5$  without additions. In this temperature window of the system, six different solid phases can be recognised. The first phase to precipitate when the silica level is less than 40 wt-% is olivine. When the silica concentration is between 40 wt-% and 42.5 wt-%  $\text{SiO}_2$  clinopyroxene is the first precipitating phase from the slag at the ratio of  $\text{Fe/MgO}$  of 4 and 6. At higher silica concentrations and in the case when  $\text{Fe/MgO} = 5$  tridymite and cristoballite are the primary precipitates.

Figures 10 and 11 show the precipitating phases at the  $\text{Fe/MgO}$  ratio 4 with an addition of either 5 wt-%  $\text{CaO}$  (figure 10) or 5 wt-%  $\text{Al}_2\text{O}_3$  (figure 11). For silica concentration less than 42.5 wt-% olivine is the first precipitating phase. Between 42.5 and 47.5 wt-%  $\text{SiO}_2$  clinopyroxene is the primary precipitating phase and when the silica concentration still increases tridymite will be the primary precipitating phase. In the case of 5 wt-%  $\text{Al}_2\text{O}_3$  cristoballite will start to precipitate at 50 wt-% of silica at 1480 °C.

## DISCUSSION

The purpose of this work has been to establish the impact of silica on the liquidus and phase precipitation temperatures for a typical slag treated in an electrical furnace for nickel slag cleaning. The slag consists of the quaternary system  $\text{FeO}_x\text{-MgO-SiO}_2$  with modifying additions of  $\text{CaO}$  and  $\text{Al}_2\text{O}_3$ . When evaluating the system it can be seen that when operating in the conventional area of smelting in terms of sulphide concentrate quality ( $\text{Fe/MgO} = 4$  to 6) the increase of silica over 40 wt-%, will lead to precipitation of tridymite and to a rapid increase of the liquidus temperature. The results obtained are in good agreement with the recent analysis by Kongoli /5, 6/.

The calculated phase diagrams indicate that the liquidus line tends to rise somewhat during the reduction in EF. No solid compounds were, however, found to precipitate from the slag at 1400 °C as the oxygen partial pressure is lowered from primary matte smelting  $P_{\text{O}_2} = 10^{-6...7}$  bar to the end point of slag cleaning with  $P_{\text{O}_2} = 10^{-9...10}$  bar. It is therefore safe to operate at high silica concentration levels with 30 to 35 wt-%  $\text{SiO}_2$  in the slag without any tendency of formation of a solid cover on top of the EF slag.

The calculations show that in EF conditions the impact of silica in the region of 40 to 50 wt-%  $\text{SiO}_2$  is very drastic on the liquidus temperature, as expected. In the case of  $\text{Fe/MgO} = 4$  without any additions of  $\text{CaO}$  or  $\text{Al}_2\text{O}_3$  it was seen, that when the silica concentration was increased, the liquidus temperature slightly increased from 1400 °C ( $\text{SiO}_2 = 20$  wt-%) to 1440 °C ( $\text{SiO}_2 = 27.5$  wt-%). After this, the liquidus temperature decreased to 1320 °C ( $\text{SiO}_2 = 40 - 42.5$  wt-%) and then steeply increased. The higher the  $\text{Fe/MgO}$  ratio was, the lower was the liquidus temperature for the system when the silica concentration was below 40 wt-%, but after passing this fluxing ratio the higher  $\text{Fe/MgO}$  ratio increased the liquidus much more rapidly than the lower ratio. The effect of the silica concentration on the solidus temperature was found to be small and a higher silica concentration in the slag, had no significant impact on the solidus temperature. The primary precipitating phase from the slag was olivine at silica concentrations less than 40 wt-%. Causing the steep increase of the liquidus temperature at high silica concentrations are the primary crystallising phases tridymite and cristoballite ( $\text{SiO}_2$ ).

Increasing  $\text{CaO}$  in the slag decreased the local liquidus maximum from 1440 °C, when the silica concentration was around 27.5 wt-%  $\text{SiO}_2$ , by 40 °C with the 5 wt-% addition and by 70 °C for the 10 wt-% addition, respectively. The  $\text{CaO}$  decreased the liquidus temperatures at high silica concentrations and smoothed the steep slope of the liquidus temperatures. The

impact on the solidus line by the CaO addition was clear. The solidus for silica concentrations over 32.5 wt-% decreases 150 °C with the addition of 5 wt-% of CaO and when the addition of CaO is 10 wt-% the solidus line will be 140 °C lower. The primarily precipitating phases are olivine at silica concentrations below 42.5 wt-% and clinopyroxenes at silica concentrations between 42.5 to 47.5 wt-% SiO<sub>2</sub>. At higher silica concentrations the primary precipitating phase is tridymite.

Additions of Al<sub>2</sub>O<sub>3</sub> in the slag decreased the local liquidus maximum from 1440 °C at the silica concentration around 27.5 wt-% by 10 °C at the 5 wt-% addition of Al<sub>2</sub>O<sub>3</sub> and by 50 °C at the 10 wt-% addition. The Al<sub>2</sub>O<sub>3</sub> addition lowers the liquidus temperatures more clearly than CaO in the silica concentration range 40 to 45 wt-%. When the silica concentration increases from this, the liquidus temperature behaves like the unmodified cases and increases sharply. The solidus line at silica concentrations over 32.5 wt-% decreases 150 °C with the addition of 5 or 10 wt-% of CaO. The primarily precipitating phases are olivine for silica concentrations under 42.5 wt-% SiO<sub>2</sub> and then clinopyroxene for silica concentrations between 42.5 to 45 wt-%. When the silica concentration increases even further the primary precipitating phase from the liquid slag is tridymite or cristoballite.

## ACKNOWLEDGMENT

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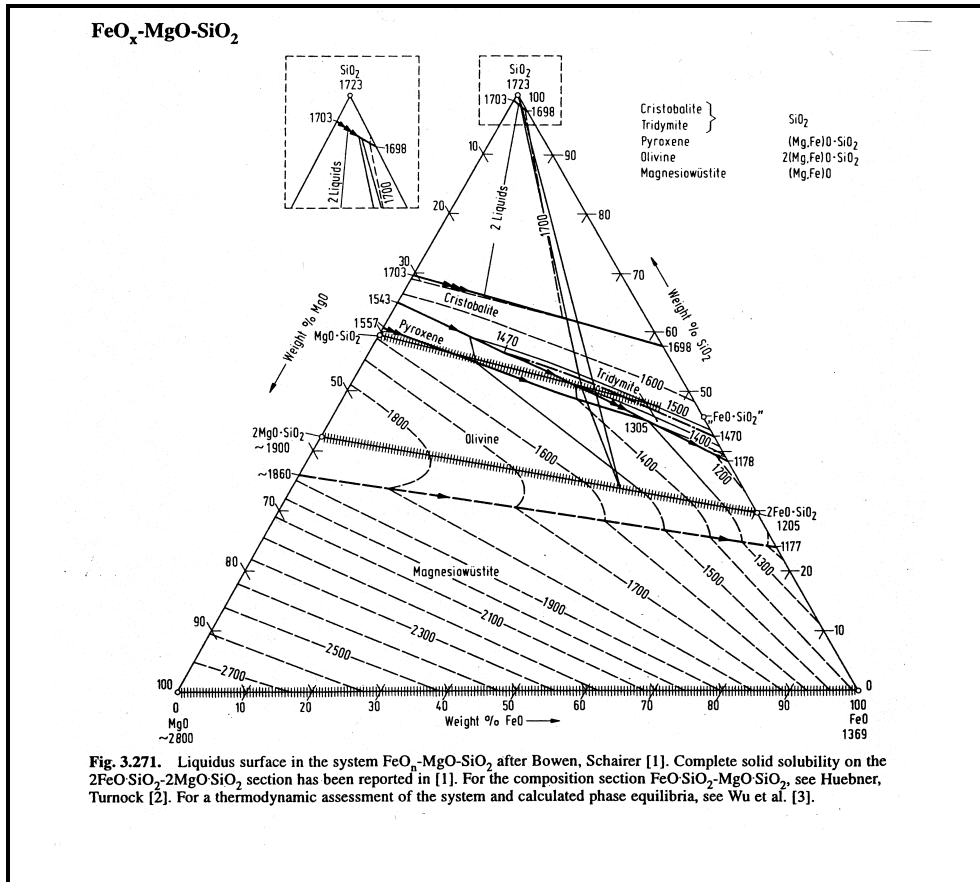


Figure 1. Phase diagram of the slag FeO<sub>x</sub>-SiO<sub>2</sub>-MgO at equilibrium with metallic iron. /1/

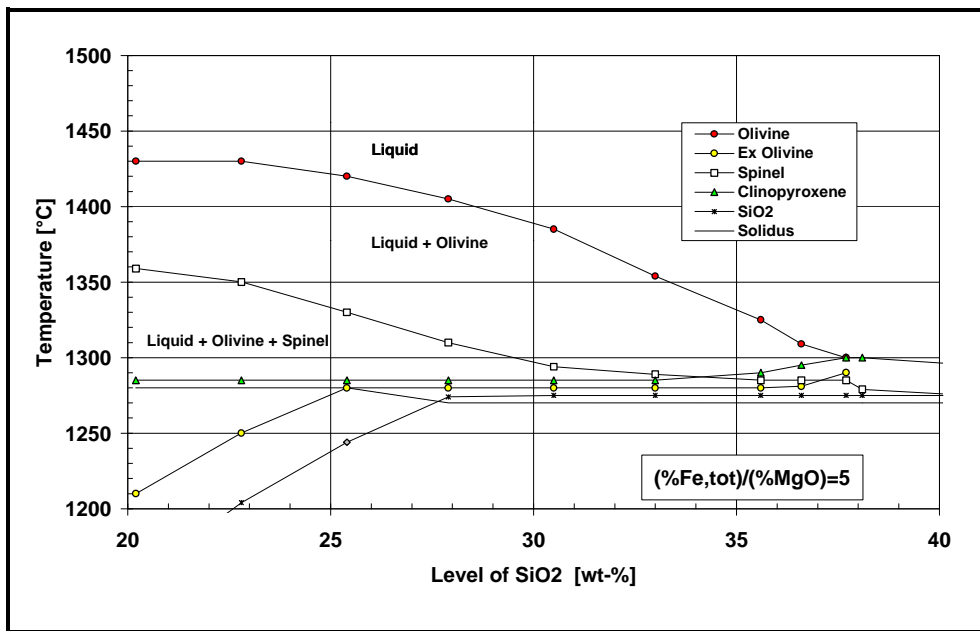


Figure 2. A calculated isopleth of the system  $\text{FeO}_x\text{-MgO-SiO}_2$  at  $P_{\text{O}_2} = 5.5 \cdot 10^{-7}$  bar and a constant Fe/MgO ratio; the oxygen partial pressure corresponds to a high-grade nickel matte smelting environment with 4 wt-% Fe in the Ni-Cu-Fe-S matte in a DON furnace, Ex\_Olivine refers to disappearance of olivine in cooling.

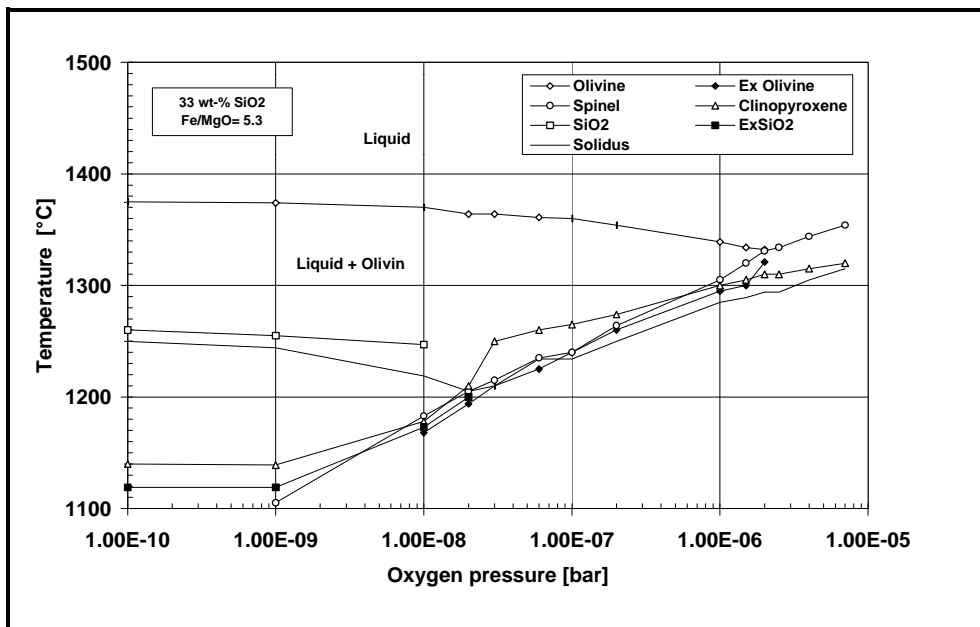


Figure 3. The development of phase equilibria under reduction of an EF  $\text{FeO}_x\text{-MgO-SiO}_2$  slag, Ex\_Olivine refers to disappearance of olivine in cooling.



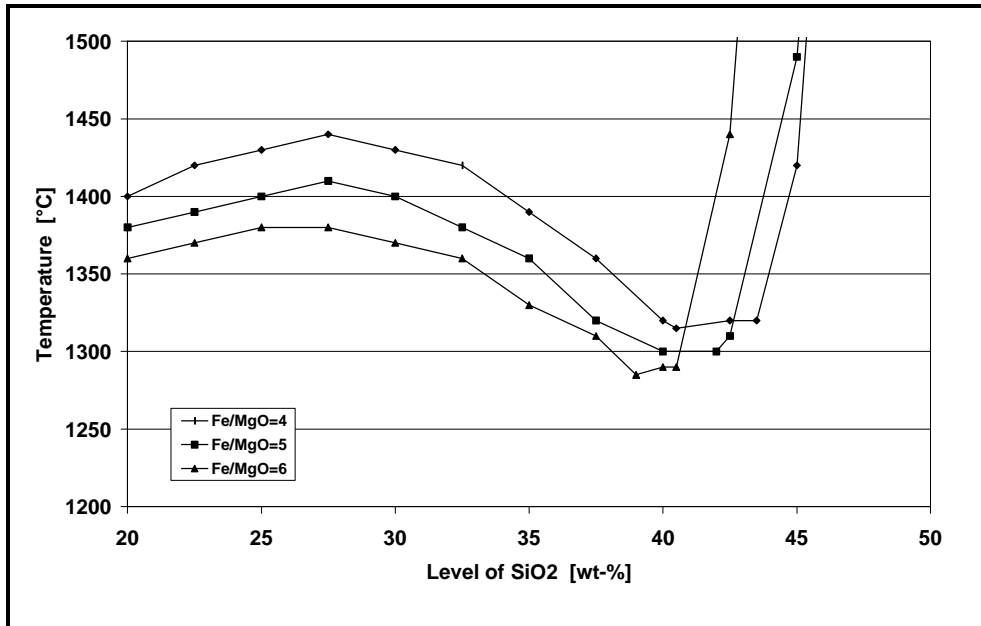


Figure 4. The calculated liquidus for Fe/MgO = 4, 5 and 6 as a function of silica concentration.

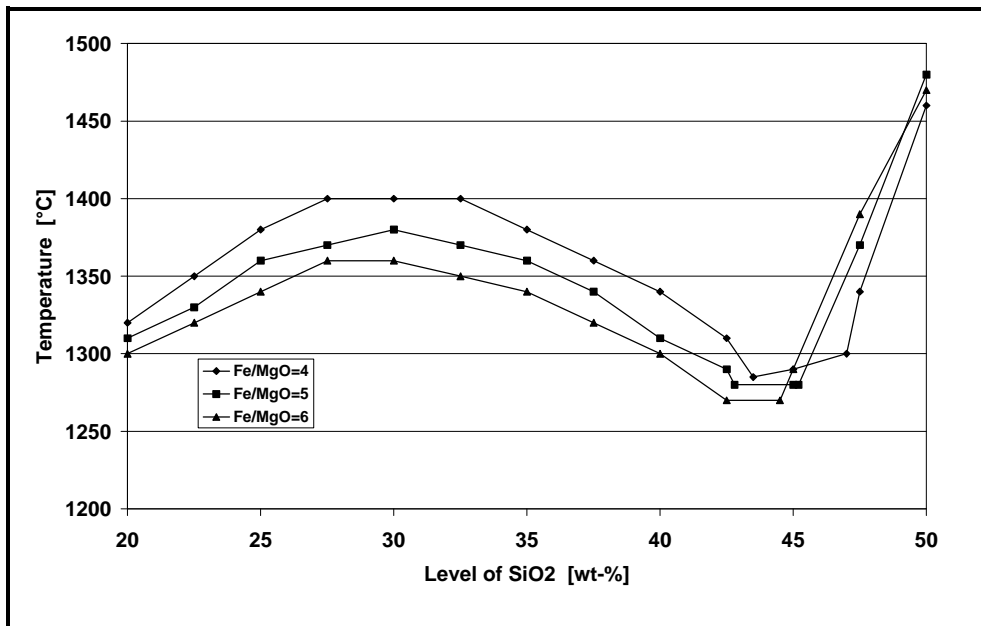


Figure 5. The calculated liquidus for Fe/MgO = 4, 5 and 6 at a constant lime concentration of 5 wt-% CaO.

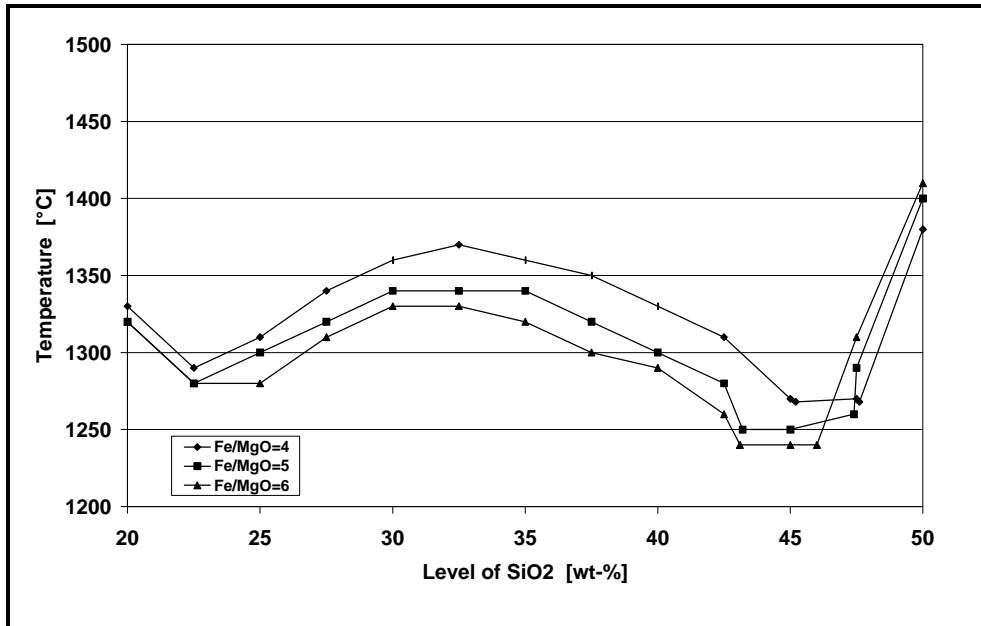


Figure 6. The calculated liquidus for Fe/MgO = 4, 5 and 6 at a constant lime concentration of 10 wt-% CaO.

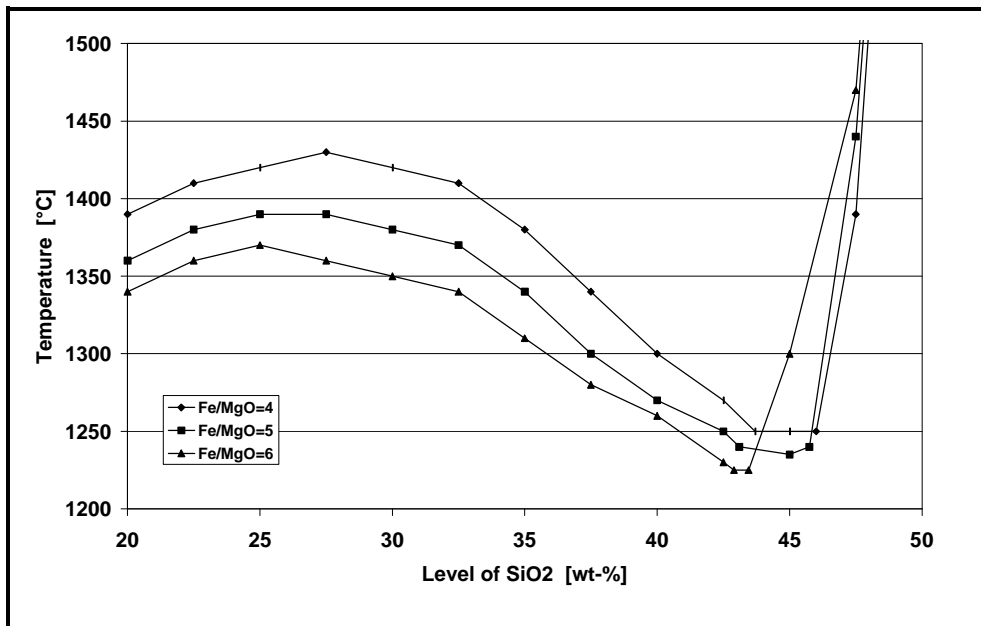


Figure 7. The calculated liquidus for Fe/MgO = 4, 5 and 6 at a constant alumina concentration of 5 wt-% Al<sub>2</sub>O<sub>3</sub>.

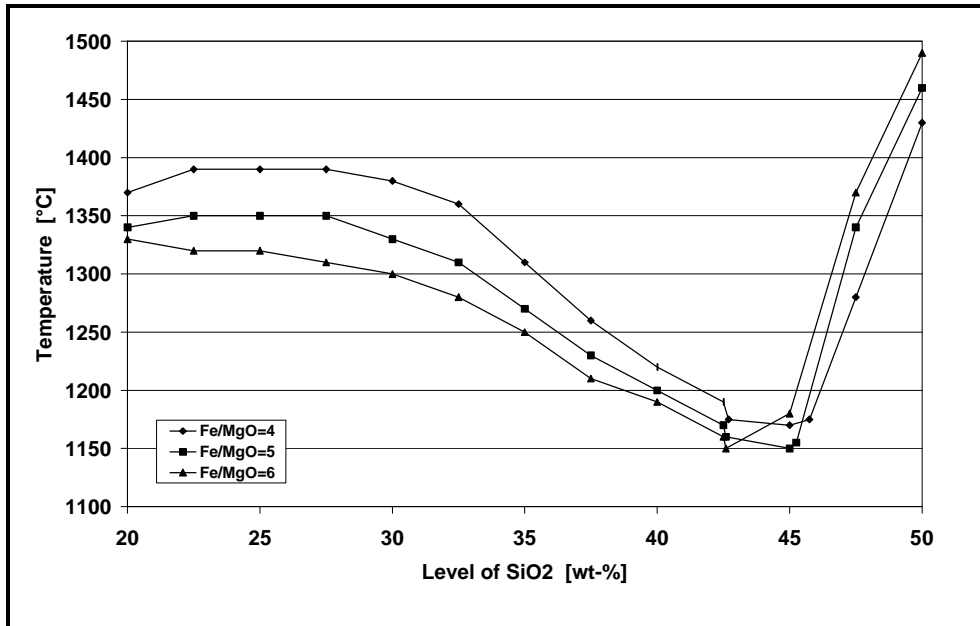


Figure 8. The calculated liquidus for Fe/MgO = 4, 5 and 6 at a constant alumina concentration of 10 wt-%  $\text{Al}_2\text{O}_3$ .

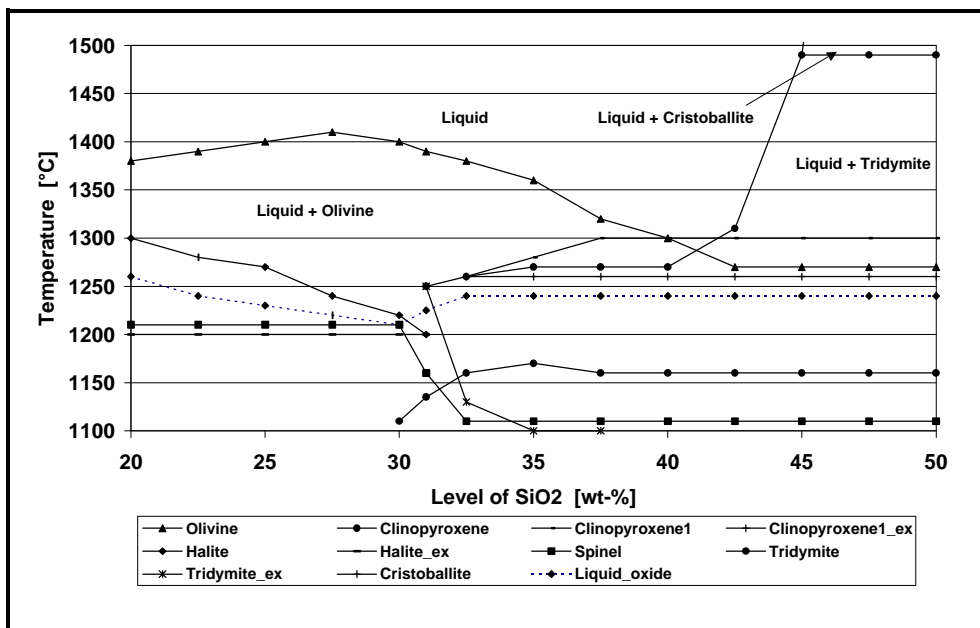


Figure 9. The precipitating phases from the melt at Fe/MgO = 5, “ex” refers to disappearance of the phase in question during cooling.

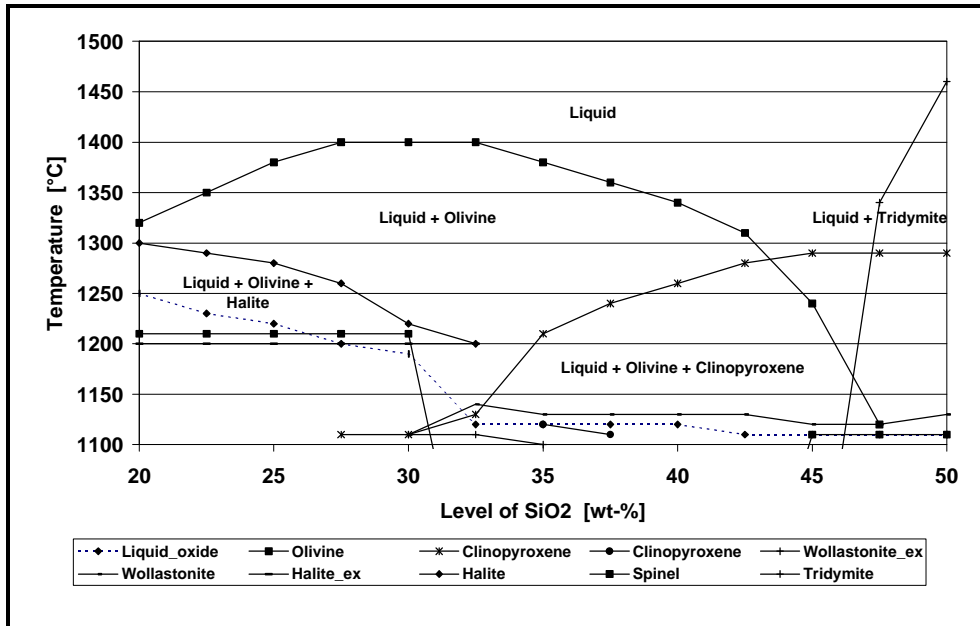


Figure 10. The phases precipitating from the melt at Fe/MgO = 4 (+ 5 wt-% CaO), “ex” refers to disappearance of the phase in question during cooling.

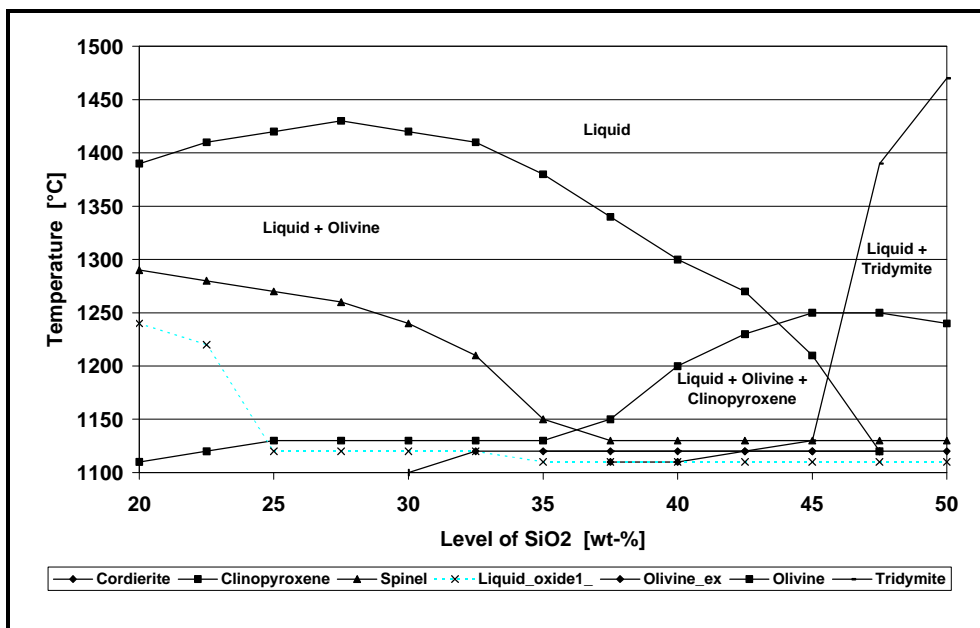


Figure 11. The phases precipitating from the melt at Fe/MgO = 4 (+ 5 wt-% Al<sub>2</sub>O<sub>3</sub>), “ex” refers to disappearance of the phase in question during cooling.

SiO <sub>2</sub>	20	30	40	50
Fe	49.02	42.89	36.76	30.64
MgO	12.25	10.72	9.19	7.66
O <sub>2</sub>	18.73	16.38	14.04	11.70
Sum:	100.00	100.00	100.00	100.00

[illegible][illegible]

Table 4. Phases, substances, status and models in the calculations, case 1.

PHASE	SPECIES		STATUS	MODEL
METAL_LIQUI	Fe		NORMAL	PURE SUBSTANCE
LIQUID_OXID	FeO; FeO1.5; FeO3Si; Fe2O4Si; MgO; Mg2O4Si; O2Si		1 M-G*	REDLICH-KISTER
OLIVINE	Fe/+2:1; Mg/+2:1; Fe/+2:2; Mg/+2:2; O4Si/-4:3	(1:1:1)	1 M-G*	SUBLATTICE
CLINOPYROXE	Fe/+2:1; Mg/+2:1; FeSi/+7:2; FeSi/+6:2; MgSi/+6:2; O6Si/-8:3	(1:1:1)	1 M-G*	SUBLATTICE
HALITE	Fe/+3:1; Fe/+2:1; Mg/+2:1; Va:1; O/-2:2	(1:1)	1 M-G*	SUBLATTICE
SPINEL	Fe/+3:1; Fe/+2:1; Mg/+2:1; Fe/+3:2; Fe/+2:2; Mg/+2:2; Va:2; Fe/+2:3; Mg/+2:3; Va:3; O/-2:4	(1:2:2:4)	NORMAL	SUBLATTICE
BCC_A2	Fe		NORMAL	PURE SUBSTANCE
CRISTOBALIT	O2Si		NORMAL	PURE SUBSTANCE
TRIDYMIT	O2Si		NORMAL	PURE SUBSTANCE
GAS	O; O2; O3		NORMAL	IDEAL GAS

\*miscibility gap

Table 5. Phases, substances, status and models in the calculations, case 2.

PHASE	SPECIES		STATUS	MODEL
LIQUID_OXIDE	CaO; CaO3Si; Ca2O4Si; FeO; FeO1.5; FeO3Si; Fe2O4Si; MgO; Mg2O4Si; O2Si		1 M-G	REDLICH-KISTER
OLIVINE	Ca/+2:1; Fe/+2:1; Mg/+2:1; Ca/+2:2; Fe/+2:2; Mg/+2:2; O4Si/-4:3	(1:1:1)	1 M-G	SUBLATTICE
CLINOPYROXE	Ca/+2:1; Fe/+2:1; Mg/+2:1; FeSi/+7:2; FeSi/+6:2; MgSi/+6:2; O6Si/-8:3	(1:1:1)	1 M-G	SUBLATTICE
HALITE	Ca/+2:1; Fe/+3:1; Fe/+2:1; Mg/+2:1; Va:1; O/-2:2	(1:1)	1 M-G	SUBLATTICE
SPINEL	Fe/+3:1; Fe/+2:1; Mg/+2:1; Ca/+2:2; Fe/+3:2; Fe/+2:2; Mg/+2:2; Va:2; Fe/+2:3; Mg/+2:3; Va:3; O/-2:4	(1:2:2:4)	NORMAL	SUBLATTICE
WOLLASTONIT	CaO3Si; FeO3Si; MgO3Si		NORMAL	REDLICH-KISTER
METAL_LIQUID	Fe		NORMAL	PURE SUBSTANCE
BCC_A2	Fe		NORMAL	PURE SUBSTANCE
CRISTOBALIT	O2Si		NORMAL	PURE SUBSTANCE
TRIDYMIT	O2Si		NORMAL	PURE SUBSTANCE
GAS	O; O2; O3		NORMAL	IDEAL GAS

Table 6. Phases, substances, status and models in the calculations, case 3.

PHASE	SPECIES		STATUS	MODEL
CORDIERITE	Al4Fe2O18Si5; Al4Mg2O18Si5		NORMAL	REDLICH-KISTER
CLINOPYROXE	Fe/+2:1; Mg/+2:1; Al2/+6:2; FeSi/+7:2; FeSi/+6:2; MgSi/+6:2; O6Si/-8:3	(1:1:1)	1 M-G	SUBLATTICE
SPINEL	Al/+3:1; Fe/+3:1; Fe/+2:1; Mg/+2:1; Al/+3:2; Fe/+3:2; Fe/+2:2; Mg/+2:2; Va:2; Fe/+2:3; Mg/+2:3; Va:3; O/-2:4	(1:2:2:4)	1 M-G	SUBLATTICE
LIQUID_OXID	AlO1.5; Al1.333333O4Si; FeO; FeO1.5; FeO3Si; Fe2O4Si; MgO; Mg2O4Si; O2Si		1 M-G	REDLICH-KISTER
METAL_LIQUI	Fe		NORMAL	PURE SUBSTANCE
OLIVINE	Fe/+2:1; Mg/+2:1; Fe/+2:2; Mg/+2:2; O4Si/-4:3	(1:1:1)	1 M-G	SUBLATTICE
BCC_A2	Fe		NORMAL	PURE SUBSTANCE
CRISTOBALIT	O2Si		NORMAL	PURE SUBSTANCE
TRIDYMIT	O2Si		NORMAL	PURE SUBSTANCE
GAS	O; O2; O3		NORMAL	IDEAL GAS