

# Addition of $K_2O$ and $Na_2O$ to the $Al_2O_3$ - $CaO$ - $FeO_x$ - $MgO$ - $SiO_2$ Oxide System

GTT-Technologies, Herzogenrath

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# Contents of presentation

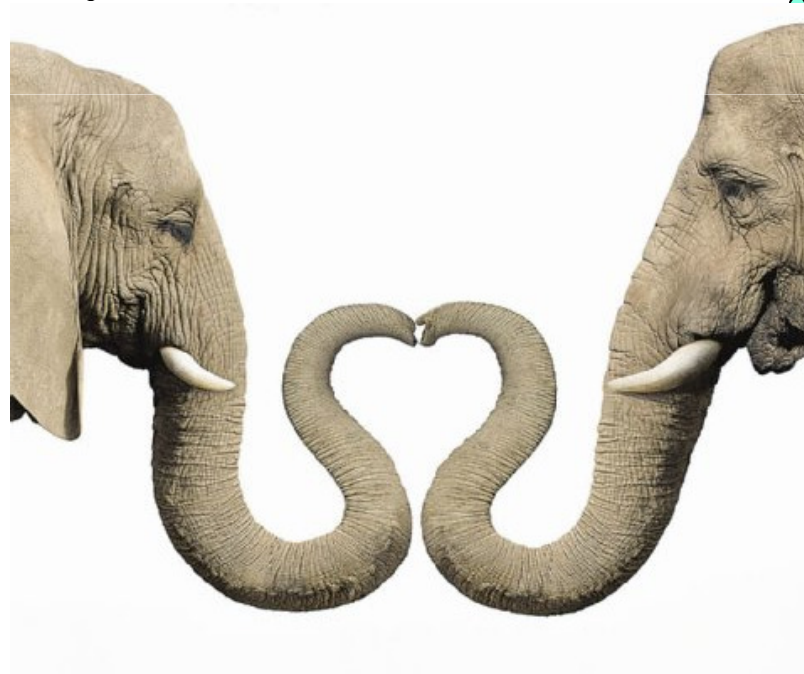
GTT-Technologies

- Introduction
- The  $\text{FeO}_x$ - $\text{K}_2\text{O}$  and  $\text{FeO}_x$ - $\text{Na}_2\text{O}$  binary systems
- The  $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{K}_2\text{O}$  ternary system
- The  $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{Na}_2\text{O}$  ternary system
- The proposed  $\text{AlFeO}_2$ - $\text{AlKO}_2$  isoplethal section
- The  $\text{AlFeO}_2$ - $\text{AlNaO}_2$  isoplethal section
- The  $\text{Al}_2\text{O}_3$ - $\text{K}_2\text{O}$ - $\text{MgO}$  ternary system
- The  $\text{Al}_2\text{O}_3$ - $\text{MgO}$ - $\text{Na}_2\text{O}$  ternary system
- The  $\text{CaO}$ - $\text{Na}_2\text{O}$ - $\text{SiO}_2$  ternary system
- The  $\text{Fe}_2\text{O}_3$ - $\text{K}_2\text{O}$ - $\text{SiO}_2$ - $\text{O}_2$  system
- The  $\text{Fe}_2\text{O}_3$ - $\text{Na}_2\text{O}$ - $\text{SiO}_2$ - $\text{O}_2$  system
- The  $\text{FeO}$ - $\text{K}_2\text{O}$ - $\text{SiO}_2$ - $\text{Fe}$  system
- The  $\text{MgO}$ - $\text{Na}_2\text{O}$ - $\text{SiO}_2$  ternary system
- The behaviour of  $(\text{K,N})_2\text{C}_3\text{A}_5$  in  $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{K}_2\text{O}$ - $\text{Na}_2\text{O}$
- The  $\text{Al}_2\text{O}_3$ - $\text{Fe}_2\text{O}_3$ - $\text{K}_2\text{O}$ - $\text{SiO}_2$  quaternary system
- Conclusions



# Elephant's wedding

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# Introduction

The **associate species** containing K or Na were added in order to describe the liquid phase in the  $\text{Al}_2\text{O}_3$ -CaO- $\text{FeO}_x$ -MgO- $\text{SiO}_2$  system containing  $\text{K}_2\text{O}$  or  $\text{Na}_2\text{O}$ .

The **composition of the liquid oxide species** are as introduced by Spear taking two moles of cations per associate.

System	Associate species
$\text{FeO}_x - \text{K}_2\text{O}$	$\text{FeKO}_2$
$\text{FeO}_x - \text{Na}_2\text{O}$	$\text{FeNaO}_2, (\text{FeNa}_2\text{O}_2):1.5$
$\text{Al}_2\text{O}_3 - \text{CaO} - \text{Na}_2\text{O}$	$(\text{Al}_{10}\text{Ca}_3\text{Na}_4\text{O}_{20}):8.5$
$\text{CaO} - \text{Na}_2\text{O} - \text{SiO}_2$	$(\text{Na}_2\text{Ca}_3\text{Si}_6\text{O}_{16}):5.5$
$\text{FeO}_x - \text{Na}_2\text{O} - \text{SiO}_2$	$(\text{FeSiNa}_2\text{O}_4):2$



# Modelling of new phases in binary sub-systems

System	Phase	Description	Work	Used data
FeO <sub>x</sub> -K <sub>2</sub> O	FeKO <sub>2</sub> -HT	(Fe <sup>3+</sup> )( <u>K</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	Cp data from SGPS are used
	FeKO <sub>2</sub> -LT	(Fe <sup>3+</sup> )( <u>K</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	Fe <sub>12</sub> K <sub>2</sub> O <sub>19</sub> Fe <sub>22</sub> K <sub>2</sub> O <sub>34</sub>	stoichiometric stoichiometric	GTT GTT	
FeO <sub>x</sub> -Na <sub>2</sub> O	FeNaO <sub>2</sub> (s4)	stoichiometric	GTT	FeNaO <sub>2</sub> (s) from SGPS is used as basic
	FeNaO <sub>2</sub> -HT	(Fe <sup>3+</sup> )( <u>Na</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	FeNaO <sub>2</sub> -LT	(Fe <sup>3+</sup> )( <u>Na</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	FeNaO <sub>2</sub> (s)	stoichiometric	GTT	
	FeNa <sub>2</sub> O <sub>2</sub>	stoichiometric	GTT	H <sub>f</sub> [84Dai2]
	FeNa <sub>4</sub> O <sub>3</sub> Fe <sub>16</sub> Na <sub>10</sub> O <sub>29</sub>	stoichiometric stoichiometric	GTT GTT	



# Modelling of new phases in ternary systems

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<i>System</i>	<i>Phase</i>	<i>Description</i>	<i>Work</i>	<i>Used data</i>
<b>Al<sub>2</sub>O<sub>3</sub>-CaO-K<sub>2</sub>O</b>	K2C3A5	(K <sup>1+</sup> , Va)(Ca <sup>2+</sup> , K <sup>1+</sup> )(Al <sup>3+</sup> ) <sub>2</sub> (O <sup>2-</sup> ) <sub>4</sub>	GTT	
<b>Al<sub>2</sub>O<sub>3</sub>-CaO-Na<sub>2</sub>O</b>	N2C3A5	(Na <sup>1+</sup> , Va)(Ca <sup>2+</sup> , Na <sup>1+</sup> )(Al <sup>3+</sup> ) <sub>2</sub> (O <sup>2-</sup> ) <sub>4</sub>	GTT	
	NC3A8	Na <sub>2</sub> Ca <sub>3</sub> Al <sub>16</sub> O <sub>28</sub>	GTT	
	NC8A3	Na <sub>2</sub> Ca <sub>8</sub> Al <sub>6</sub> O <sub>18</sub>	GTT	
<b>Al<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O</b>	(Fe,Al)KO2-HT	( <u>Fe</u> <sup>3+</sup> , <u>Al</u> <sup>3+</sup> )( <u>K</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	AlKO <sub>2</sub> (s2)FZJ AlKO <sub>2</sub> (s) FZJ
	(Fe,Al)KO2-LT	( <u>Fe</u> <sup>3+</sup> , <u>Al</u> <sup>3+</sup> )( <u>K</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>		
<b>Al<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O</b>	(Fe,Al)NaO2-HT	( <u>Fe</u> <sup>3+</sup> , <u>Al</u> <sup>3+</sup> )( <u>Na</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	AlNaO <sub>2</sub> (s2)FZJ AlNaO <sub>2</sub> (s) FZJ
	(Fe,Al)NaO2-LT	( <u>Fe</u> <sup>3+</sup> , <u>Al</u> <sup>3+</sup> )( <u>Na</u> <sup>1+</sup> , Va)(O <sup>2-</sup> ) <sub>2</sub>		



# Modelling of new phases in ternary systems

System	Phase	Description	Work	Used data
<b>Al<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-MgO</b>	Beta-prime	$(K^{1+})_2(\underline{Al}^{3+}, Va)_2(Mg^{2+}, \underline{Va})_3(Al_{10}O_{19}^{8-})$	GTT	K <sub>2</sub> Al <sub>12</sub> O <sub>19</sub> (Jülich)
	Beta-tri	$(\underline{O}^{2-}, Va)_3(\underline{Al}^{3+}, K^{1+})_2(\underline{Al}^{3+}, Mg^{2+})_2$ $(Al_{40}K_4Mg_5O_{70}^{6-})$	GTT	
<b>Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O</b>	Beta-prime	$(Na^{1+})_2(\underline{Al}^{3+}, Va)_2(Mg^{2+}, \underline{Va})_3(Al_{10}O_{19}^{8-})$	GTT	Na <sub>2</sub> Al <sub>12</sub> O <sub>19</sub> (Jülich)
	Beta-tri	$(O^{2-}, Va)_3(Al^{3+}, Na^{1+})_2(Al^{3+}, Mg^{2+})_2$ $(Al_{40}Na_4Mg_5O_{70}^{6-})$	GTT	
<b>CaO-Na<sub>2</sub>O-SiO<sub>2</sub></b>	NC2S3	$(Na^{1+}, \underline{Va})_2(\underline{Ca}^{2+}, Va) (Na_2CaSi_3O_9)^{2-}$	GTT	
	111	Na <sub>2</sub> CaSiO <sub>4</sub>	GTT	
	115	Na <sub>2</sub> CaSi <sub>5</sub> O <sub>12</sub>	(GTT)	Spear data
	122	Na <sub>2</sub> Ca <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>	GTT	
	136	Na <sub>2</sub> Ca <sub>3</sub> Si <sub>6</sub> O <sub>16</sub>	(GTT)	Spear data
	213	Na <sub>4</sub> CaSi <sub>3</sub> O <sub>9</sub>	(GTT)	Spear data



# Modelling of new phases in ternary systems

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System	Phase	Description	Work	Used data
<b>Fe<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-SiO<sub>2</sub></b>	FeKO2-HT	( <u>Fe<sup>3+</sup></u> , Si <sup>4+</sup> )( <u>K<sup>1+</sup></u> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	FeKO2-LT	( <u>Fe<sup>3+</sup></u> , Si <sup>4+</sup> )( <u>K<sup>1+</sup></u> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	K2F2S3	Fe <sub>4</sub> K <sub>4</sub> Si <sub>3</sub> O <sub>14</sub>	GTT	
	Kaliophilite-HT	Fe <sub>2</sub> K <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>	GTT	
	Kaliophilite-LT	Fe <sub>2</sub> K <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>	GTT	
	Iron-Leucite	Fe <sub>2</sub> K <sub>2</sub> Si <sub>4</sub> O <sub>12</sub>	GTT	
	Iron-Orthoclase	Fe <sub>2</sub> K <sub>2</sub> Si <sub>6</sub> O <sub>16</sub>		
<b>Fe<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O-SiO<sub>2</sub></b>	FeNaO2-δ	( <u>Fe<sup>3+</sup></u> , Si <sup>4+</sup> )( <u>Na<sup>1+</sup></u> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	FeNaO2-HT	( <u>Fe<sup>3+</sup></u> , Si <sup>4+</sup> )( <u>Na<sup>1+</sup></u> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	FeNaO2-LT	( <u>Fe<sup>3+</sup></u> , Si <sup>4+</sup> )( <u>Na<sup>1+</sup></u> , Va)(O <sup>2-</sup> ) <sub>2</sub>	GTT	
	Acmite	Fe <sub>2</sub> Si <sub>4</sub> Na <sub>2</sub> O <sub>12</sub>	GTT	
	N5F1S8	Fe <sub>2</sub> Si <sub>8</sub> Na <sub>10</sub> O <sub>24</sub>	GTT	
	N6F4S5	Fe <sub>8</sub> Si <sub>5</sub> Na <sub>12</sub> O <sub>28</sub>	GTT	
<b>FeO-Na<sub>2</sub>O-SiO<sub>2</sub></b>	NFS	FeSiNa <sub>2</sub> O <sub>4</sub>	GTT	
<b>MgO-Na<sub>2</sub>O-SiO<sub>2</sub></b>	Roedderite	Na <sub>2</sub> Mg <sub>5</sub> Si <sub>12</sub> O <sub>30</sub>	GTT	
	NM2S6	Na <sub>2</sub> Mg <sub>2</sub> Si <sub>6</sub> O <sub>15</sub>	GTT	
	NMS4	Na <sub>2</sub> MgSi <sub>4</sub> O <sub>10</sub>	GTT	
	NMS	Na <sub>2</sub> MgSiO <sub>4</sub>	GTT	
	N2M2S3	Na <sub>4</sub> Mg <sub>2</sub> Si <sub>3</sub> O <sub>10</sub>	GTT	





# Modelling of new phases in quaternary systems

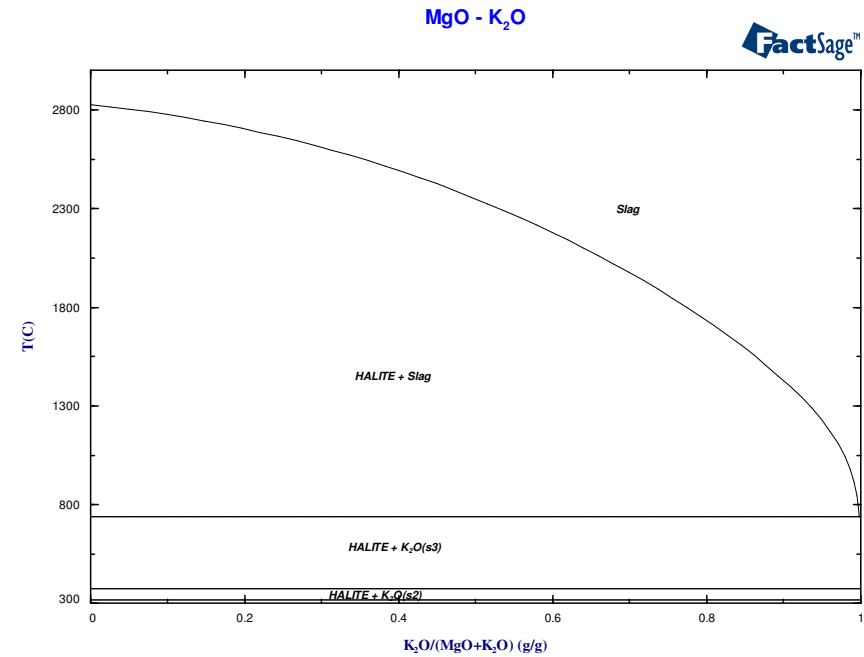
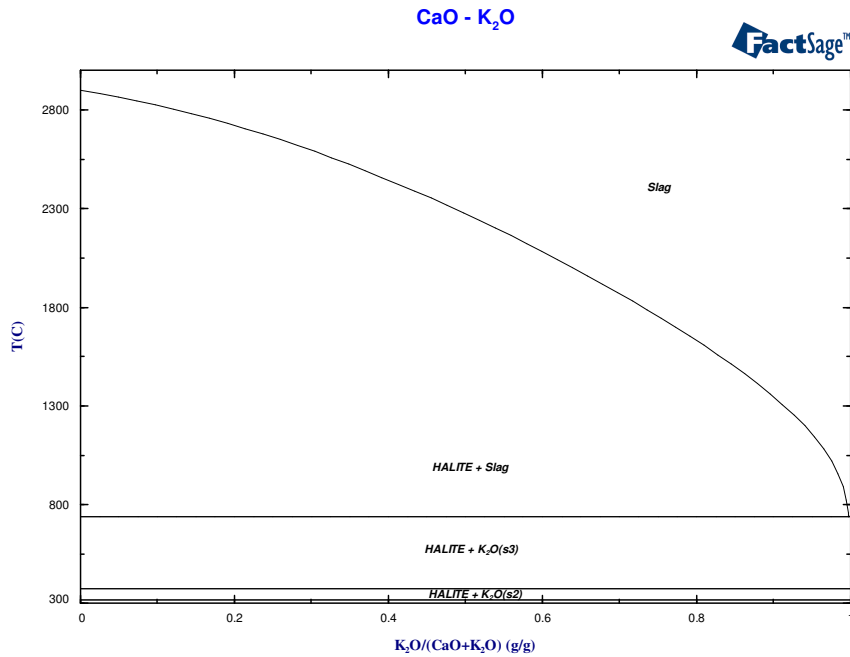
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System	Phase	Description	Used data
$\text{Al}_2\text{O}_3\text{-K}_2\text{O-MgO-Na}_2\text{O}$	Beta-prime	$(\text{K}^{1+}, \text{Na}^{1+})_2(\underline{\text{Al}}^{3+}, \underline{\text{Va}})_2(\text{Mg}^{2+}, \underline{\text{Va}})_3$ $(\text{Al}_{10}\text{O}_{19}^{8-})$	$\text{Al}_{12}\text{K}_2\text{O}_{19}(\text{s})$ $\text{Al}_{12}\text{Na}_2\text{O}_{19}(\text{s})$ from FZJ
	Beta-tri	$(\underline{\text{O}}^{2-}, \underline{\text{Va}})_3(\underline{\text{Al}}^{3+}, \text{K}^{1+}, \text{Na}^{1+})_2(\underline{\text{Al}}^{3+}, \text{Mg}^{2+})_2$ $(\text{Al}_{40}\text{K}_4\text{Mg}_5\text{O}_{70}^{6-}, \text{Al}_{40}\text{Na}_4\text{Mg}_5\text{O}_{70}^{6-})$	
$\text{Al}_2\text{O}_3\text{-Fe}_2\text{O}_3\text{-K}_2\text{O-Na}_2\text{O-SiO}_2$	$(\text{Al}, \text{Fe})(\text{K}, \text{Na})\text{O}_2\text{-HT}$	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+}, \text{Si}^{4+})(\underline{\text{K}}^{1+}, \underline{\text{Na}}^{1+}, \underline{\text{Va}})(\underline{\text{O}}^{2-})_2$	$\text{Al}_2\text{O}_3\text{-K}_2\text{O-Na}_2\text{O-SiO}_2$
	$(\text{Al}, \text{Fe})(\text{K}, \text{Na})\text{O}_2\text{-LT}$	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+}, \text{Si}^{4+})(\underline{\text{K}}^{1+}, \underline{\text{Na}}^{1+}, \underline{\text{Va}})(\underline{\text{O}}^{2-})_2$	data from FZJ
$\text{Al}_2\text{O}_3\text{-Fe}_2\text{O}_3\text{-K}_2\text{O-SiO}_2$	KAF4S3	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+})_4(\text{K}^{1+})_4(\text{Si}^{4+})_3(\underline{\text{O}}^{2-})_{14}$	$\text{Al}_4\text{K}_4\text{Si}_3\text{O}_{12}(\text{s})\text{FZJ}$
	Kaliophilite-HT	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+})_2(\text{K}^{1+})_2(\text{Si}^{4+})_2(\underline{\text{O}}^{2-})_8$	$\text{Al}_2\text{K}_2\text{Si}_2\text{O}_8(\text{s}2)\text{FZJ}$
	Kaliophilite-LT	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+})_2(\text{K}^{1+})_2(\text{Si}^{4+})_2(\underline{\text{O}}^{2-})_8$	$\text{Al}_2\text{K}_2\text{Si}_2\text{O}_8(\text{s})\text{FZJ}$
	Leucite	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+})_2(\text{K}^{1+})_2(\text{Si}^{4+})_4(\underline{\text{O}}^{2-})_{12}$	$\text{Al}_2\text{K}_2\text{Si}_4\text{O}_{12}(\text{s})\text{FZJ}$
	Feldspar	$(\underline{\text{Al}}^{3+}, \underline{\text{Fe}}^{3+})(\text{K}^{1+}, \text{Na}^{1+})(\text{Si}^{4+})_3(\underline{\text{O}}^{2-})_8$	$\text{Al}(\text{K}, \text{Na})\text{Si}_3\text{O}_8\text{FZJ}$
$\text{Al}_2\text{O}_3\text{-CaO-K}_2\text{O-Na}_2\text{O}$	(K,N)2C3A5	$(\text{K}^{1+}, \text{Na}^{1+}, \underline{\text{Va}})(\text{Ca}^{2+}, \text{K}^{1+}, \text{Na}^{1+})$ $(\underline{\text{Al}}^{3+})_2(\underline{\text{O}}^{2-})_4$	



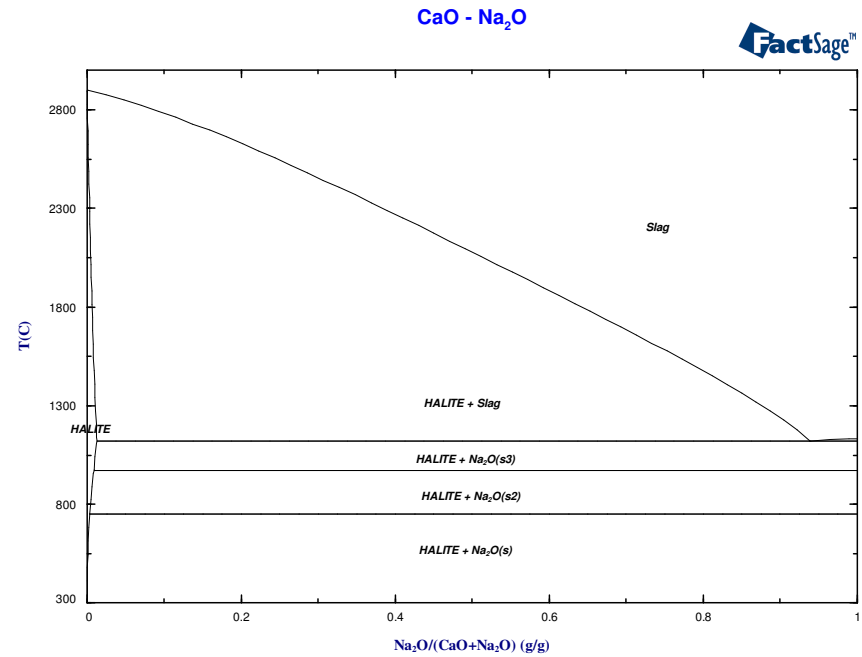
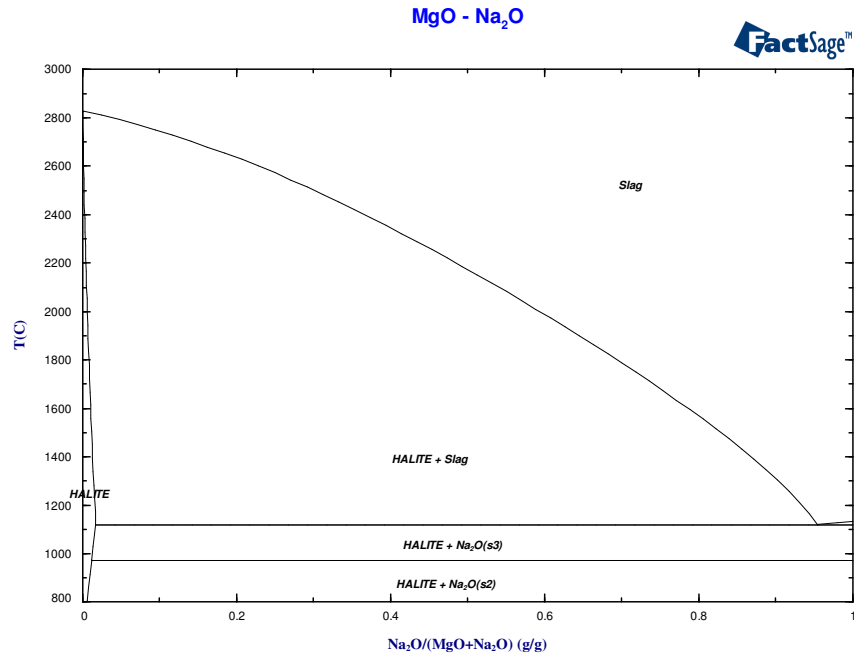
# Proposed CaO-K<sub>2</sub>O and K<sub>2</sub>O-MgO phase diagrams

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# Proposed CaO-Na<sub>2</sub>O and MgO-Na<sub>2</sub>O phase diagrams

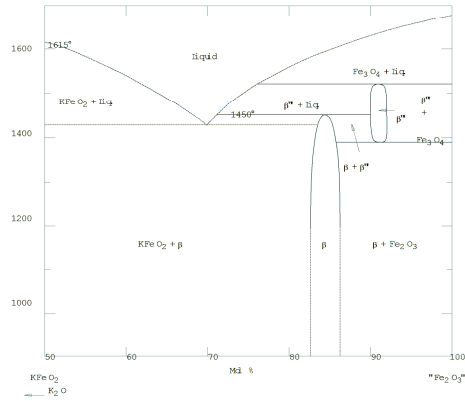
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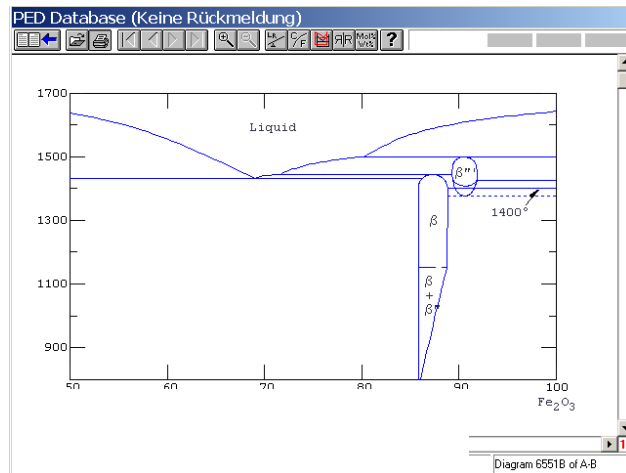
# Binary Fe<sub>2</sub>O<sub>3</sub> - K<sub>2</sub>O phase diagram in air

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*E.R. Plante, H.S. Parker, R.S. Roth, C.D. Olson, Natl. Bur. Stand. (US) Int. Rep., NBSIR 79-1767 (1979), pp.82-102.*



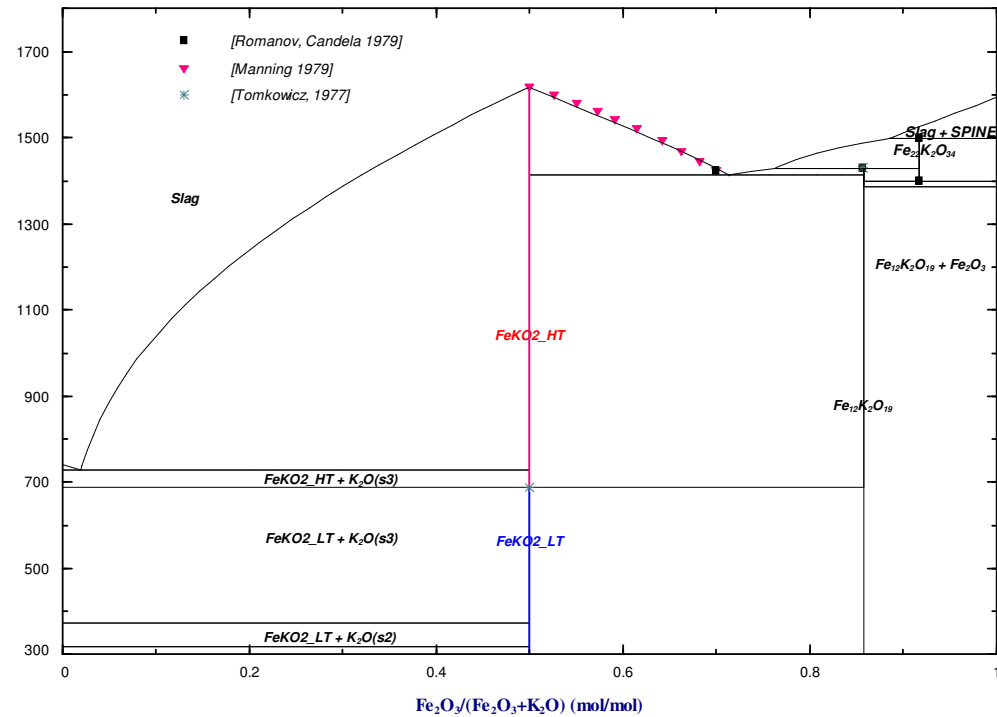
*V.P. Romanov, G.A. Candela, R.S. Roth, L.J. Schwartzengruber, J. Appl. Phys., 507 (1979), [10], pp. 6455-6458.*



687°C  
FeKO<sub>2</sub>-LT → FeKO<sub>2</sub>-HT [77Tom]

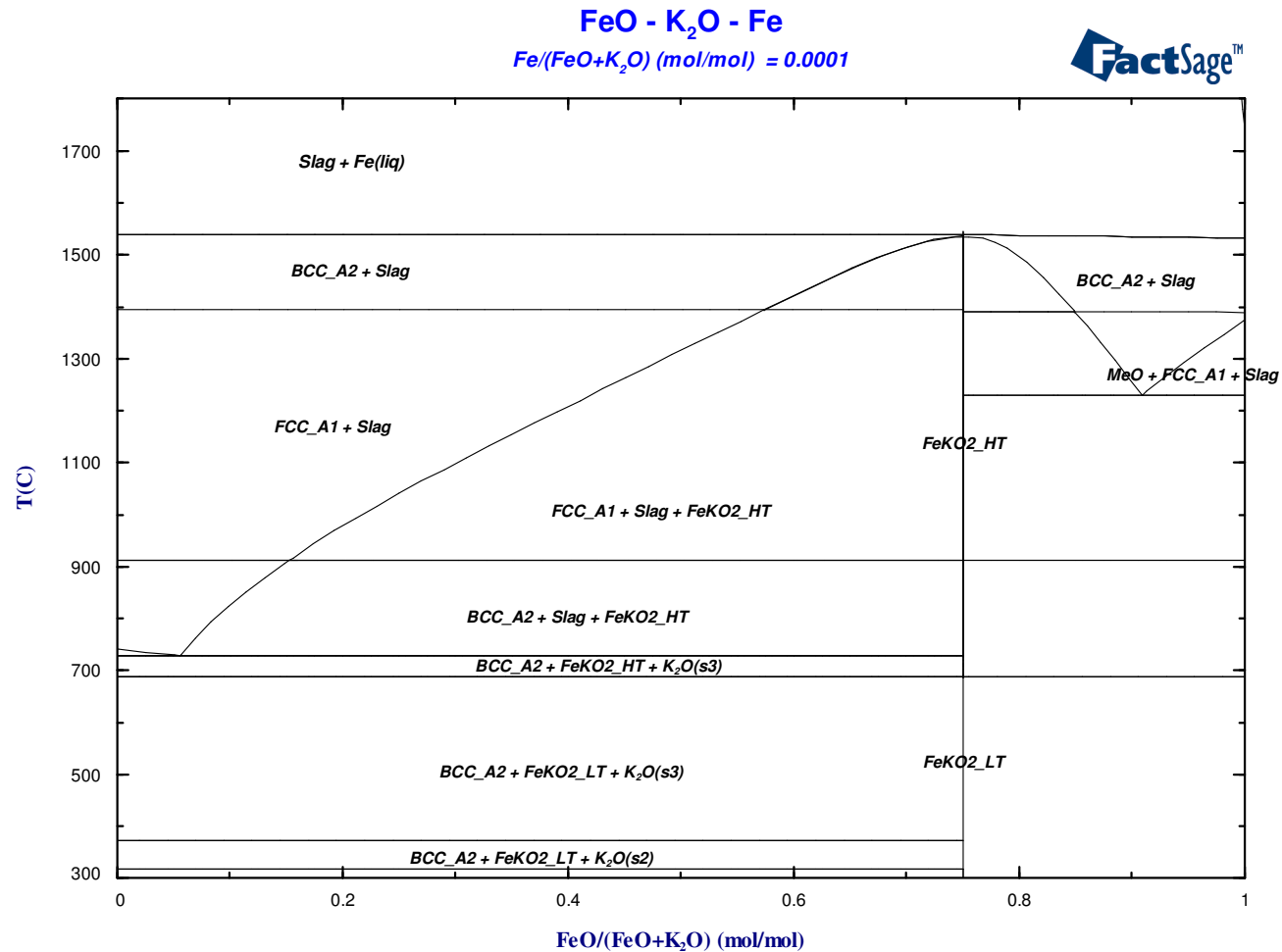
Fe<sub>2</sub>O<sub>3</sub> - K<sub>2</sub>O - O<sub>2</sub>  
p(O<sub>2</sub>) = 0.21 atm

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# FeO-K<sub>2</sub>O phase diagram for equilibrium with Fe

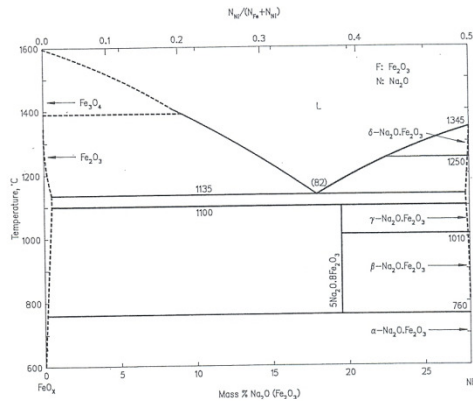
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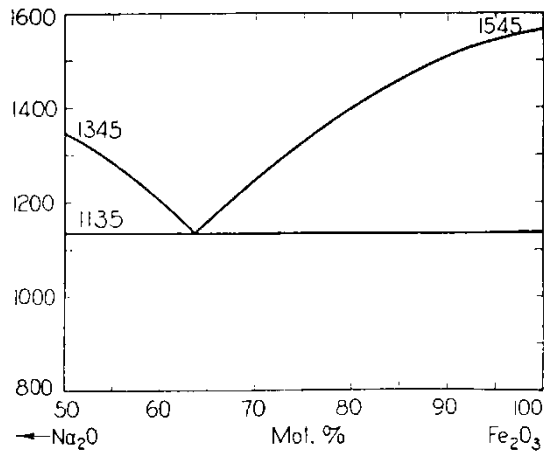
# Binary Fe<sub>2</sub>O<sub>3</sub> - Na<sub>2</sub>O phase diagram in air

GTI-Technologies

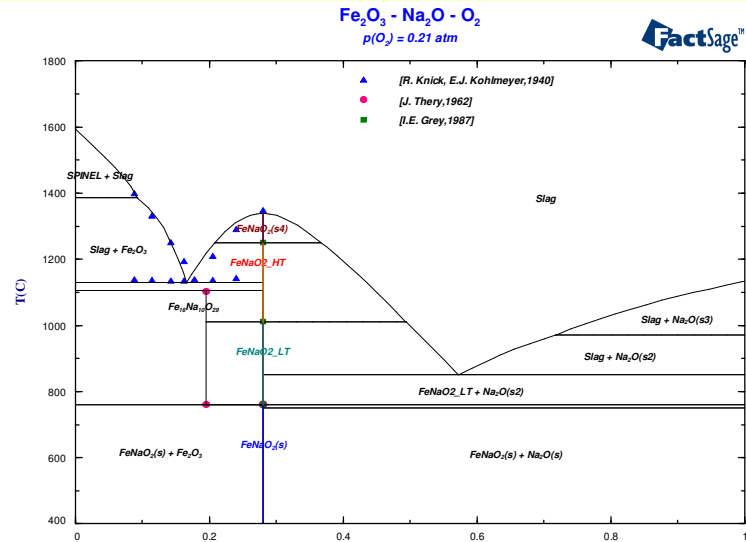
Slag Atlas (1995), p.75.



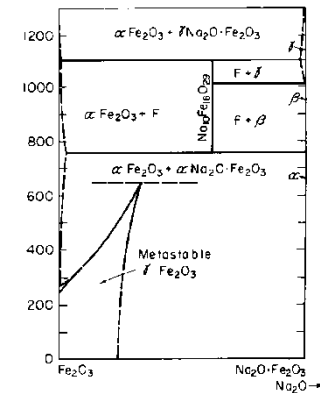
R. Knick, E.J. Kohlmeyer, Z. Anorg. Allg. Chem., 244 [1], (1940), pp.67-84.



760°C 1010°C 1250°C  
 $\text{FeNaO}_2(\text{s}) \rightarrow \text{FeNaO}_2\text{-LT} \rightarrow \text{FeNaO}_2\text{-HT} \rightarrow \text{FeNaO}_2\text{-}\delta$  [87Grey]



J. Thery, Ann. Chim. (Paris), 7 [3-4], (1962), pp.207-238.



# FeO-Na<sub>2</sub>O phase diagram for equilibrium with Fe

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W. Dai, S. Seetharamab, L.-I. Staffansson, Metall. Trans. B, 15B, (1984), No.2, pp. 319-327.

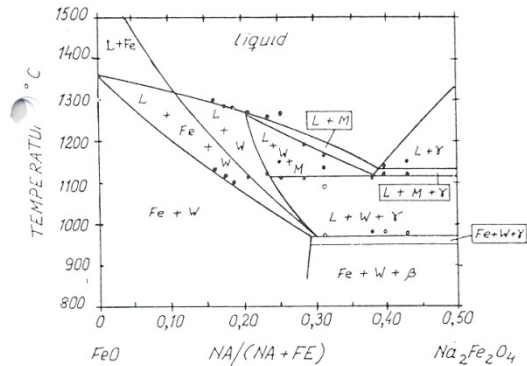


Fig. 7—Phase relations in the FeO-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub> section. W: wustite. M: magnetite. β: β-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>. γ: γ-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>.

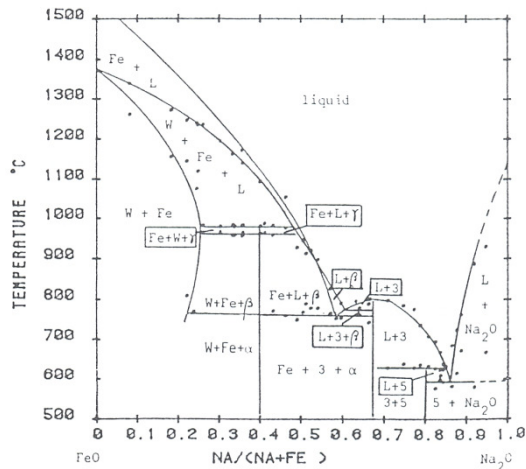
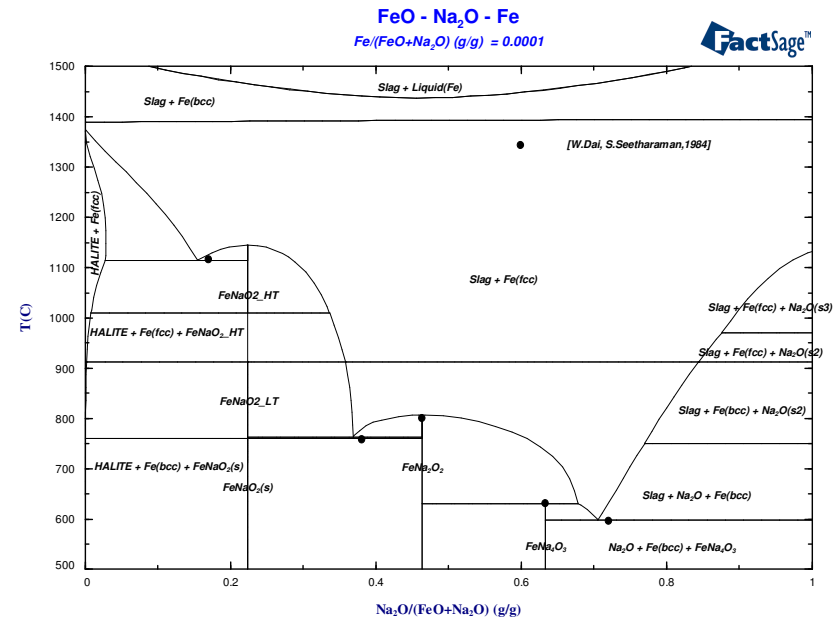


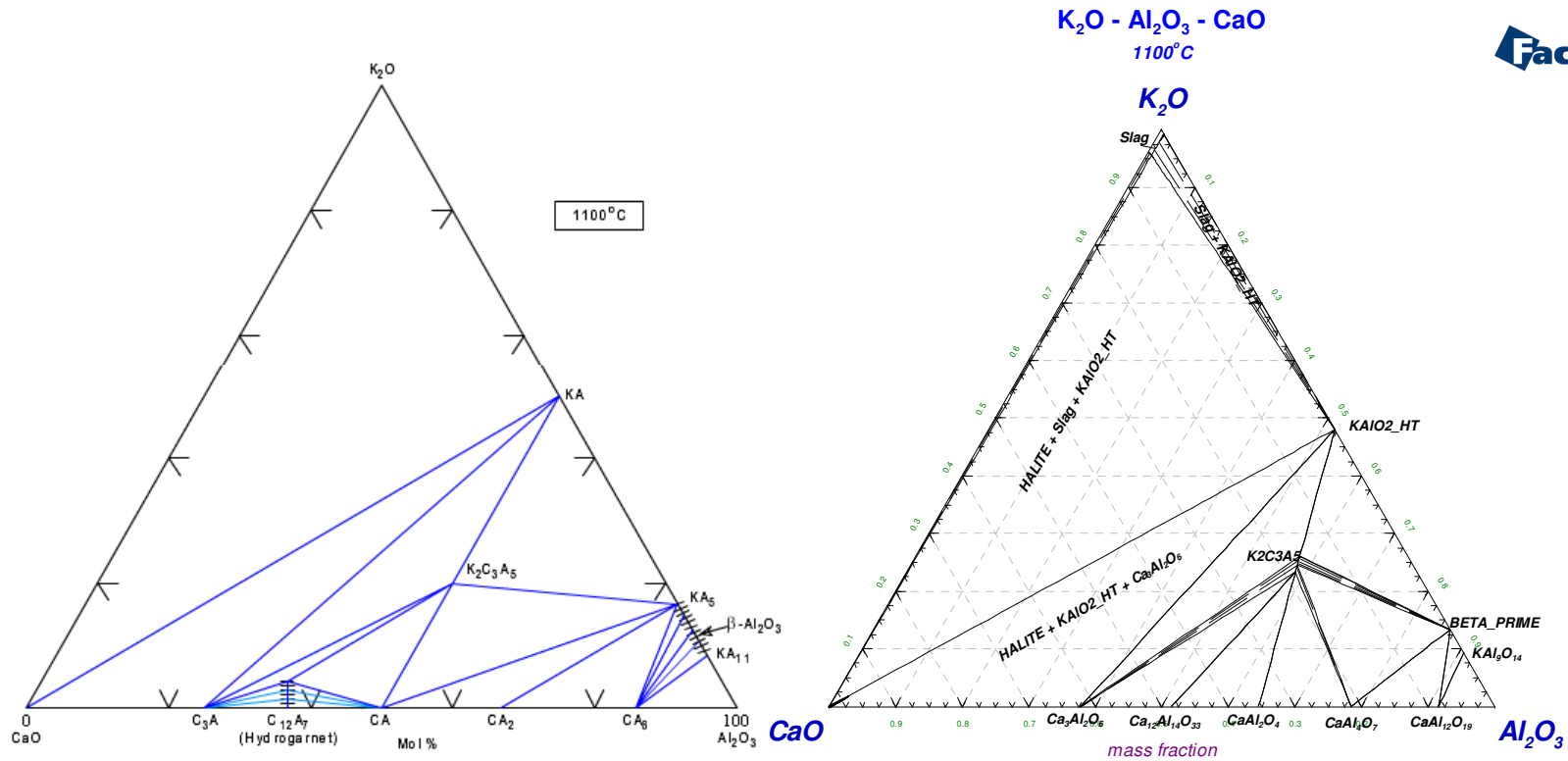
Fig. 4—The FeO-Na<sub>2</sub>O section of the Fe-Na-O system. W: wustite. α: α-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>. β: β-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>. γ: γ-Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>. 3: Na<sub>2</sub>Fe<sub>2</sub>O<sub>4</sub>. 5: Na<sub>2</sub>FeO<sub>3</sub>.



# Isothermal section at 1100°C in $\text{Al}_2\text{O}_3$ -CaO- $\text{K}_2\text{O}$

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J. A. M. Van Hoek, F. J. J. Van Loo, and R. Metselaar,  
*Mater. Sci. Monogr.*, 66B (1991), pp. 581-590.





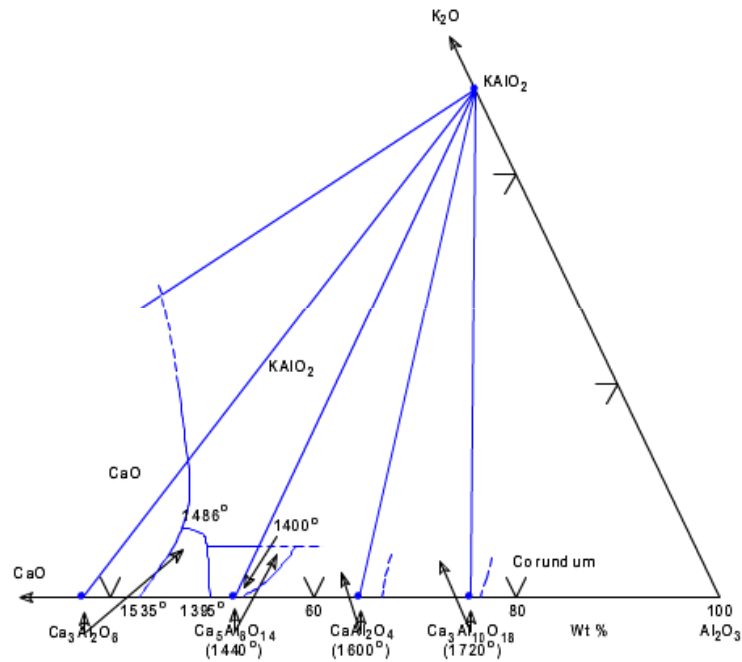
# Liquidus surface in $\text{Al}_2\text{O}_3\text{-CaO-K}_2\text{O}$

GTT-Technologies

L. T. Brownmiller, *Am. J. Sci.*, 229(29) [171] 260-277 (1935).

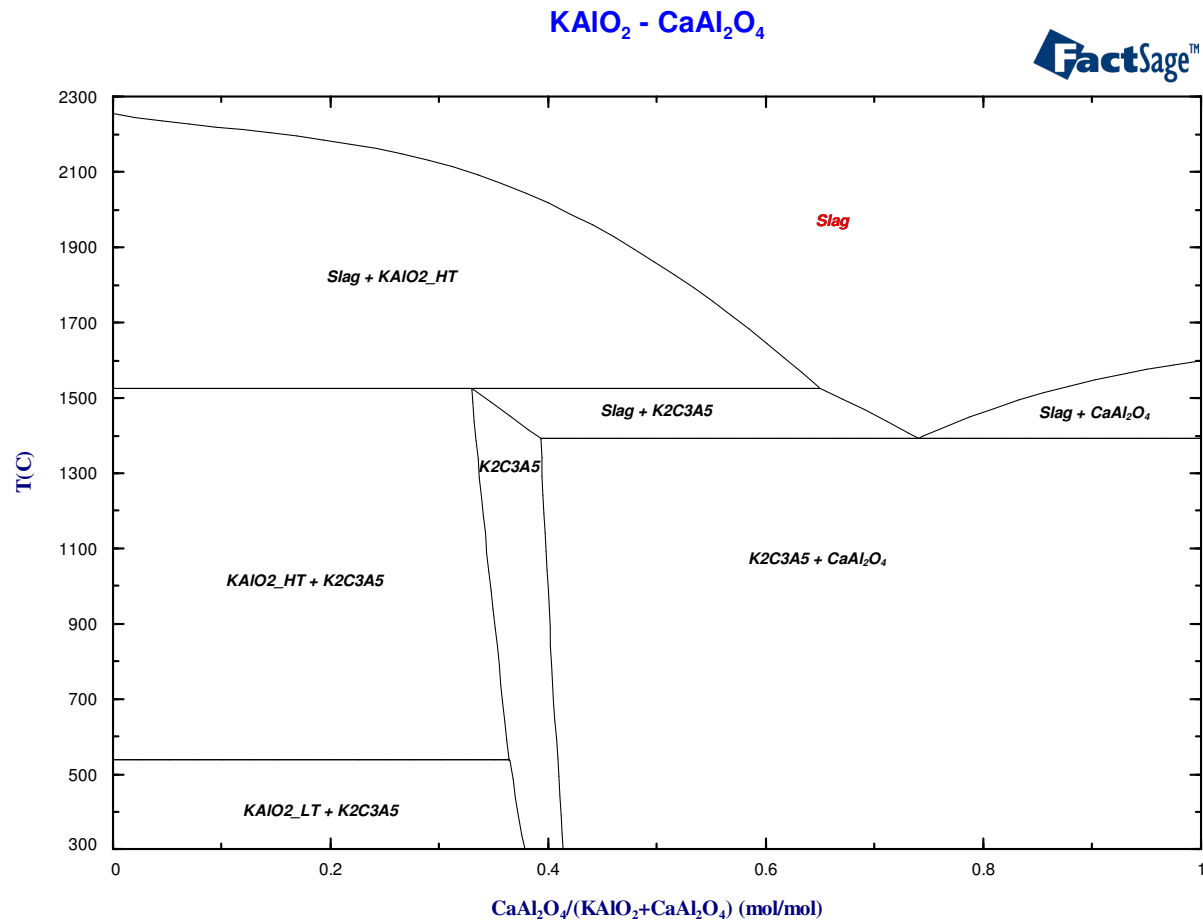
$\text{K}_2\text{O} - \text{Al}_2\text{O}_3 - \text{CaO}$   
Projection (Slag)

FactSage™



# Proposed isopleth section $K_2Al_2O_4$ - $CaAl_2O_4$

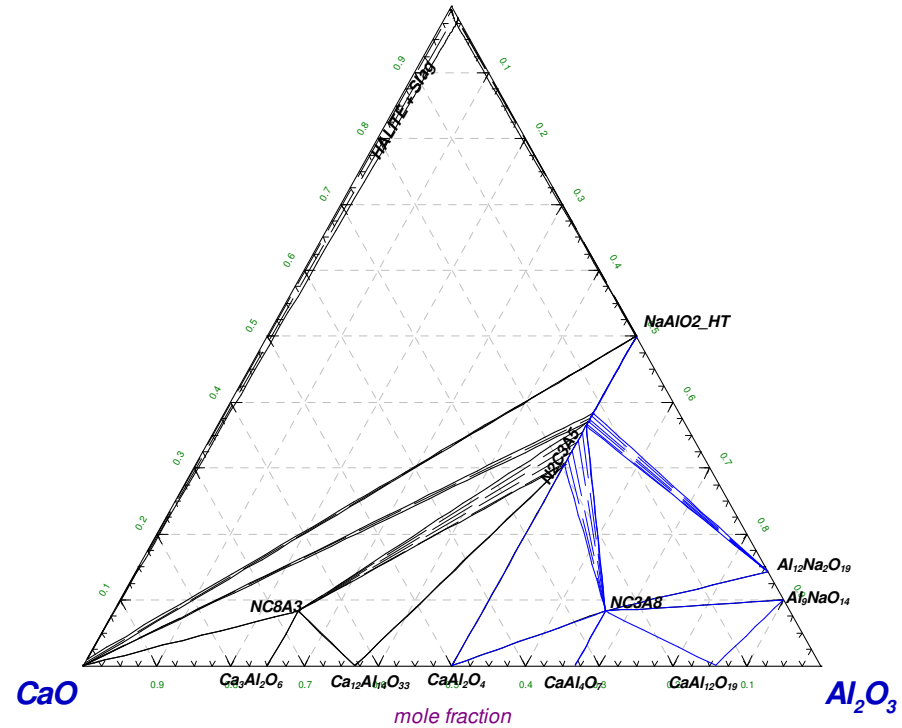
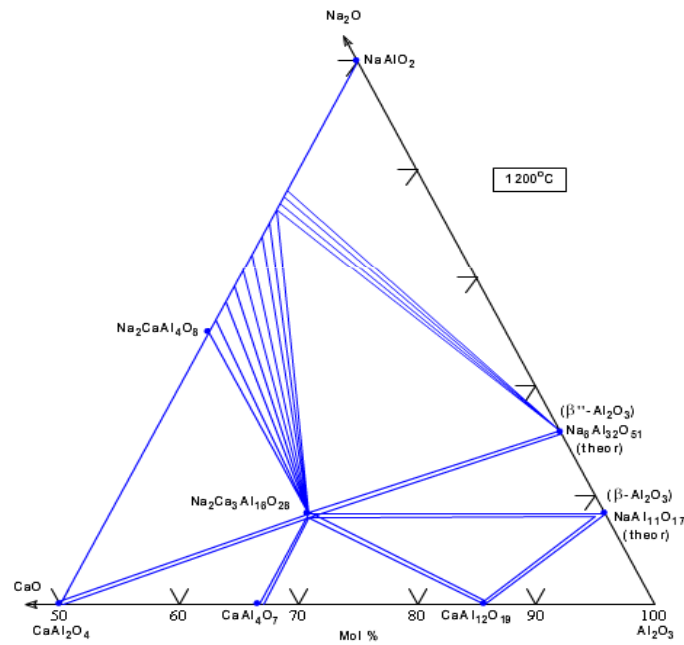
GTT-Technologies



# Isothermal section at 1200°C in $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{Na}_2\text{O}$

H. Verweij and C. M. P. M. Saris, *J. Am. Ceram. Soc.*, 69 [2] 94-98 (1986).

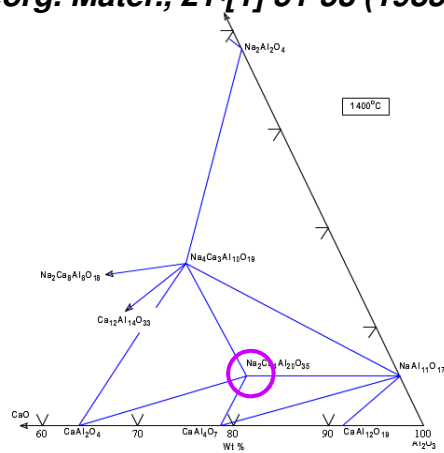
$\text{CaO} - \text{Na}_2\text{O} - \text{Al}_2\text{O}_3$   
1200°C  
 $\text{Na}_2\text{O}$



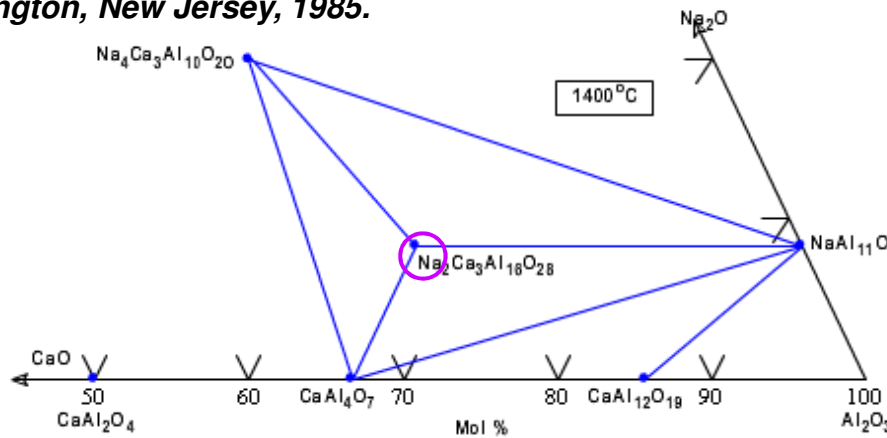
# Isothermal section at 1400°C in Al<sub>2</sub>O<sub>3</sub>-CaO-Na<sub>2</sub>O

GTT-Technologies

G. I. Zaldat, M. S. Kupriyanova, and A. L. Tubolev, *Izv. Akad. Nauk SSSR, Neorg. Mater.*, 21<sup>(1-2)</sup> [1] 51-53 (1985).

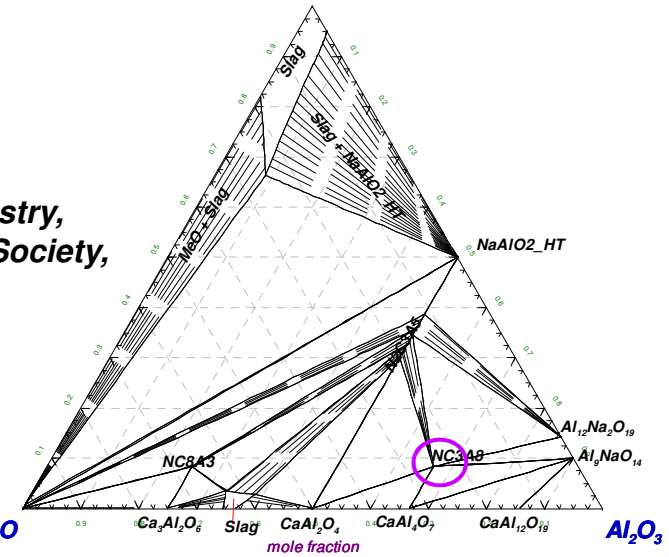


J. D. Hodge, in *Proc. - Electrochem. Soc., High Temperature Lamp Chemistry*, 1985, Vol. 85-2, pp. 261-270, Edited by E. G. Zubler, The Electrochemical Society, Inc., Pennington, New Jersey, 1985.



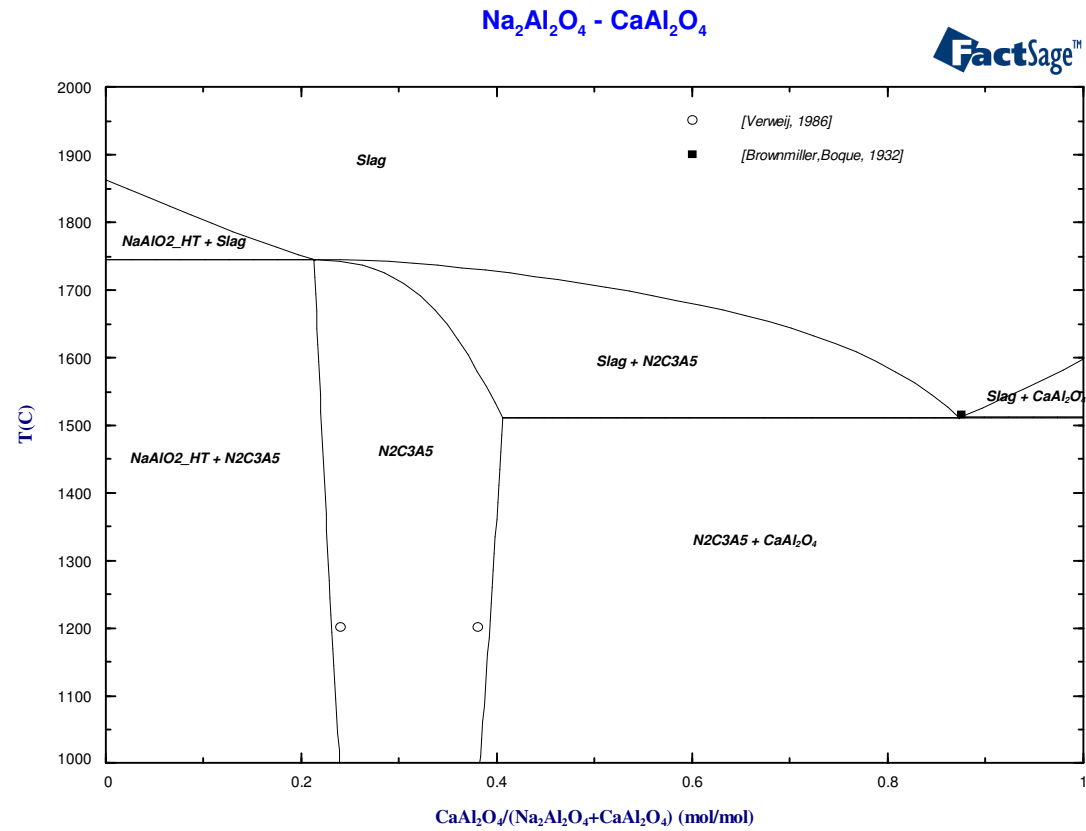
CaO - Na<sub>2</sub>O - Al<sub>2</sub>O<sub>3</sub>  
1400°C  
Na<sub>2</sub>O

FactSage™

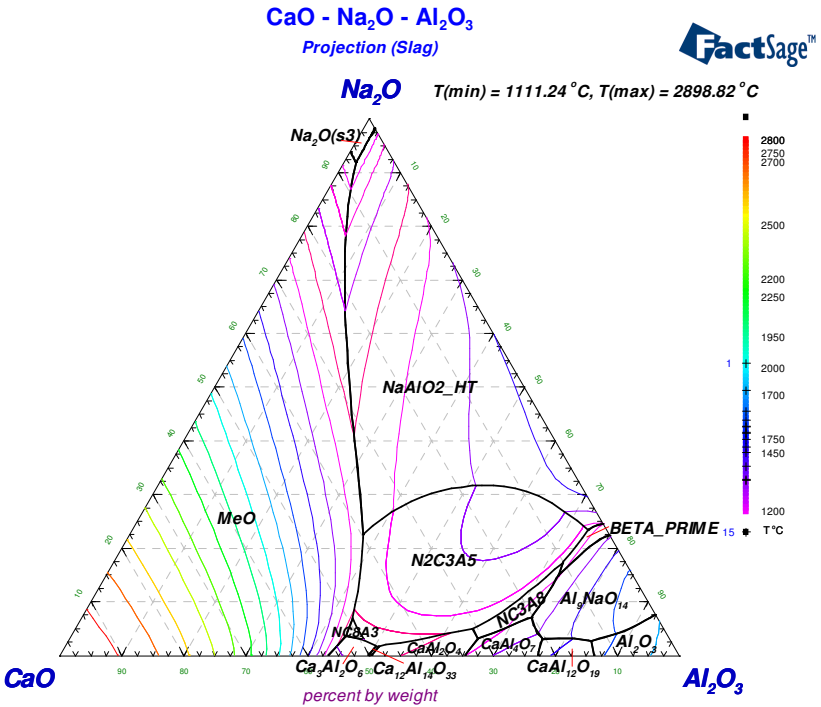
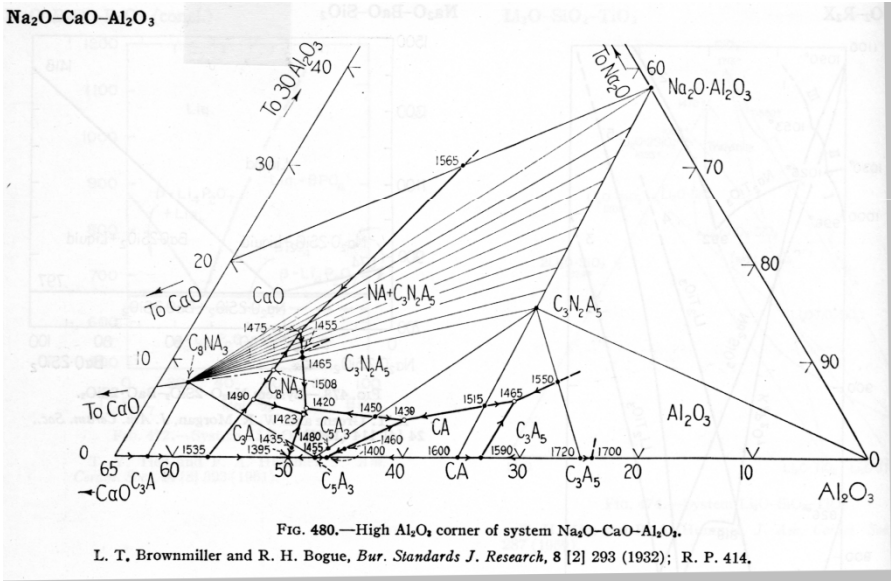


# Isopleth section $\text{Na}_2\text{Al}_2\text{O}_4$ - $\text{CaAl}_2\text{O}_4$

GTT-Technologies

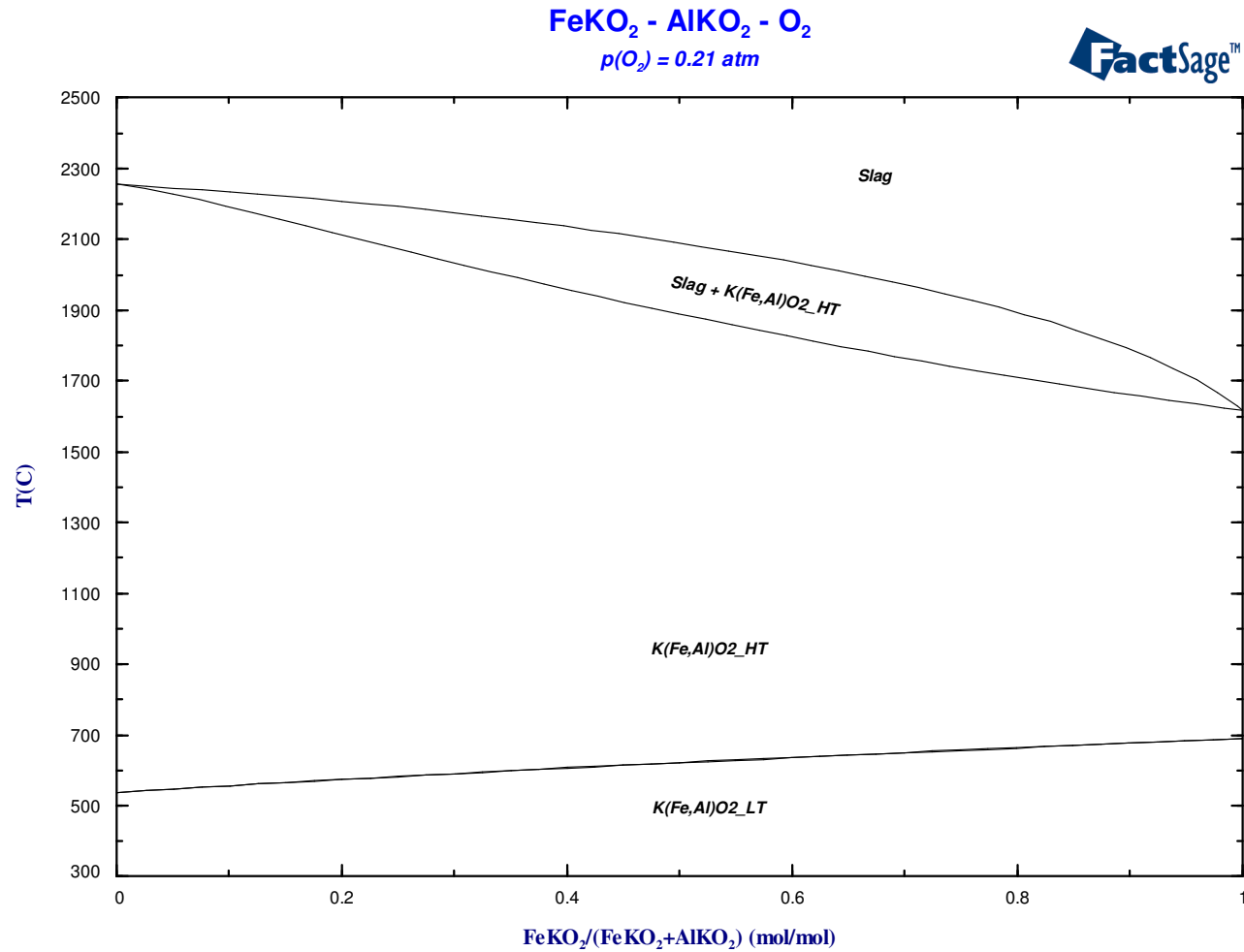


# Liquidusoberfläche in $\text{Al}_2\text{O}_3\text{-CaO-Na}_2\text{O}$



# Proposed isoplethal section $\text{FeKO}_2\text{-AlKO}_2$ in air

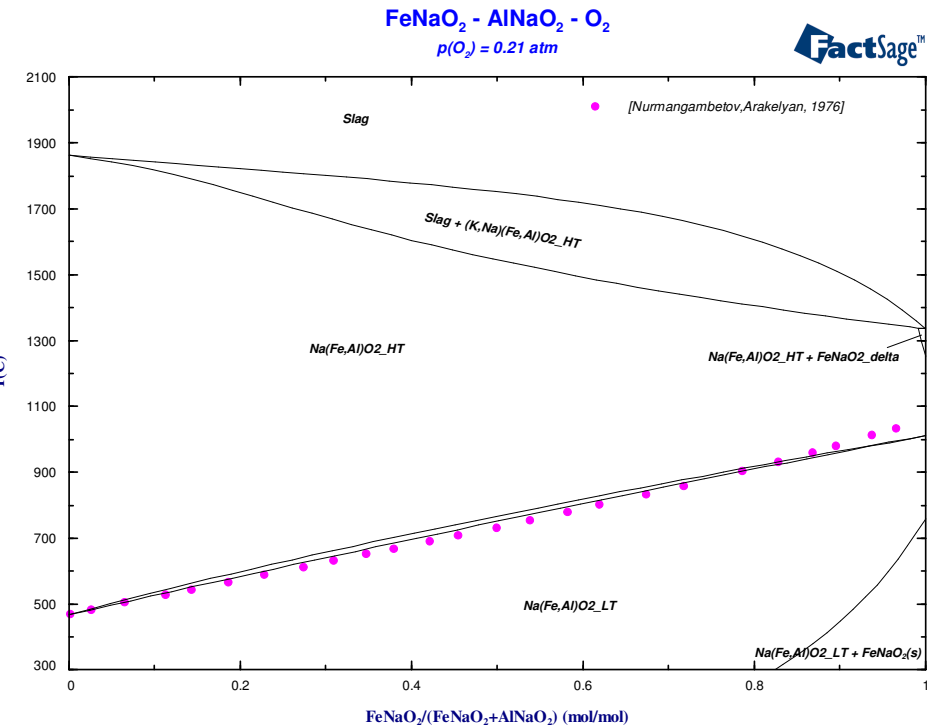
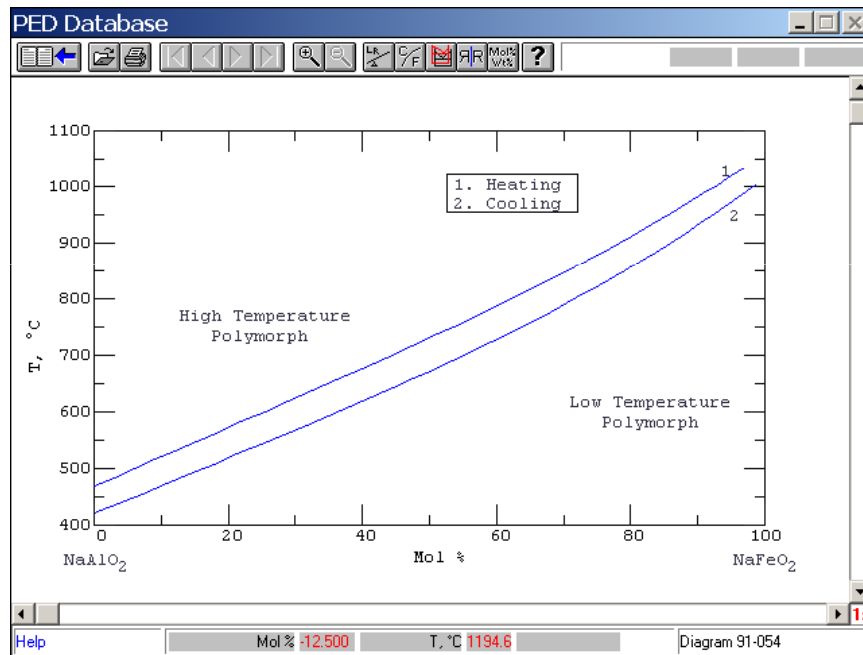
GTT-Technologies



# Isoplethal section $\text{FeNaO}_2\text{-AlNaO}_2$ in air

GTT-Technologies

Kh.N. Nurmangambetov, O.I.Arakelyan, S.A.Shcherban, Z.S.Karpenko,  
M.V.Tsvetkova, Izv. Vyssh.Uchebn,Zaved., Tsvetn. Metall., No.3,  
(1976), pp.61-65.

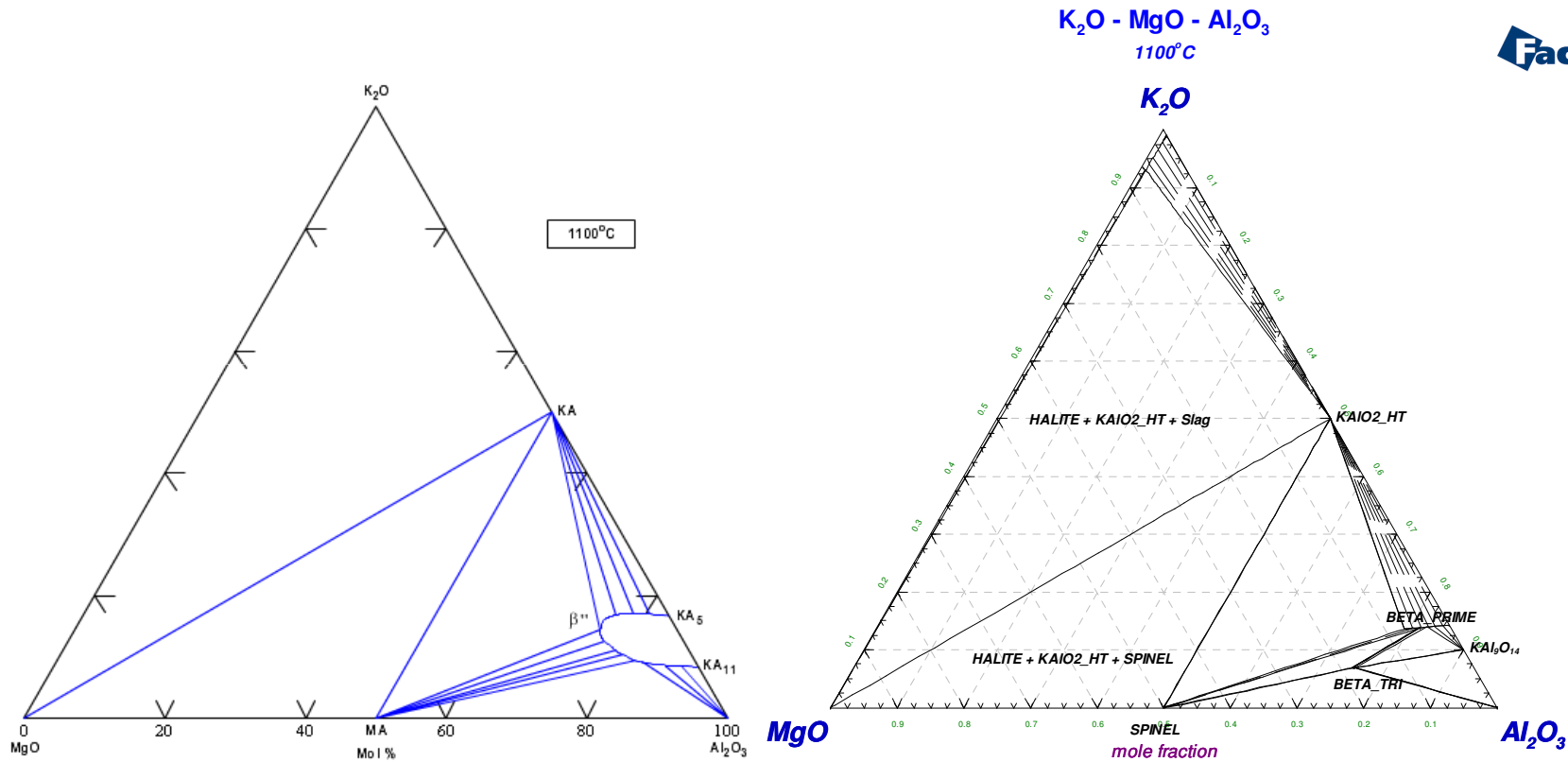




# Isothermal section at 1100°C in Al<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-MgO

GTT-Technologies

J. A. M. Van Hoek, F. J. J. Van Loo, and R. Metselaar, *Key Eng. Mater.*, 53-55 [Austceram '90] 111-119 (1991).



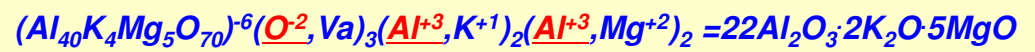
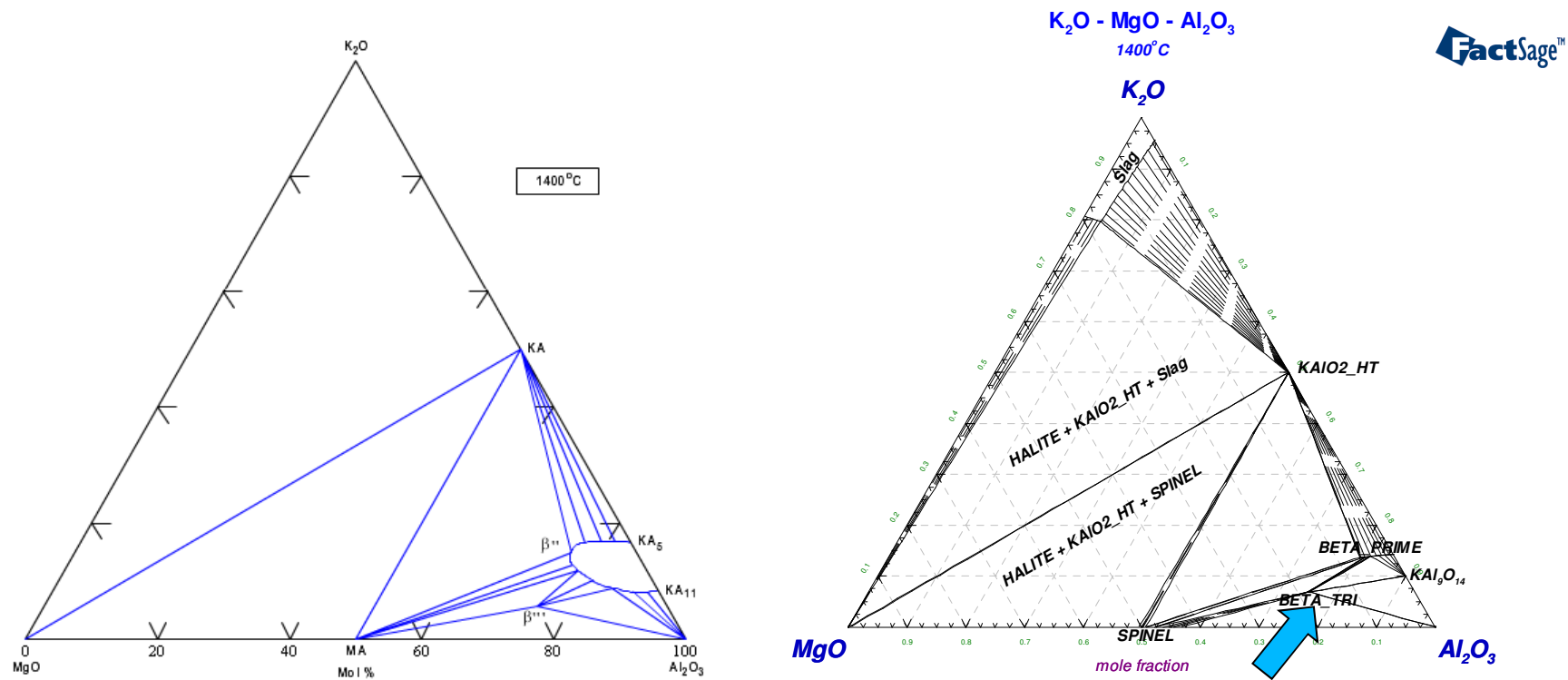
FactSage™



# Isothermal section at 1400°C in Al<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-MgO

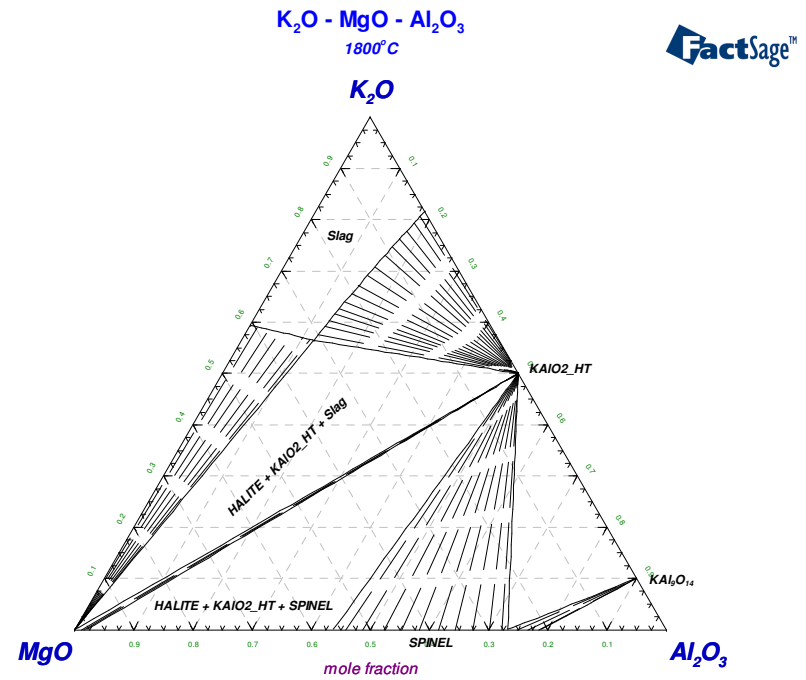
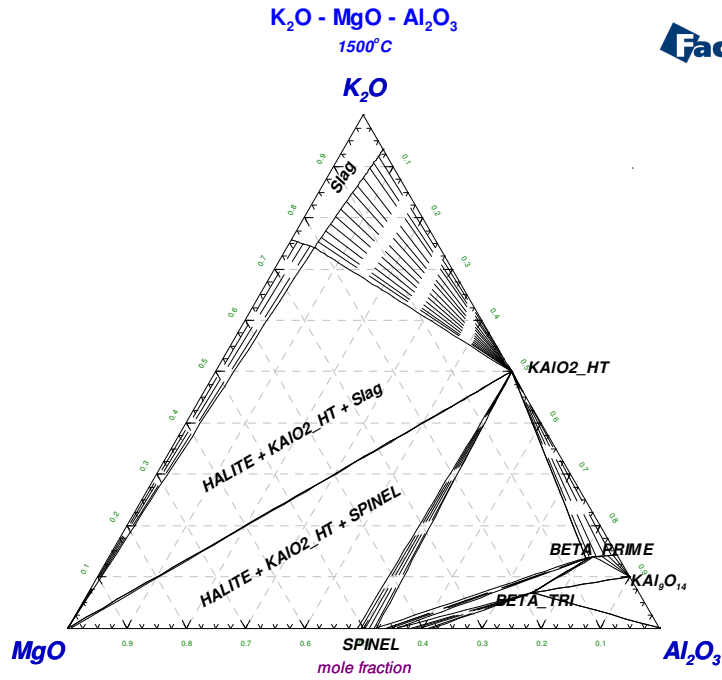
GTT-Technologies

J. A. M. Van Hoek, F. J. J. Van Loo, and R. Metselaar, *Key Eng. Mater.*, 53-55 [Austceram '90] 111-119 (1991).



# Proposed isothermal sections in $\text{Al}_2\text{O}_3$ - $\text{K}_2\text{O}$ - $\text{MgO}$

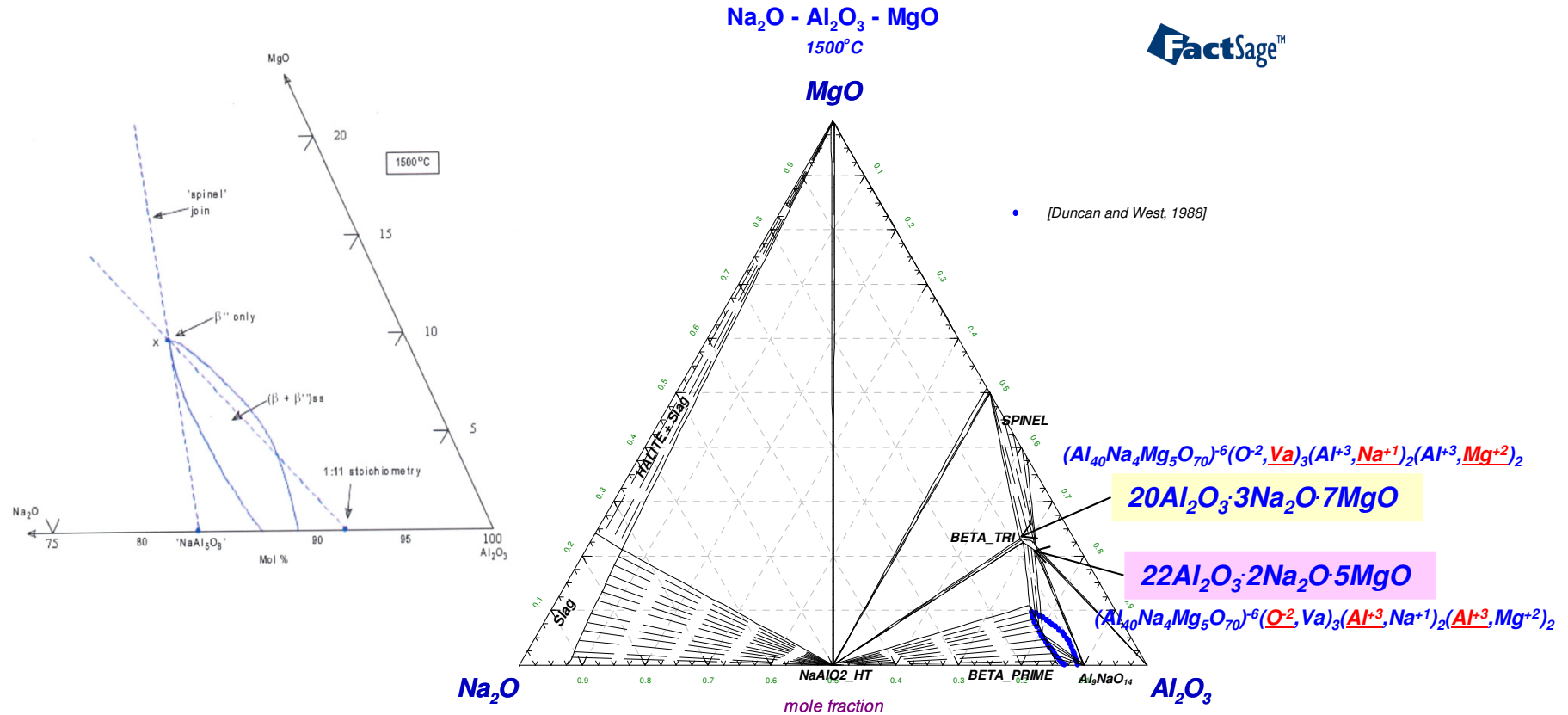
GTT-Technologies



# Isothermal section at 1500°C in Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O

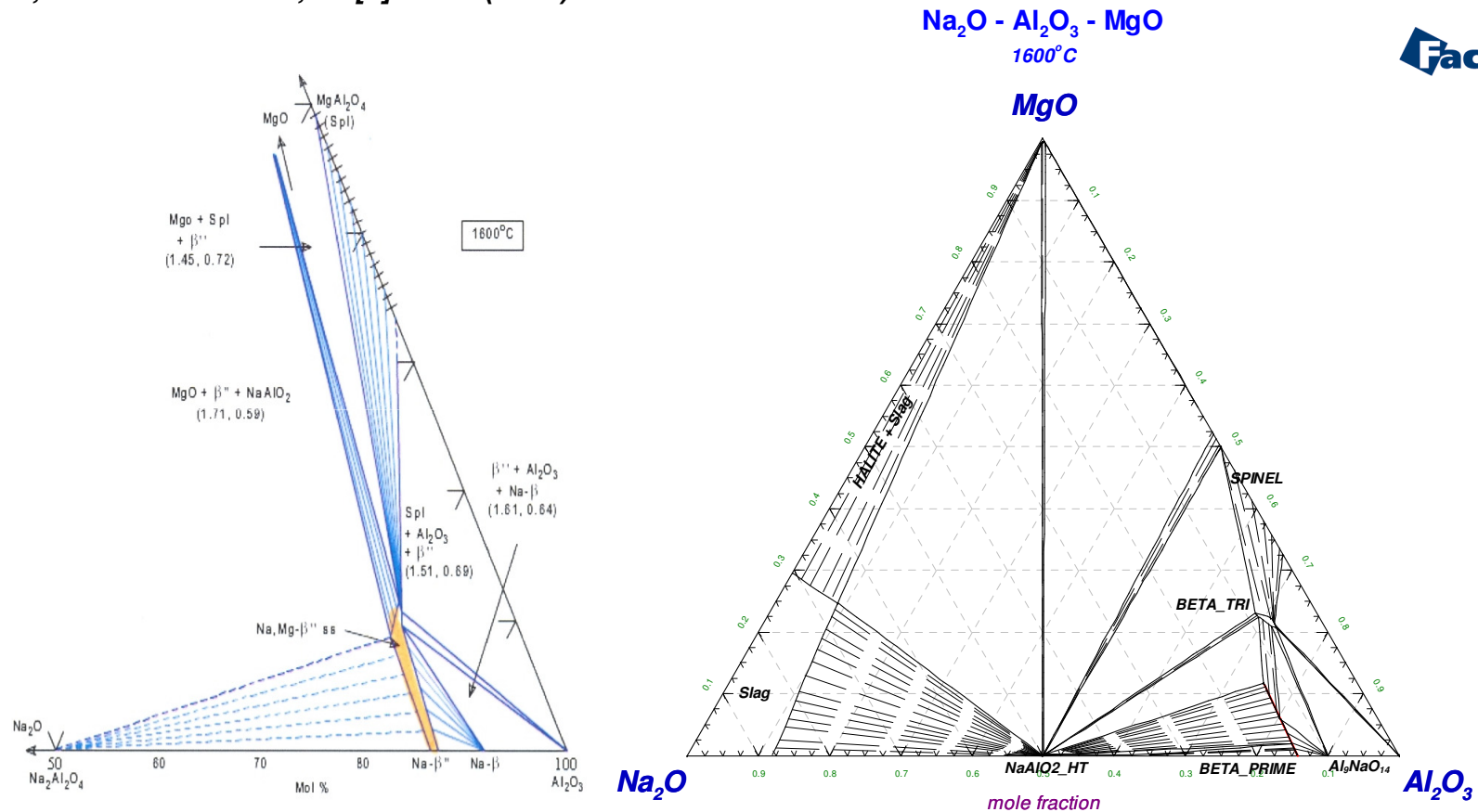
GTT-Technologies

G. K. Duncan and A. R. West, *Solid State Ionics*, 28-30 [Pt. 1] 338-343 (1988).



# Isothermal section at 1600°C in Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O

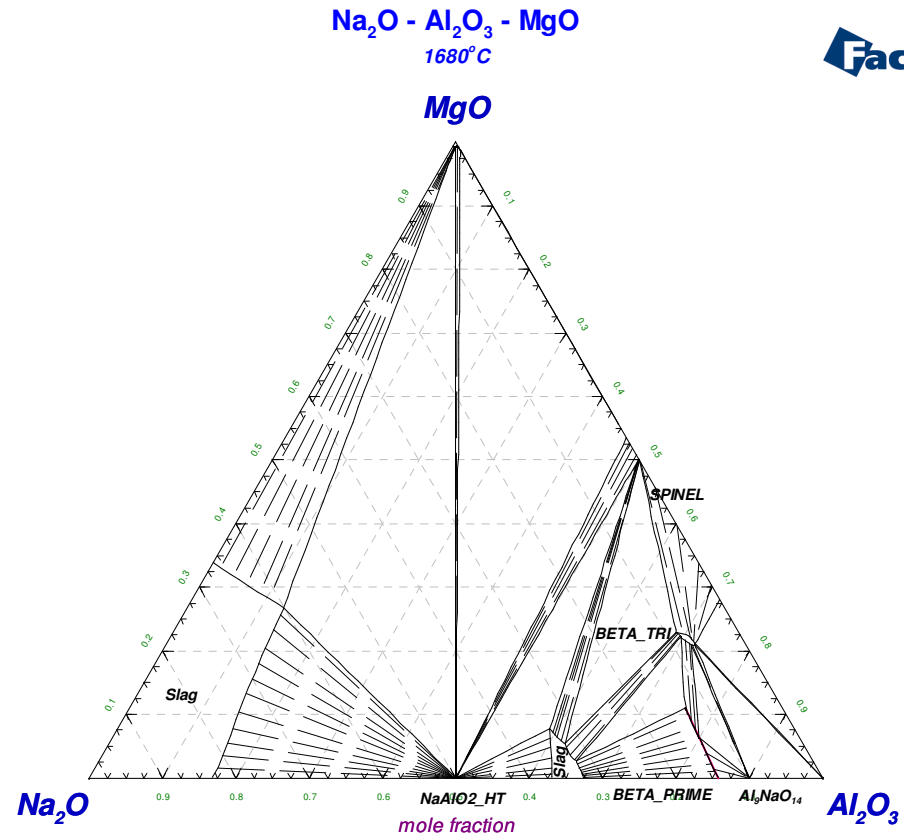
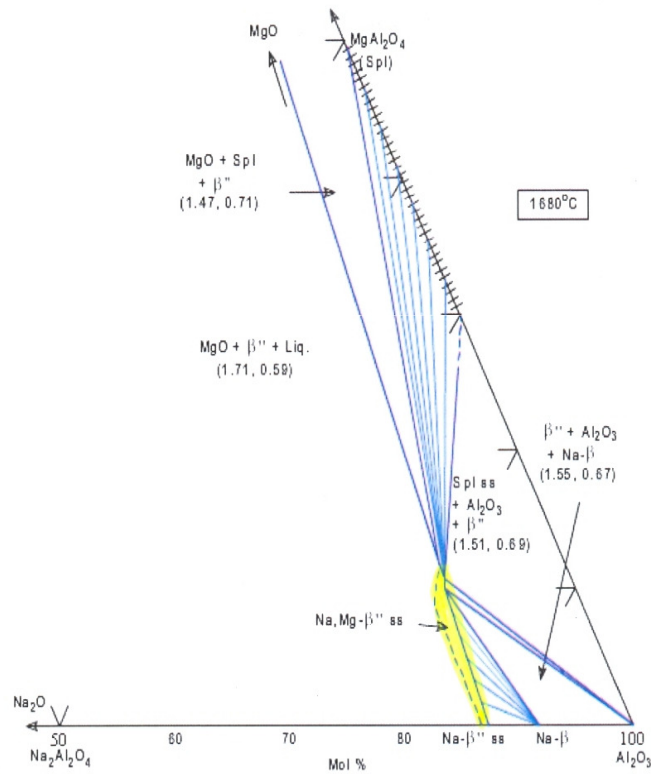
M. Alden, *Solid State Ionics*, 20 [1] 17-23 (1986).



# Isothermal section at 1680°C in Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O

GTT-Technologies

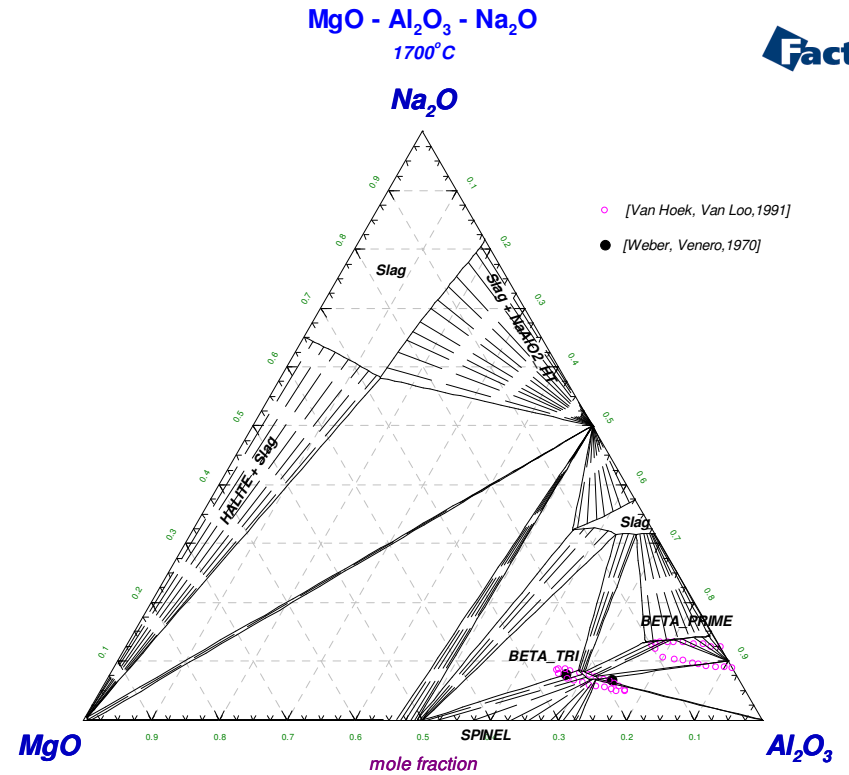
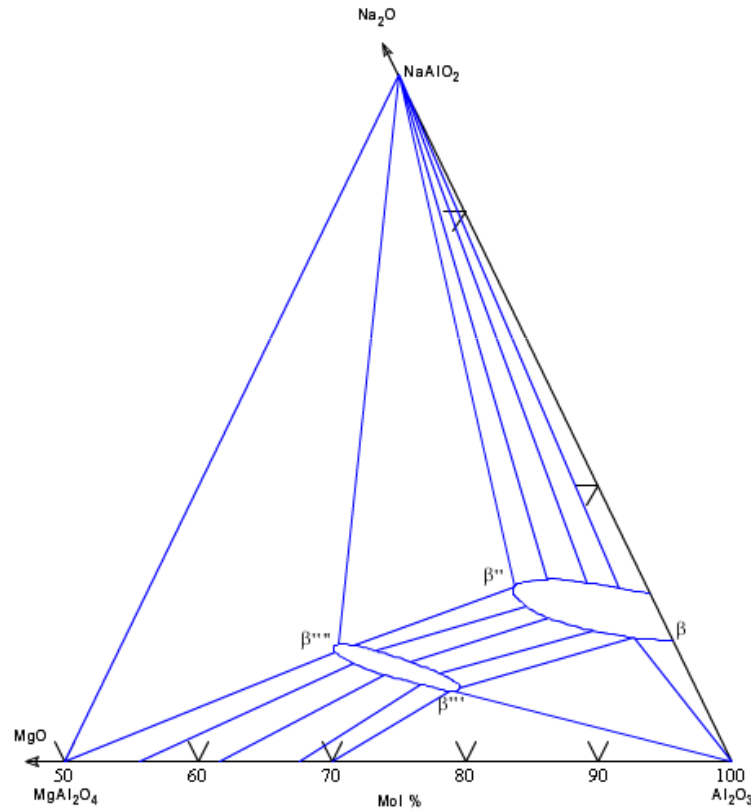
M. Alden, *Solid State Ionics*, 20 [1] 17-23 (1986).



# Isothermal section at 1700°C in Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O

GTT-Technologies

J. A. M. Van Hoek, F. J. J. Van Loo, and R. Metselaar, *Key Eng. Mater.*,53-55  
[Austceram '90] 111-119 (1991),  
7



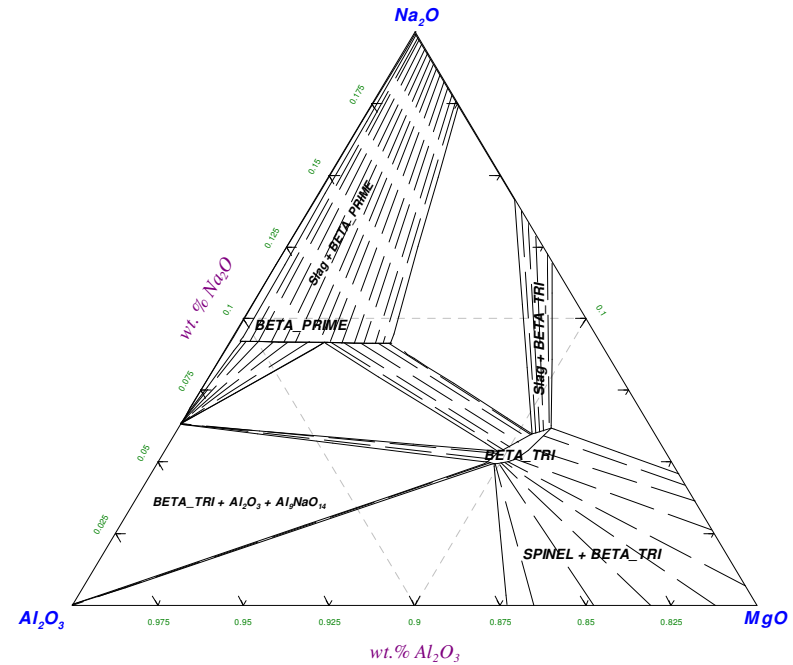
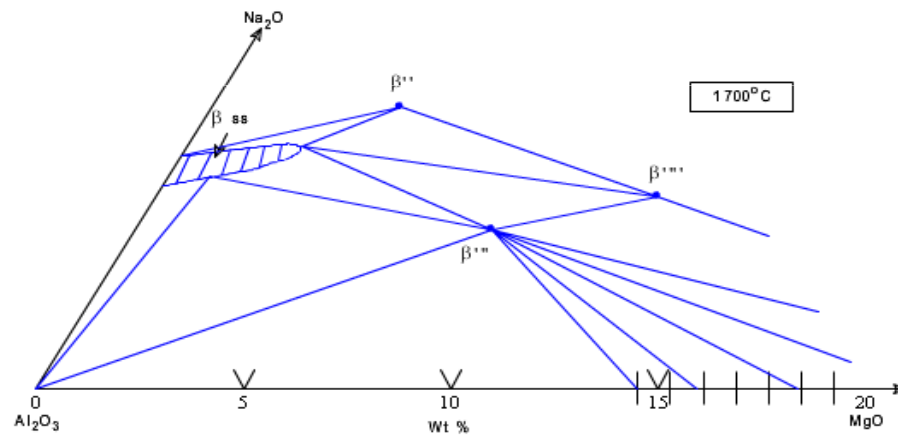
# Isothermal section at 1700°C in Al<sub>2</sub>O<sub>3</sub>-MgO-Na<sub>2</sub>O

GTT-Technologies

J. T. Kummer, "*β-Alumina Electrolytes*"; Chp. 5; pp. 141-175, in *Progress in Solid State Chemistry*, Vol. 7. Edited by H. Reiss and J. O. McCaldin. Pergamon Press (Elsevier Science Inc.), New York, New York, 1972.

Na<sub>2</sub>O - Al<sub>2</sub>O<sub>3</sub> - MgO  
1700°C

FactSage™

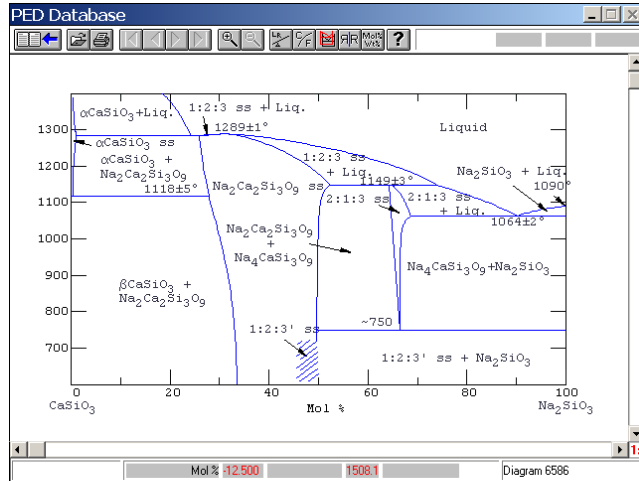




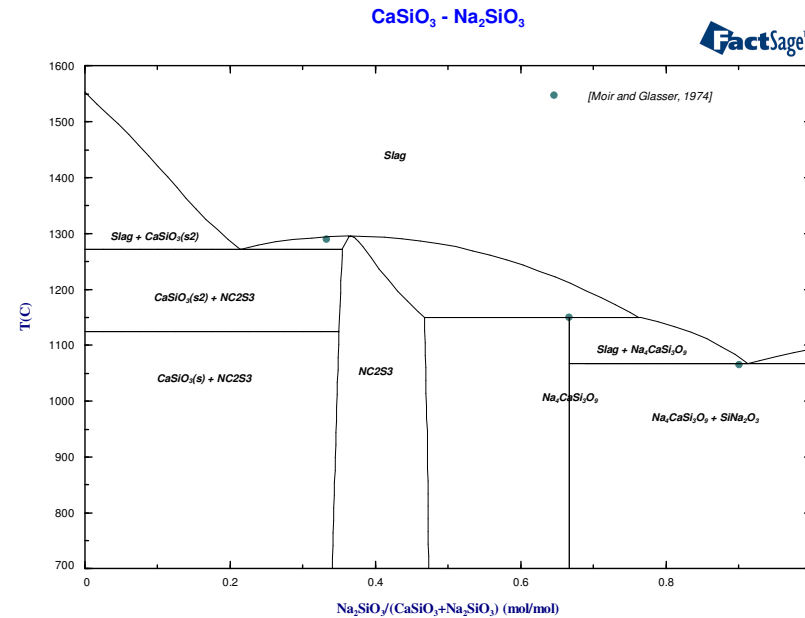
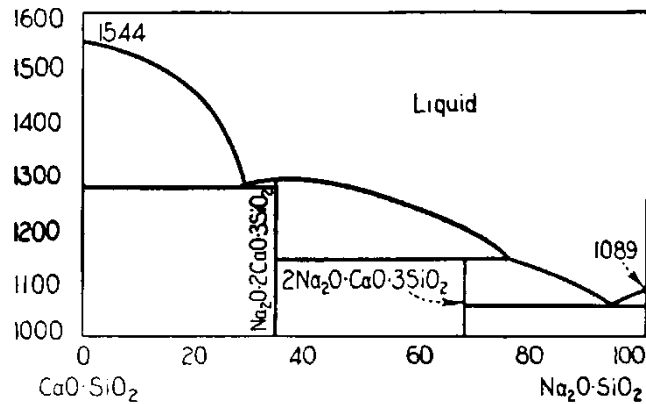
# Orthosilicate isoplethal section in $\text{CaO-Na}_2\text{O-SiO}_2$

GTT-Technologies

G. K. Moir and F. P. Glasser, *Trans. J. Br. Ceram. Soc.*, 73 [6], (1974), pp. 199-206



G. W. Morey and N. L. Bowen, *J. Soc. Glass Technol.*, 9, 226-264 (1925).

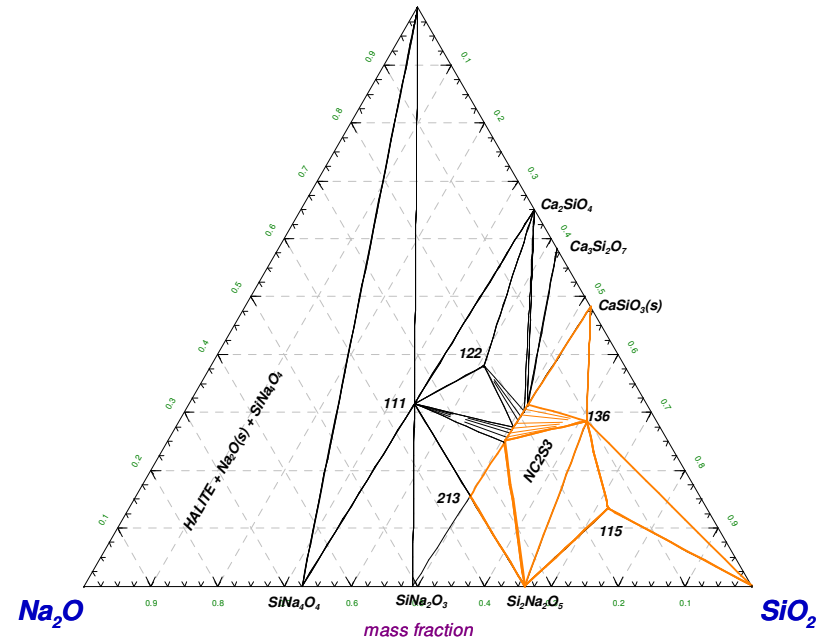
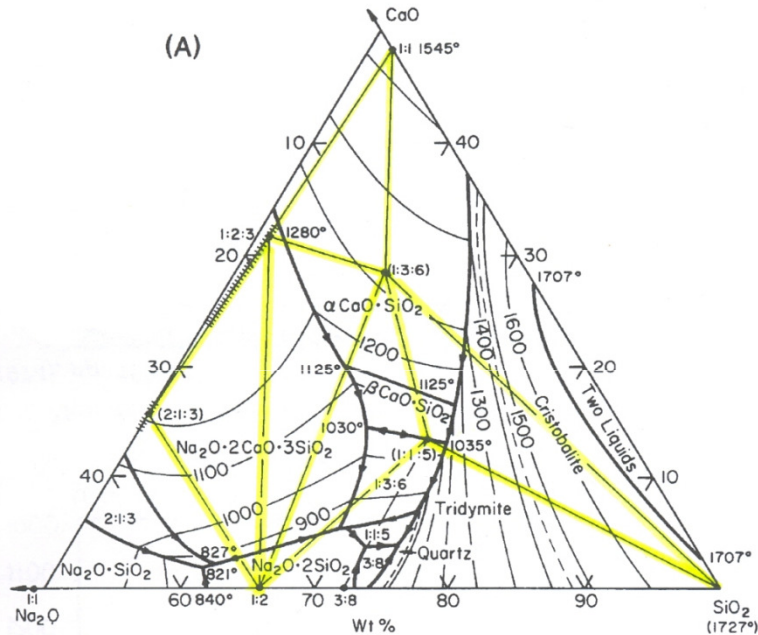


# Isothermal section at 600°C in CaO-Na<sub>2</sub>O-SiO<sub>2</sub>

GTT-Technologies

K.A. Shahid, F.P. Glasser, *Phys. Chem. Glasses*, 12 [2], (1971), pp.50-57.

CaO - Na<sub>2</sub>O - SiO<sub>2</sub>  
600°C



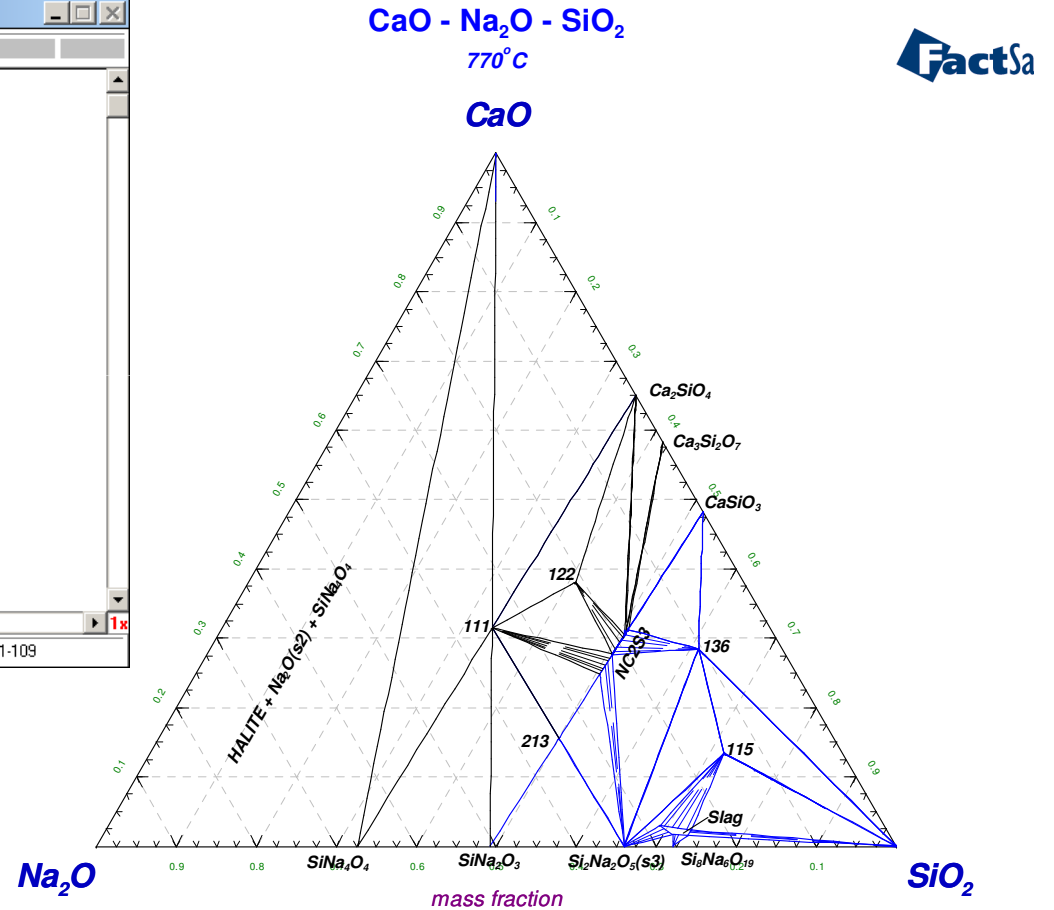
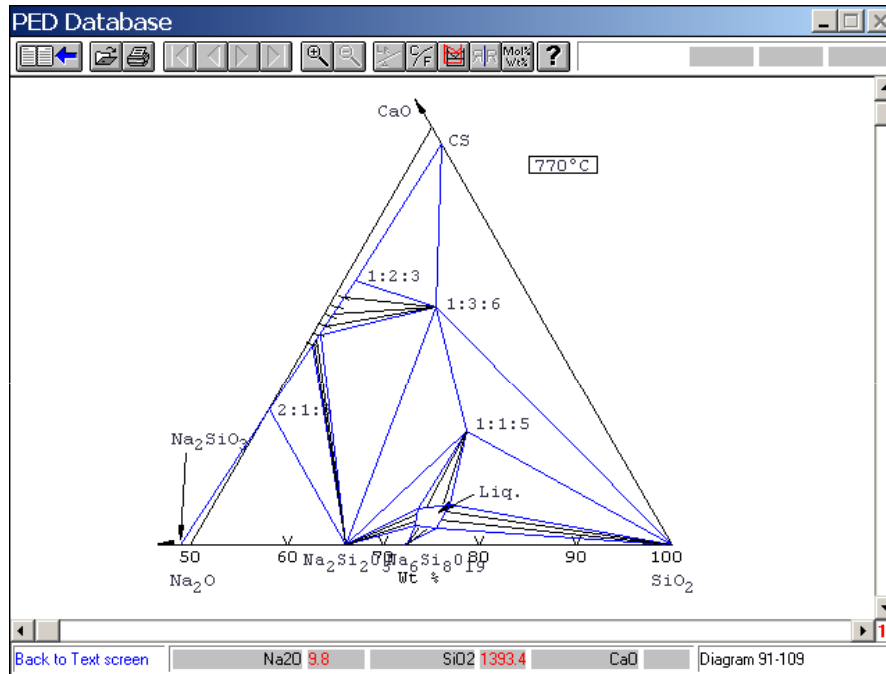
Phase	Description	Formula
111	Stoichiometric	Na <sub>2</sub> CaSiO <sub>4</sub>
115	Stoichiometric	Na <sub>2</sub> CaSi <sub>5</sub> O <sub>12</sub>
122	Stoichiometric	Na <sub>2</sub> Ca <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>
136	Stoichiometric	Na <sub>2</sub> Ca <sub>3</sub> Si <sub>6</sub> O <sub>16</sub>
213	Stoichiometric	Na <sub>4</sub> CaSi <sub>3</sub> O <sub>9</sub>
NC2S3	Solid solution	(Na <sup>1+</sup> , Va) <sub>2</sub> (Ca <sup>2+</sup> , Va)(CaNa <sub>2</sub> Si <sub>3</sub> O <sub>9</sub> <sup>2-</sup> )



# Isothermal section at 770°C in CaO-Na<sub>2</sub>O-SiO<sub>2</sub>

GTT-Technologies

G. K. Moir and F. P. Glasser, *Phys. Chem. Glasses*, 17 [3] 45-53 (1976).

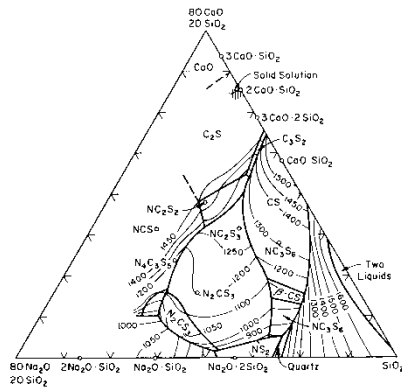


FactS<sub>8</sub>

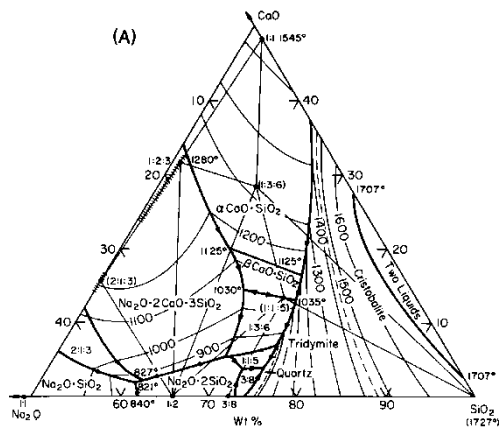


# Liquidus surface in CaO-Na<sub>2</sub>O-SiO<sub>2</sub>

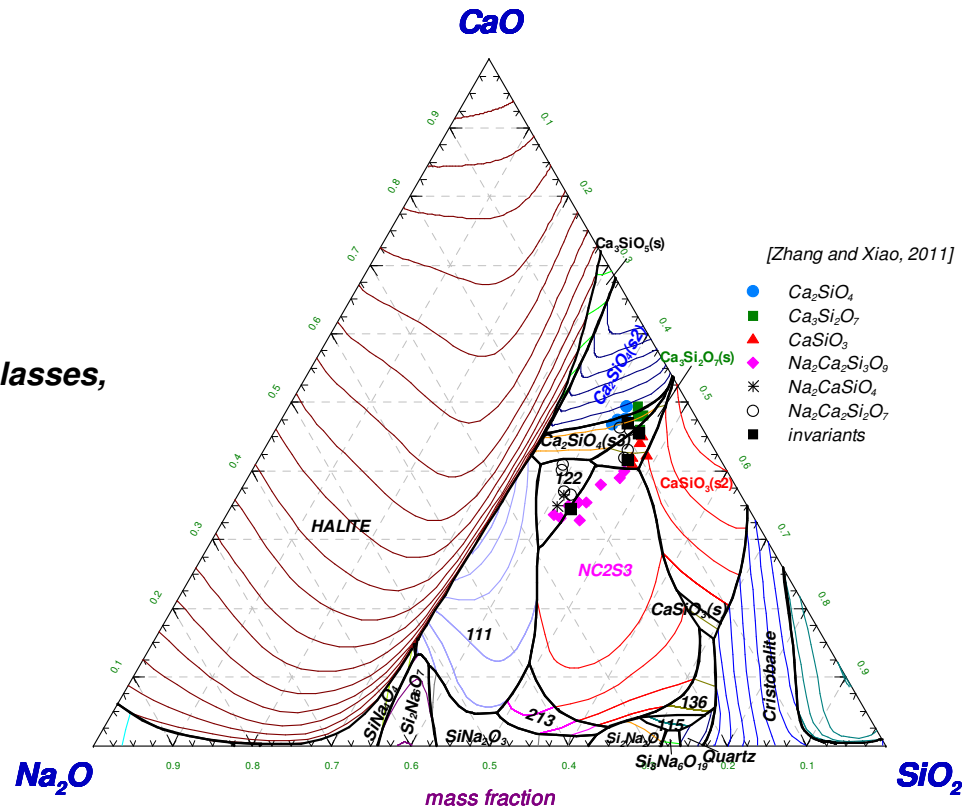
E. R. Segnit, *Am. J. Sci.*, 251 [8] 586-601 (1953).



K.A. Shahid, F.P. Glasser, *Phys. Chem. Glasses*, 12 [2], (1971), pp.50-57

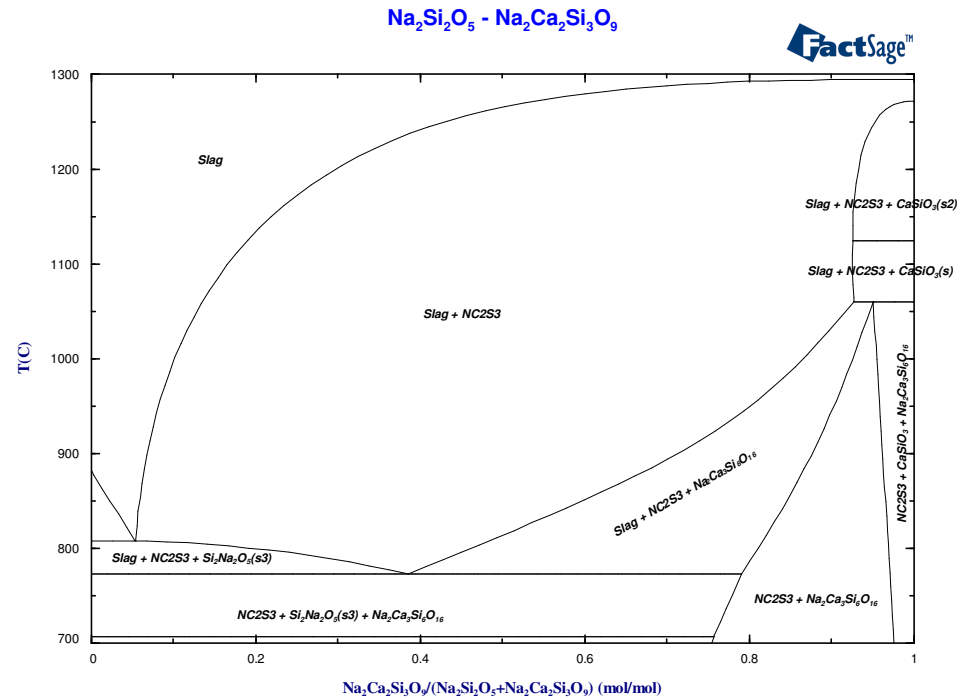
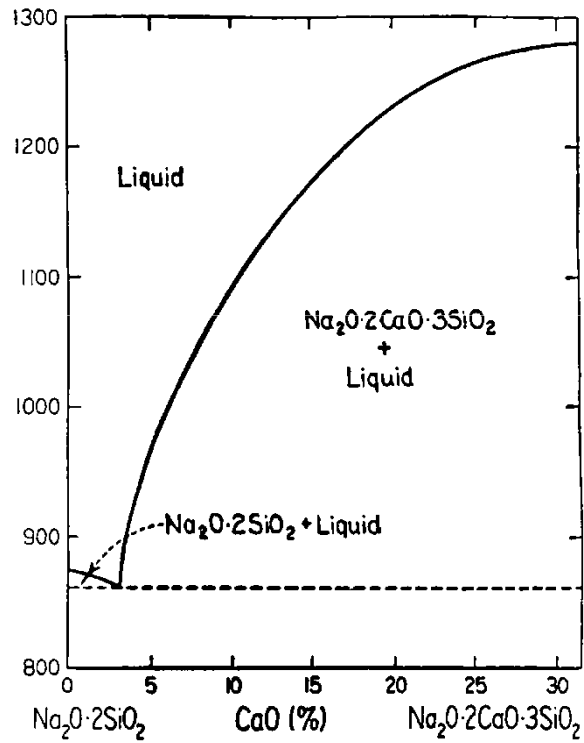


CaO - Na<sub>2</sub>O - SiO<sub>2</sub>  
Projection (Slag)



# Isoplethal section in CaO-Na<sub>2</sub>O-SiO<sub>2</sub>

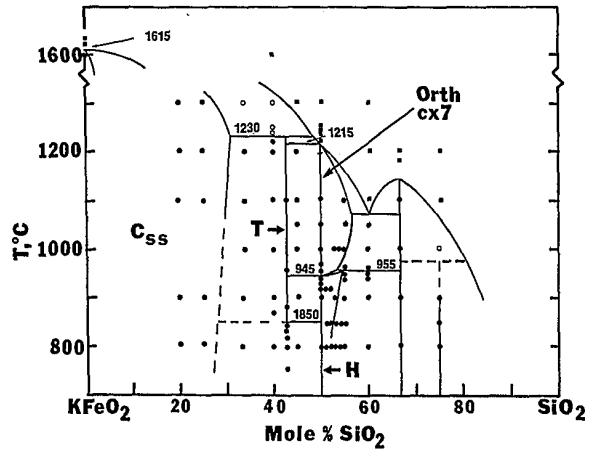
G. K. Moir and F. P. Glasser, *Trans. J. Br. Ceram. Soc.*, 73 [6], (1974), pp. 199-206



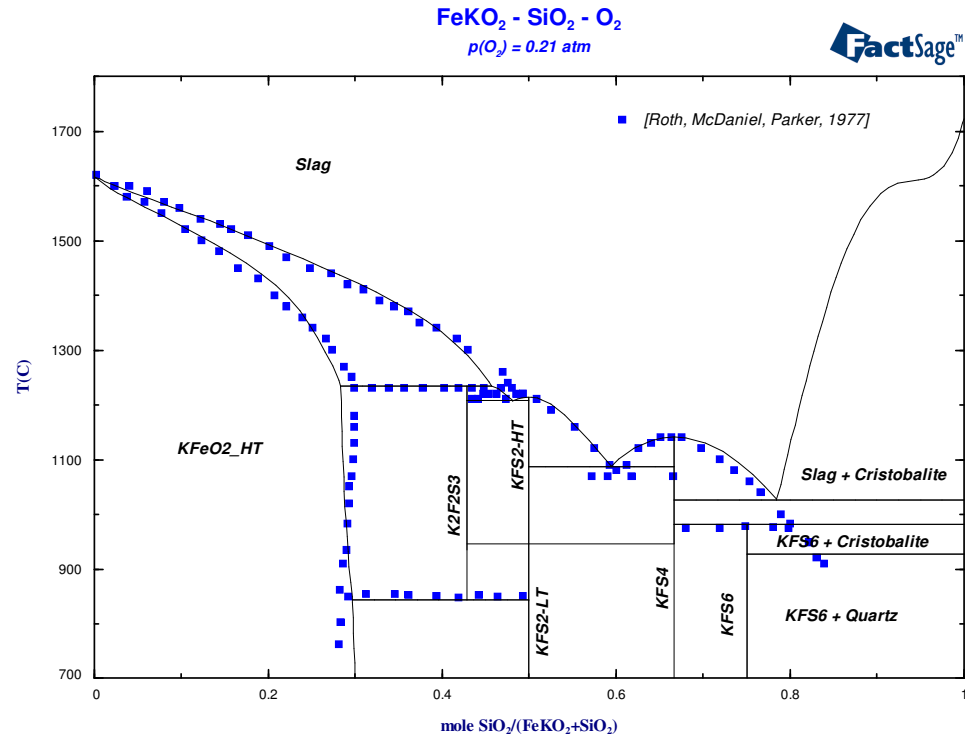
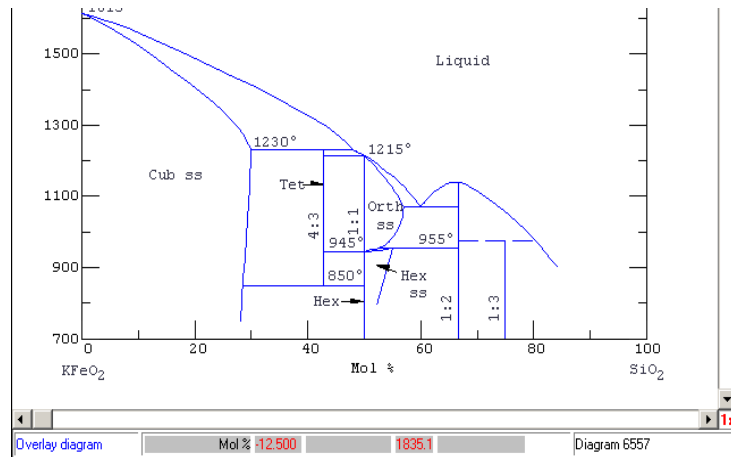
# Isoplethal section $\text{FeKO}_2\text{-SiO}_2$ in air

GTT-Technologies

R.S. Roth, *Adv. Chem. Ser., No. 186,, (1980), pp. 391-408.*



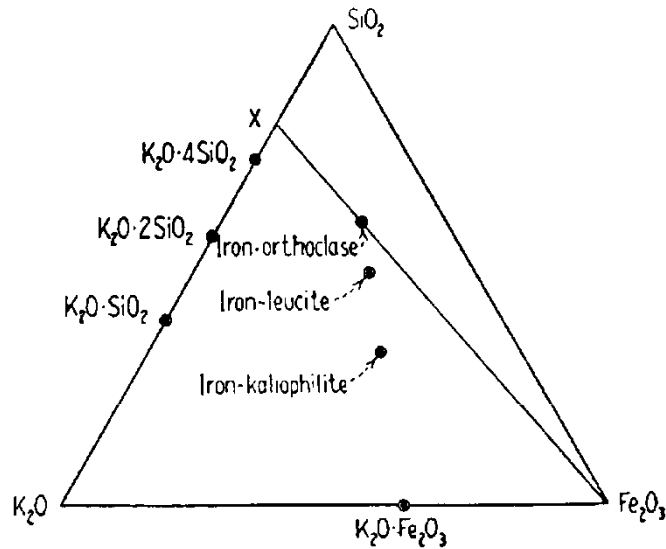
R.S. Roth, C.L. McDaniel, H.S. Parker., *Geol. Soc. Am. Abstr., 9 [7], (1977), p. 1149.*



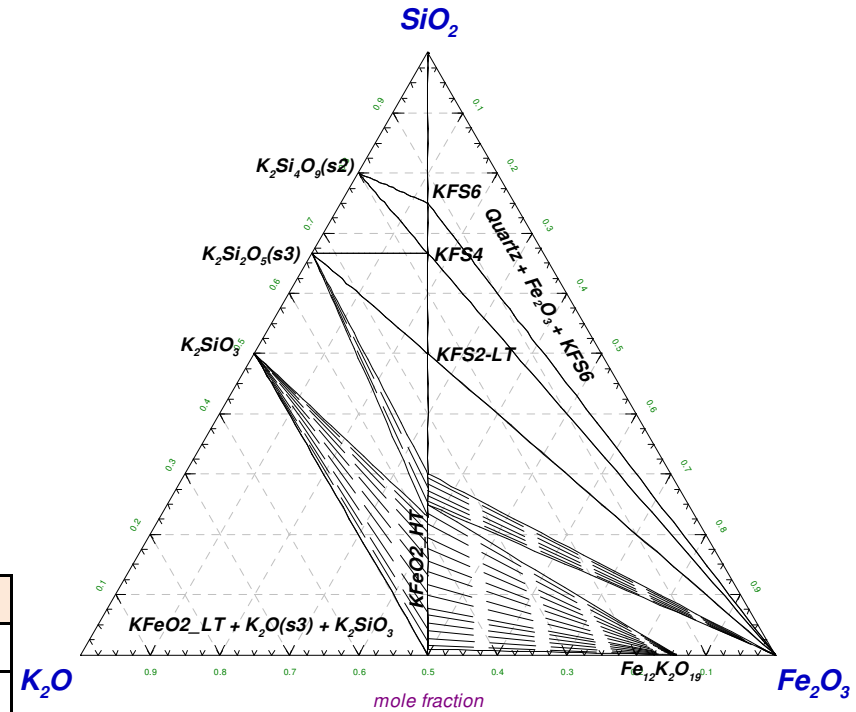
# Isothermal section at 600°C in Fe<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-SiO<sub>2</sub> in air

GTT-Technologies

G.T. Faust, *Am. Mineral*, 21 [12], (1936), pp. 735-763.



Fe<sub>2</sub>O<sub>3</sub> - K<sub>2</sub>O - SiO<sub>2</sub> - O<sub>2</sub>  
600°C, p(O<sub>2</sub>) = 0.21 atm



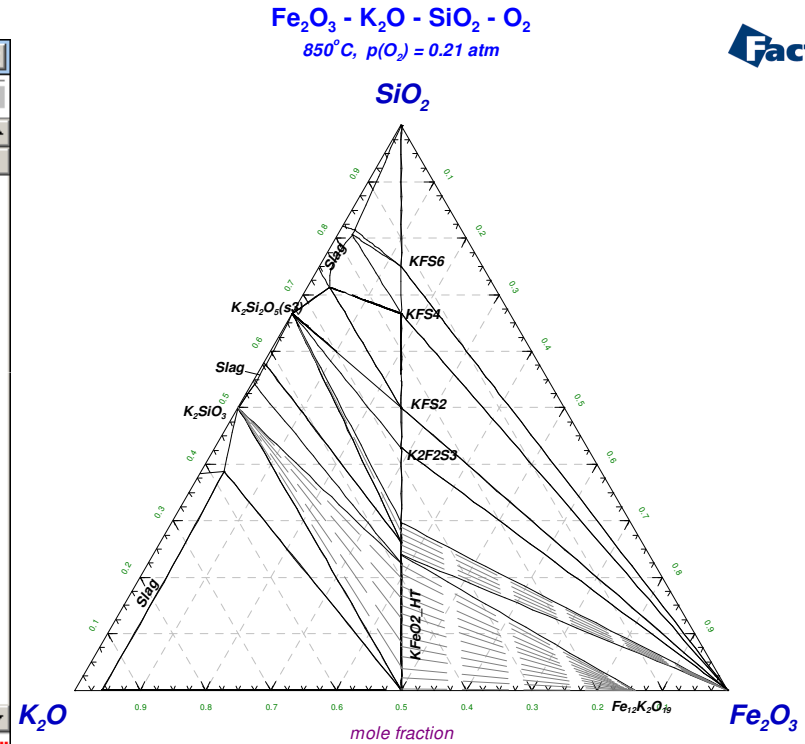
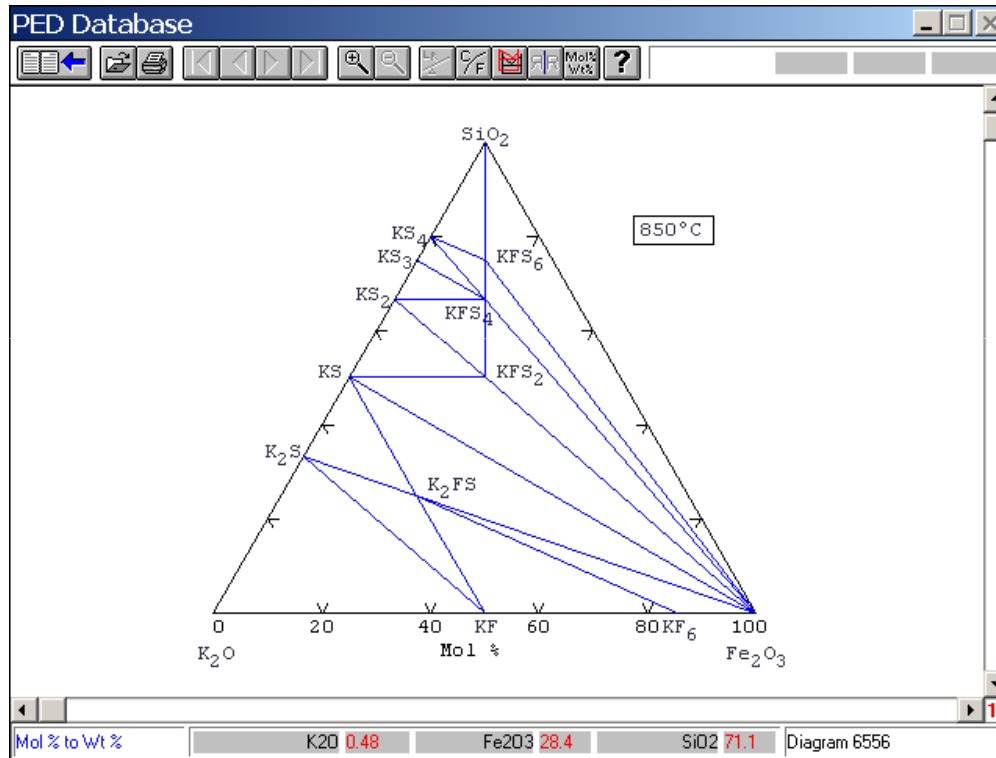
Phase	Description	Formel
KFS2-HT	Stoichiometric	Fe <sub>2</sub> K <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>
KFS2-LT	Stoichiometric	Fe <sub>2</sub> K <sub>2</sub> Si <sub>2</sub> O <sub>8</sub>
KFS4	Stoichiometric	Fe <sub>2</sub> K <sub>2</sub> Si <sub>4</sub> O <sub>12</sub>
KFS6	Stoichiometric	Fe <sub>2</sub> K <sub>2</sub> Si <sub>6</sub> O <sub>16</sub>
K2F2S3	Stoichiometric	Fe <sub>4</sub> K <sub>4</sub> Si <sub>3</sub> O <sub>14</sub>
KFeO2-HT	Solid solution	(K <sup>1+</sup> , Va)(Fe <sup>3+</sup> , Si <sup>4+</sup> )(O <sup>2-</sup> ) <sub>2</sub>
KFeO2-LT	Solid solution	(K <sup>1+</sup> , Va)(Fe <sup>3+</sup> , Si <sup>4+</sup> )(O <sup>2-</sup> ) <sub>2</sub>



# Isothermal section at 850°C in Fe<sub>2</sub>O<sub>3</sub>-K<sub>2</sub>O-SiO<sub>2</sub> in air

GTT-Technologies

A.P. Protsyuk, G.A. Konechnyi, L.G. Latysheva, *Izv. Akad. Nauk SSSR, Neorg. Mater.*, 15 [1], (1979), pp. 173-174.



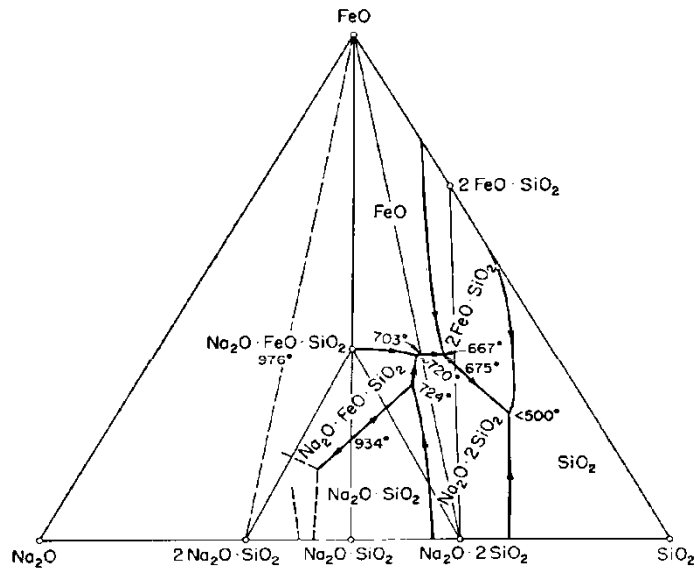


# Liquidus surface in FeO-Na<sub>2</sub>O-SiO<sub>2</sub> in equilibrium with Fe

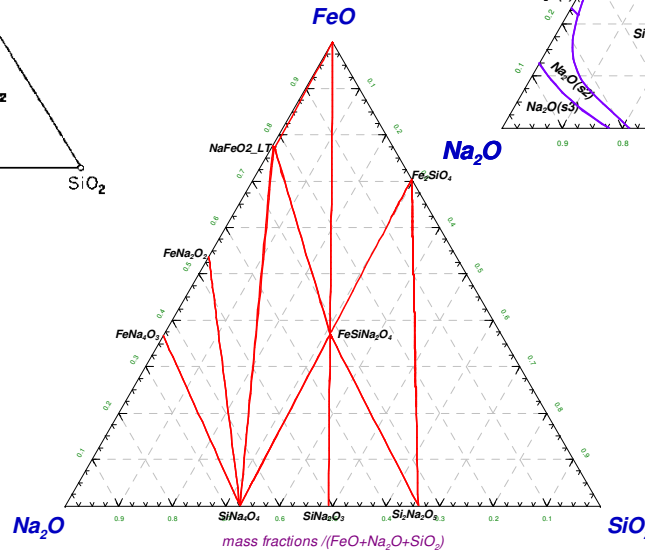
GTT-Technologies

P. T. Carter and M. Ibrahim, *J. Soc. Glass Technol.*, 36 [170] 142-163 (1952).

FeO - Na<sub>2</sub>O - SiO<sub>2</sub> - Fe  
Projection (Slag), Fe/(FeO+Na<sub>2</sub>O+SiO<sub>2</sub>) (g/g) = 0.0001



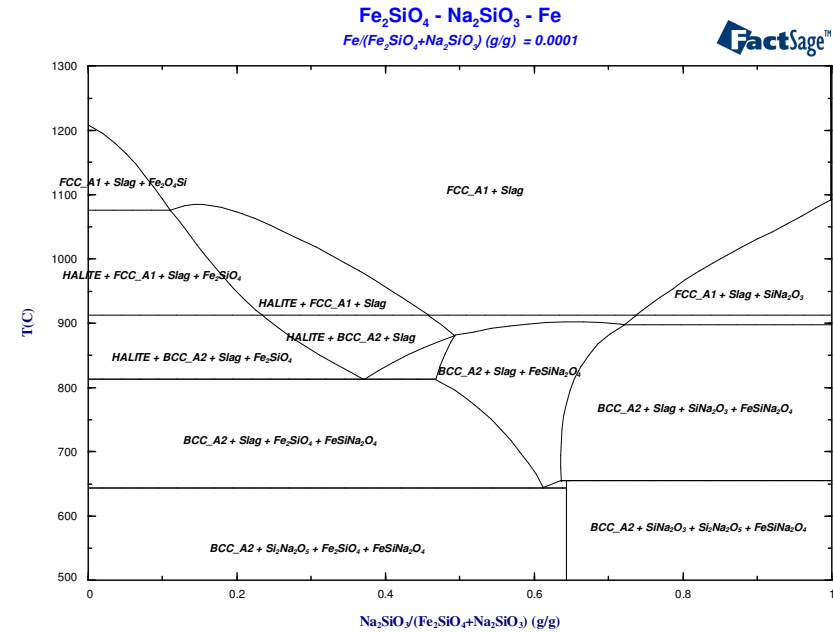
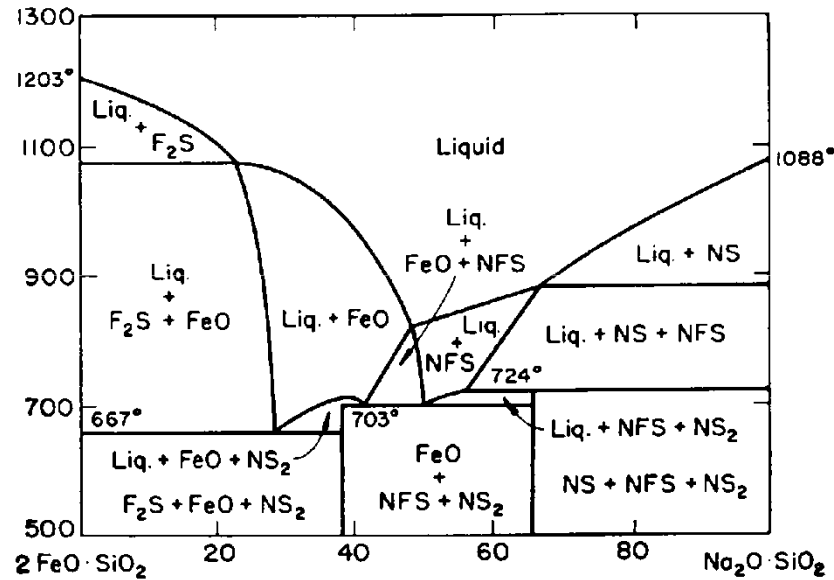
FeO - Na<sub>2</sub>O - SiO<sub>2</sub> - Fe  
580°C, Fe/(FeO+Na<sub>2</sub>O+SiO<sub>2</sub>) (g/g) = 0.0001



# Isoplethal section in $\text{Fe}_2\text{SiO}_4\text{-Na}_2\text{SiO}_3$ in equilibrium with Fe

GTT-Technologies

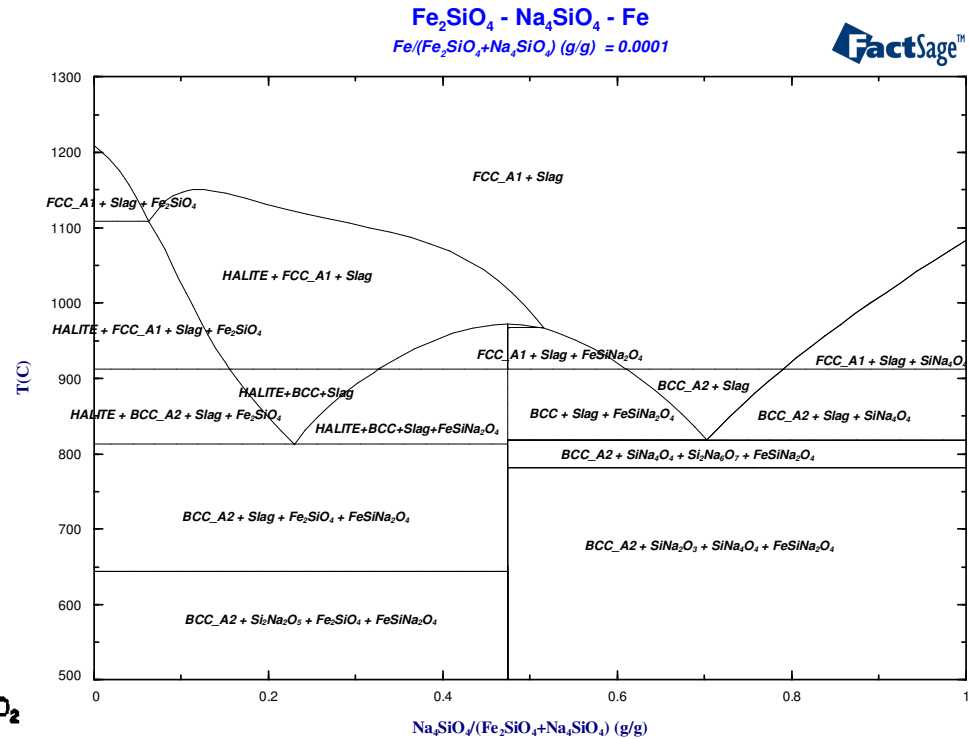
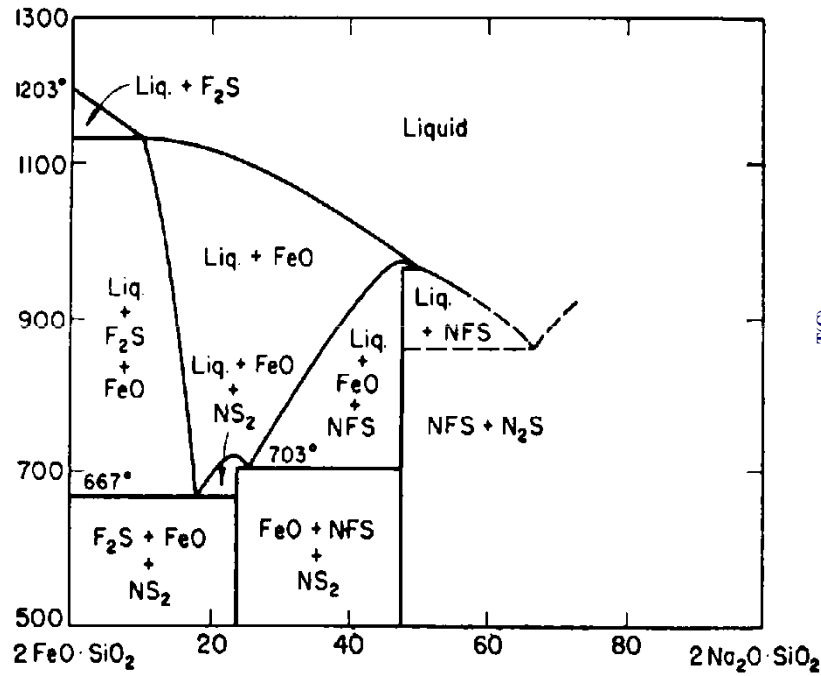
P. T. Carter and M. Ibrahim, *J. Soc. Glass Technol.*, 36 [170] 142-163 (1952).



# Isoplethal section in $\text{Fe}_2\text{SiO}_4$ - $\text{Na}_4\text{SiO}_4$ in equilibrium with Fe

GTT-Technologies

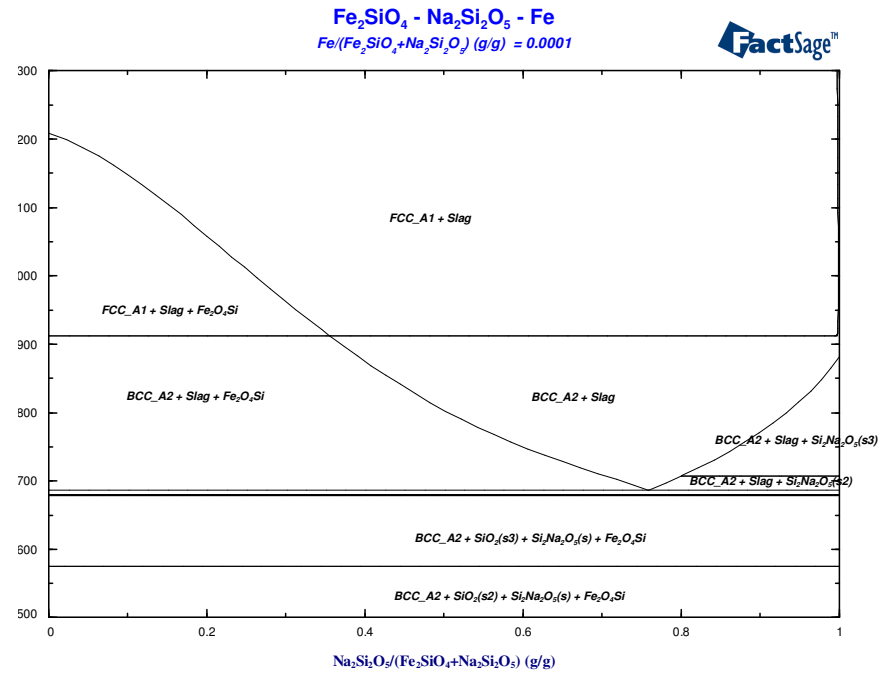
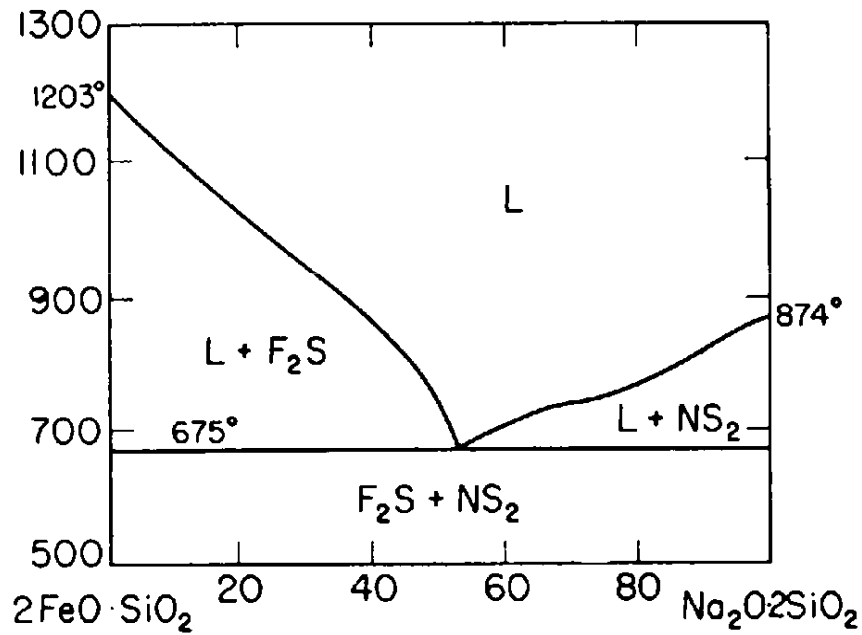
P. T. Carter and M. Ibrahim, *J. Soc. Glass Technol.*, 36 [170] 142-163 (1952).



# Isoplethal section in $\text{Fe}_2\text{SiO}_4$ - $\text{Na}_2\text{Si}_2\text{O}_5$ in equilibrium with Fe

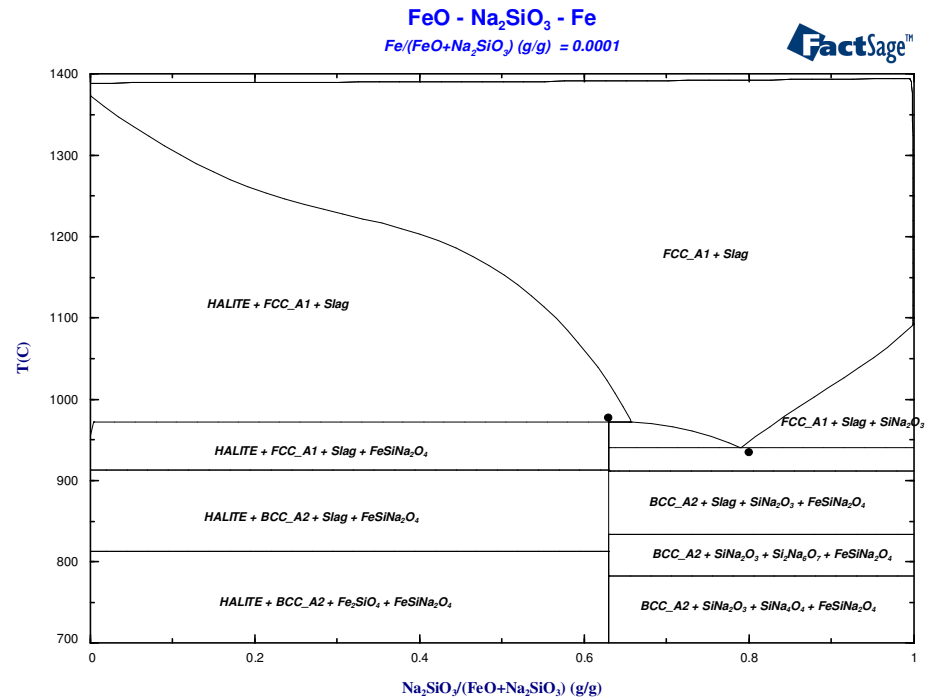
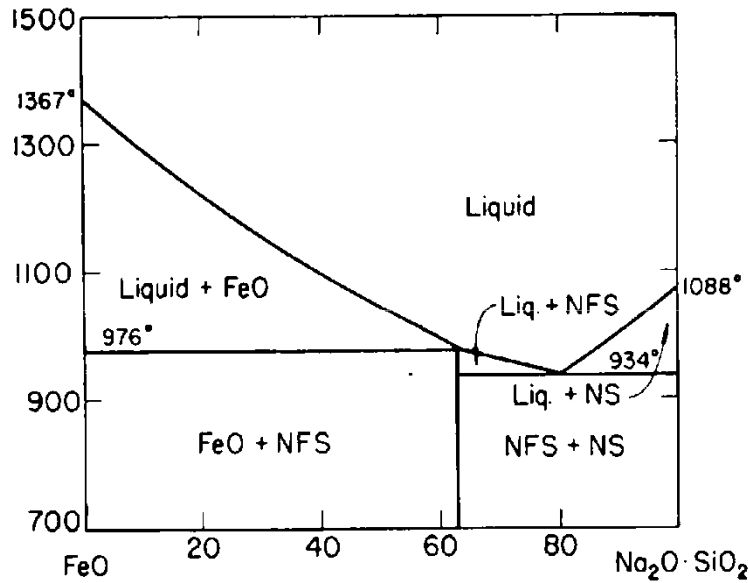
GTT-Technologies

P. T. Carter and M. Ibrahim, *J. Soc. Glass Technol.*, 36 [170] 142-163 (1952).



# Isoplethal section in Halite- $\text{Na}_2\text{SiO}_3$ in equilibrium with Fe

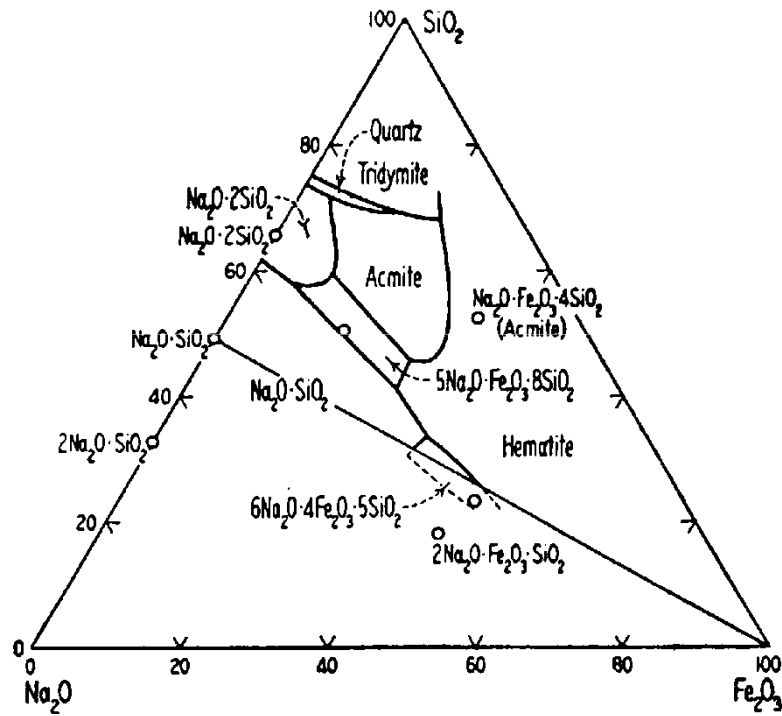
P. T. Carter and M. Ibrahim, *J. Soc. Glass Technol.*, 36 [170] 142-163 (1952).



# Liquidus surface in $\text{Fe}_2\text{O}_3\text{-Na}_2\text{O-SiO}_2$ in air

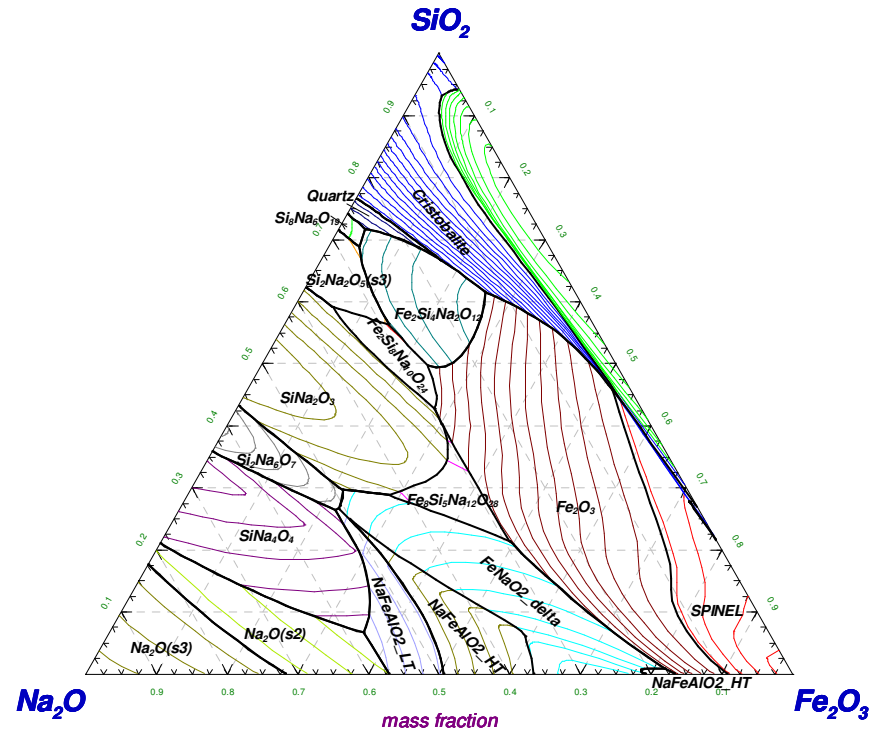
GTT-Technologies

N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220 (20), [20], (1930), pp. 405-455



$\text{SiO}_2 - \text{Fe}_2\text{O}_3 - \text{Na}_2\text{O} - \text{O}_2$   
Projection (Slag),  $p(\text{O}_2) = 0.21 \text{ atm}$

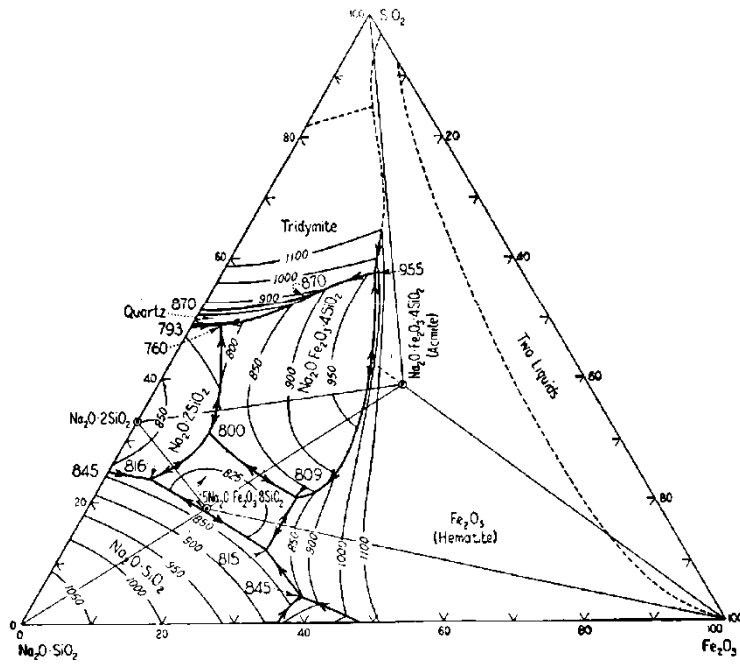
FactSage™



# Liquidus surface in $\text{Fe}_2\text{O}_3\text{-Na}_2\text{SiO}_3\text{-SiO}_2$ in air

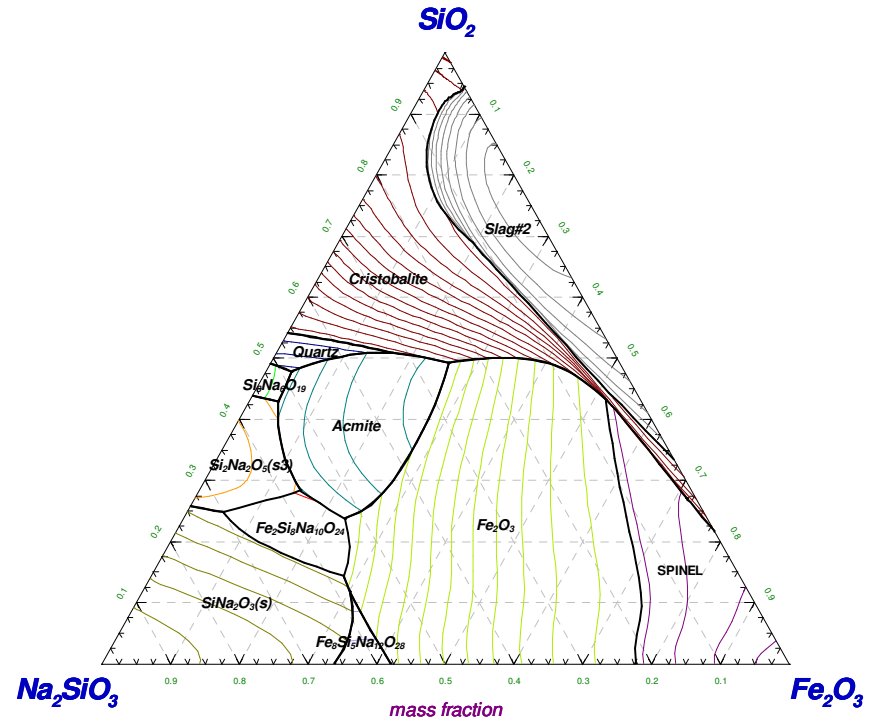
GTT-Technologies

N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



$\text{SiO}_2 - \text{Fe}_2\text{O}_3 - \text{Na}_2\text{SiO}_3 - \text{O}_2$   
Projection (Slag),  $p(\text{O}_2) = 0.21 \text{ atm}$

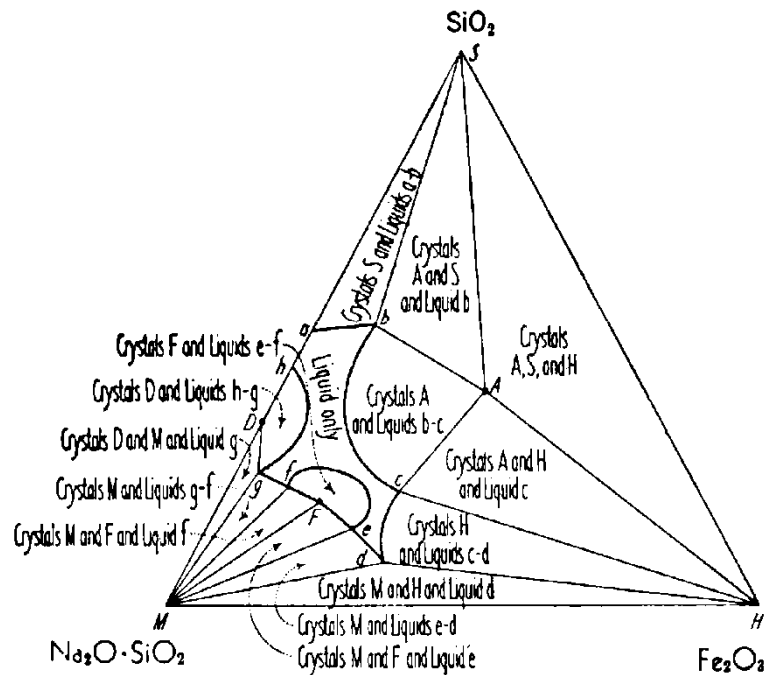
FactSage™



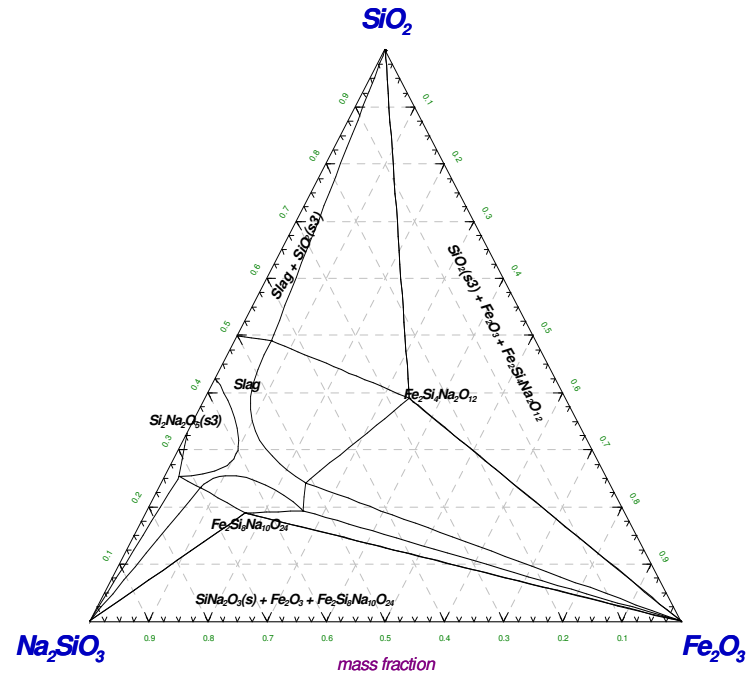
# Isothermal section at 825° C in Fe<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>SiO<sub>3</sub>-SiO<sub>2</sub> in air

GTT-Technologies

N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



SiO<sub>2</sub> - Fe<sub>2</sub>O<sub>3</sub> - Na<sub>2</sub>SiO<sub>3</sub> - O<sub>2</sub>  
825° C, p(O<sub>2</sub>) = 0.21 atm

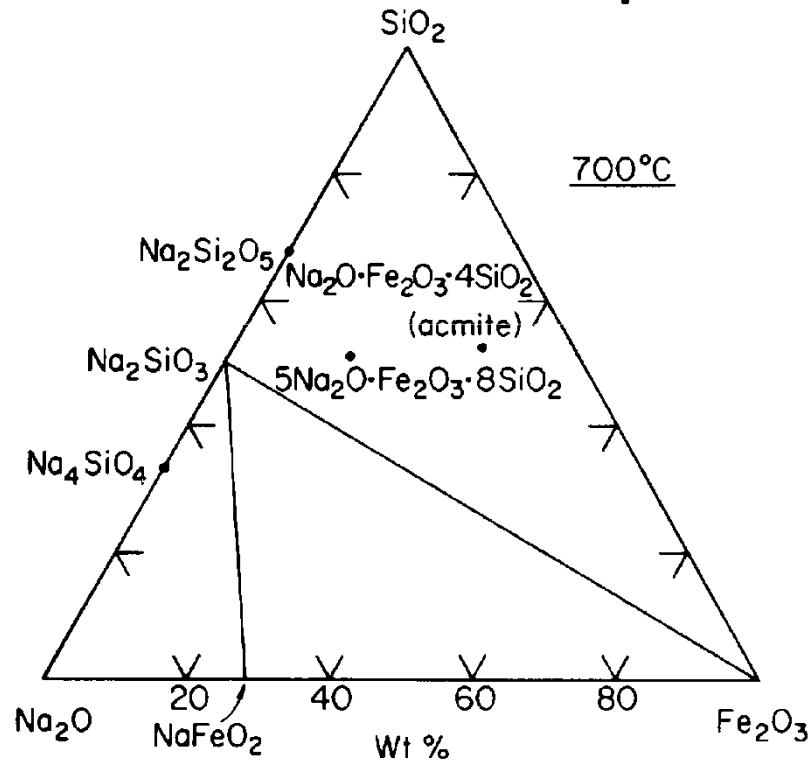




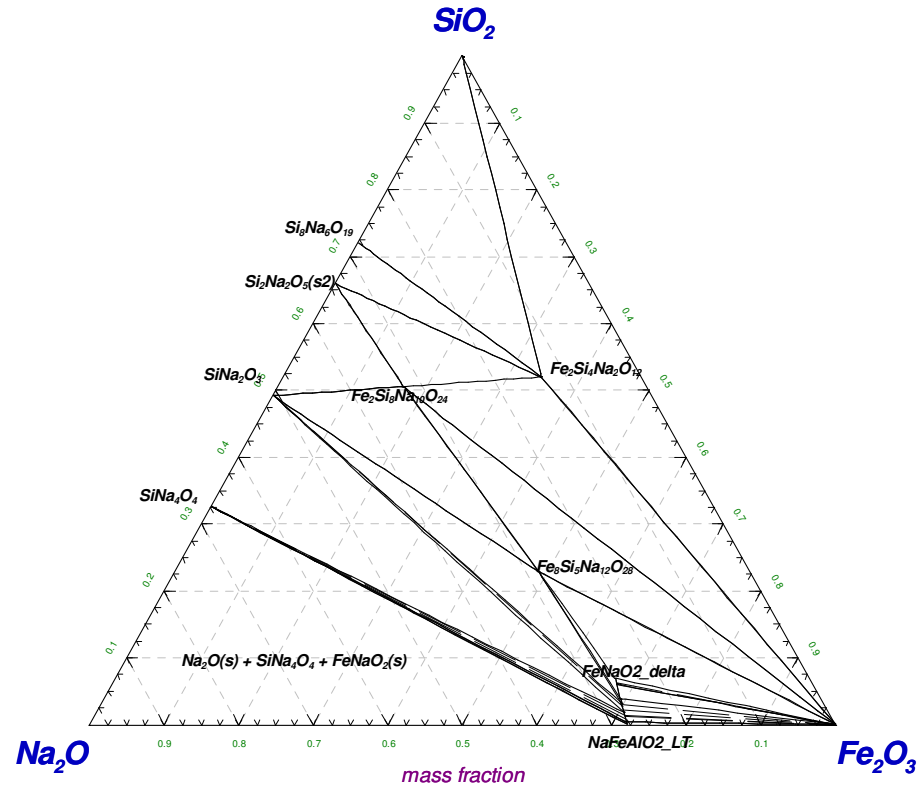
# Isothermal section at 700° C in Fe<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O-SiO<sub>2</sub> in air

GTT-Technologies

D. W. Collins and L. N. Mulay, *J. Am. Ceram. Soc.*, 53 [2] 74-76 (1970).

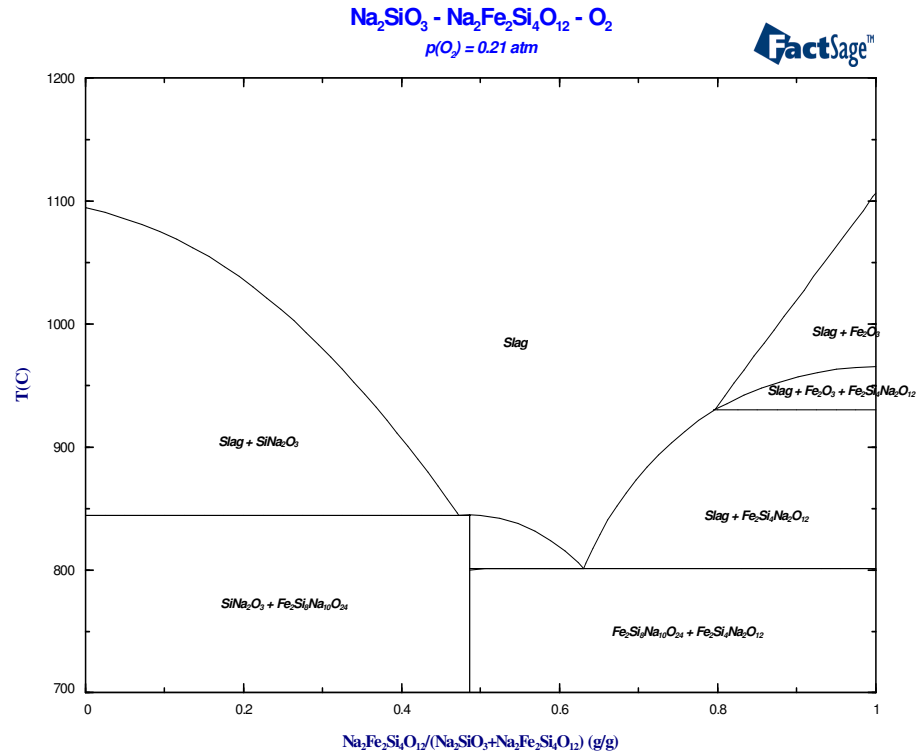
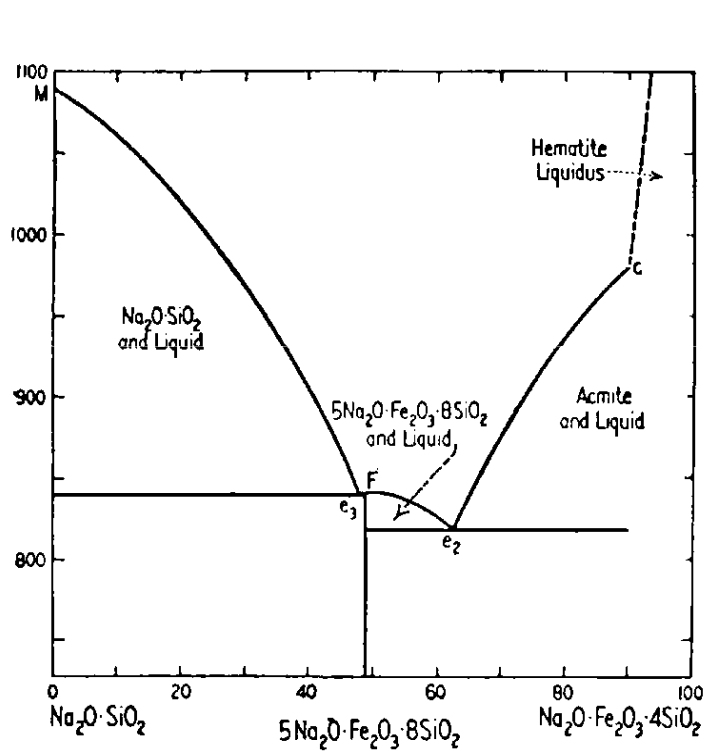


Na<sub>2</sub>O - Fe<sub>2</sub>O<sub>3</sub> - SiO<sub>2</sub> - O<sub>2</sub>  
700° C, p(O<sub>2</sub>) = 0.21 atm



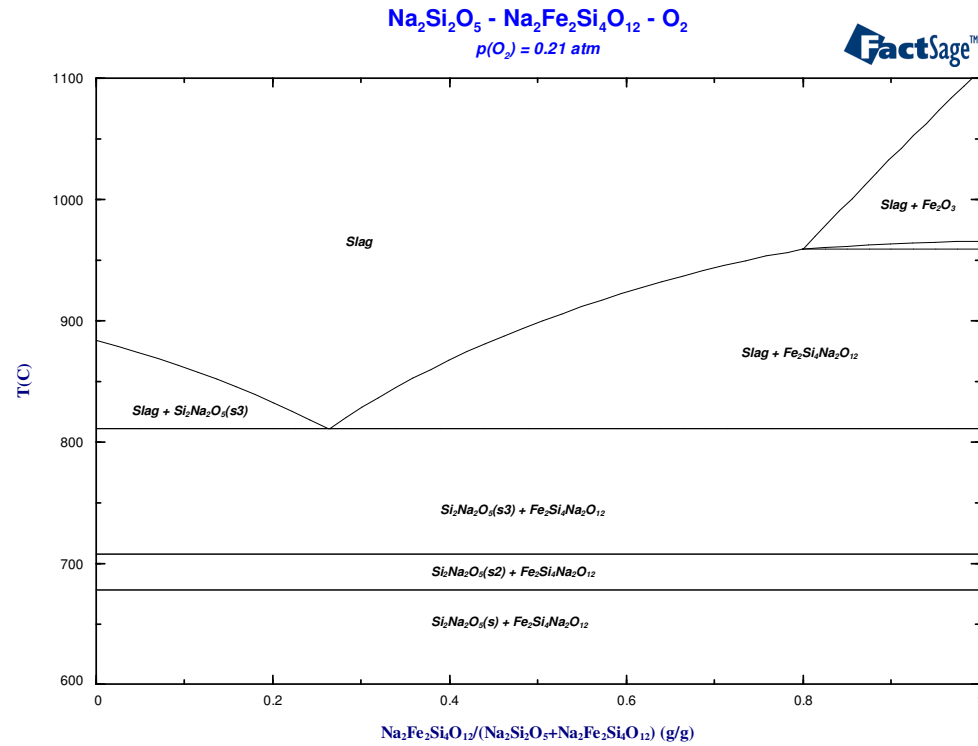
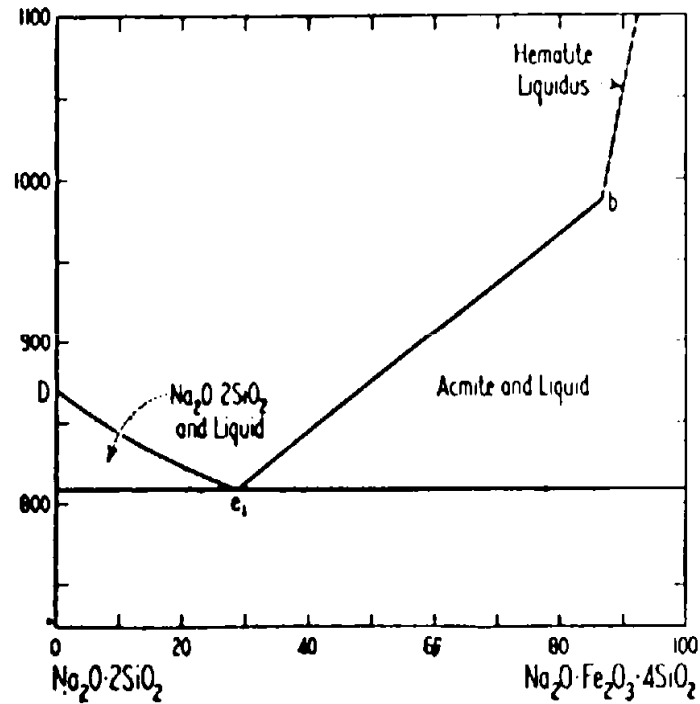
# Isoplethal section Acmite- $\text{Na}_2\text{SiO}_3$ in air

N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



# Isoplethal section Acmite- $\text{Na}_2\text{Si}_2\text{O}_5$ in air

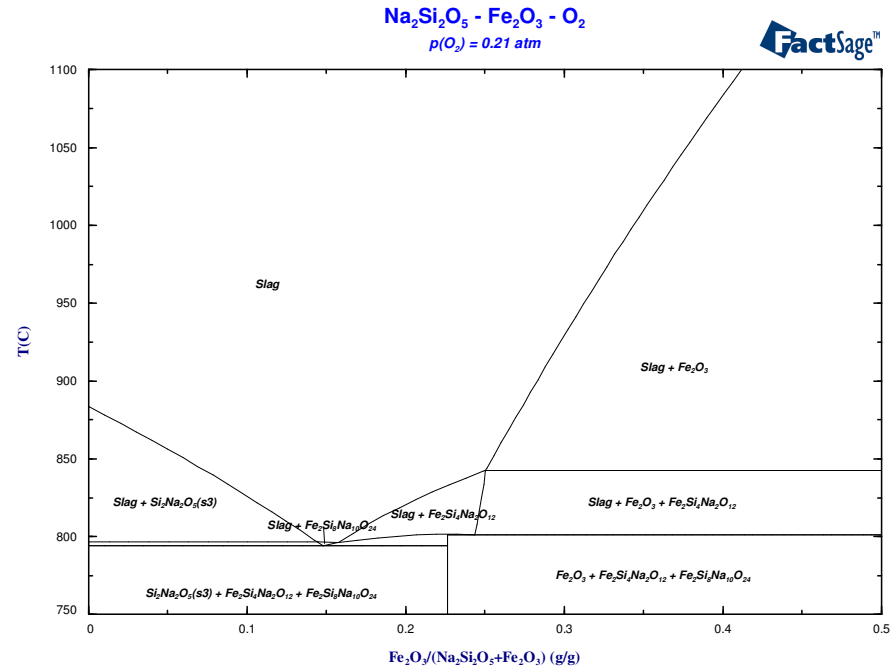
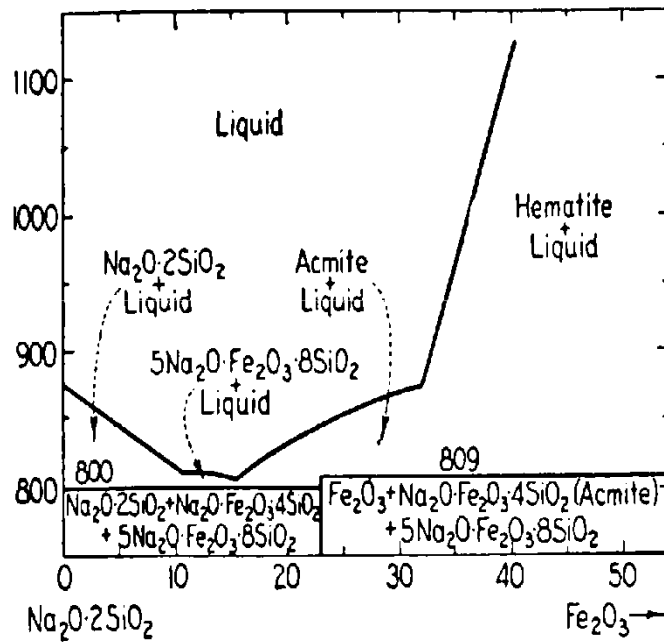
N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



# Isoplethal section $\text{Fe}_2\text{O}_3\text{-Na}_2\text{Si}_2\text{O}_5$ in air

GTT-Technologies

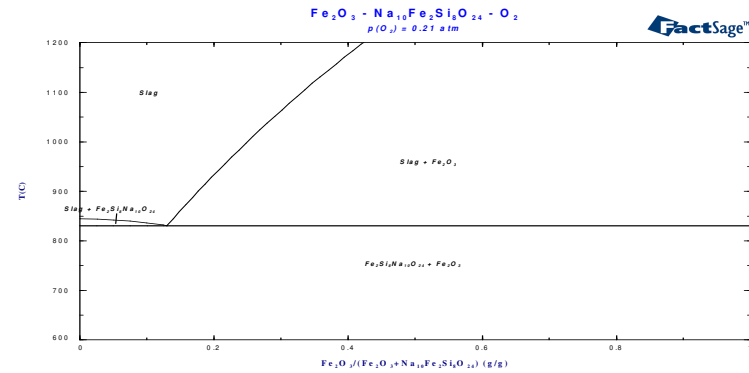
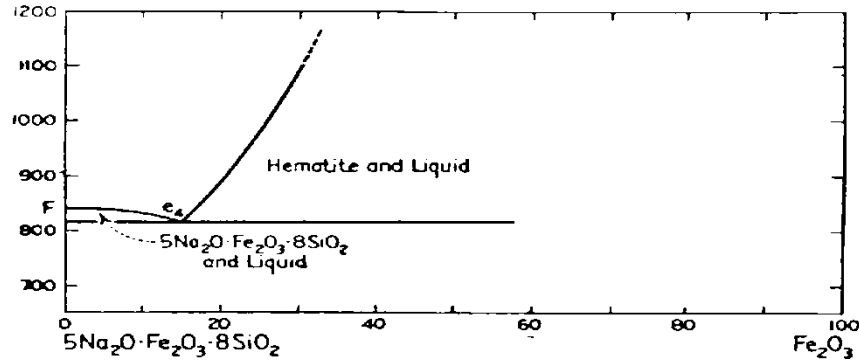
N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



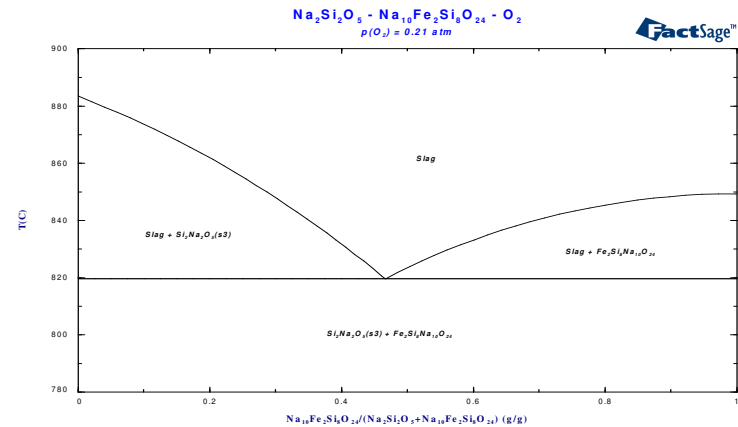
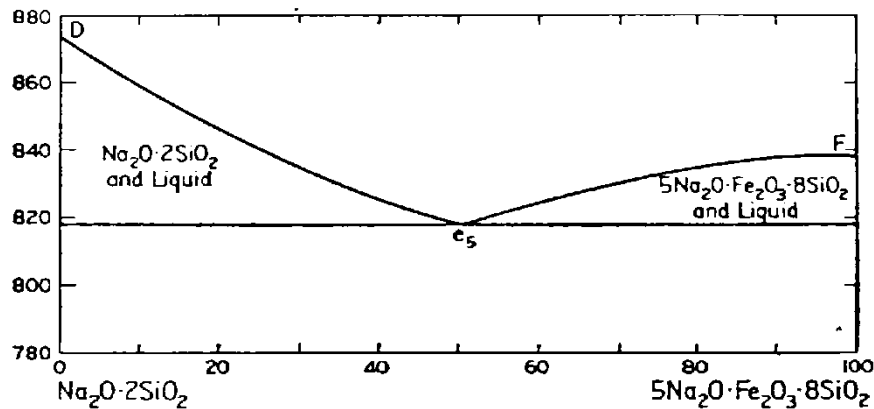
# Isoplethal sections with $5\text{Na}_2\text{O}\cdot\text{Fe}_2\text{O}_3\cdot 8\text{SiO}_2$

GTT-Technologies

N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



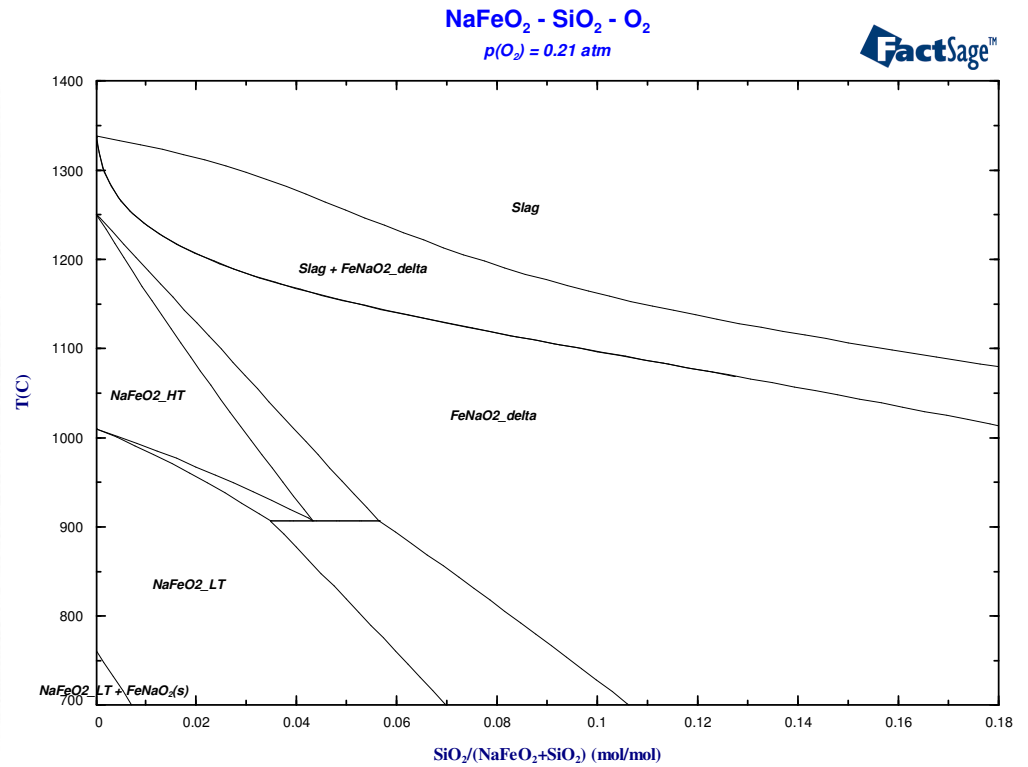
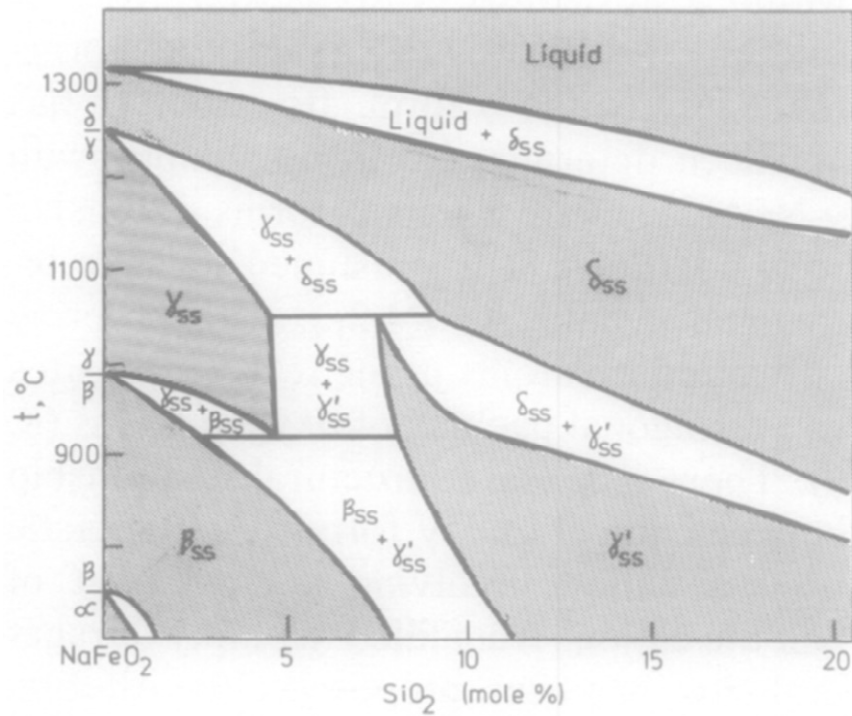
N.L. Bowen, J.F. Schairer, H.W.V. Willems, *Am. J. Sci.*, 220, [20], (1930), pp. 405-455.



# Isoplethal section $\text{FeNaO}_2\text{-SiO}_2$ in air

GTT-Technologies

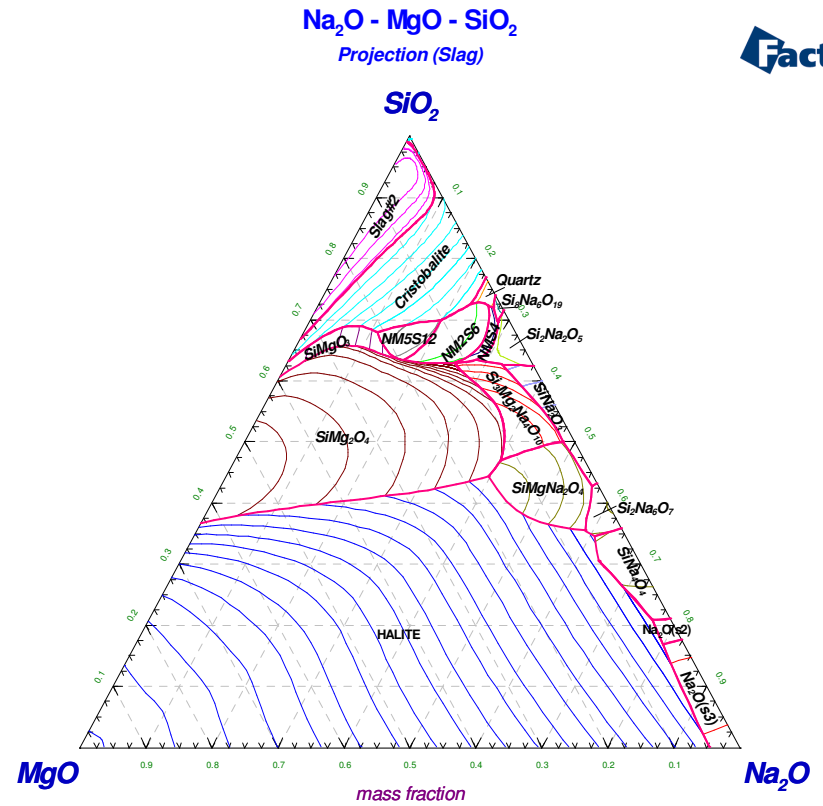
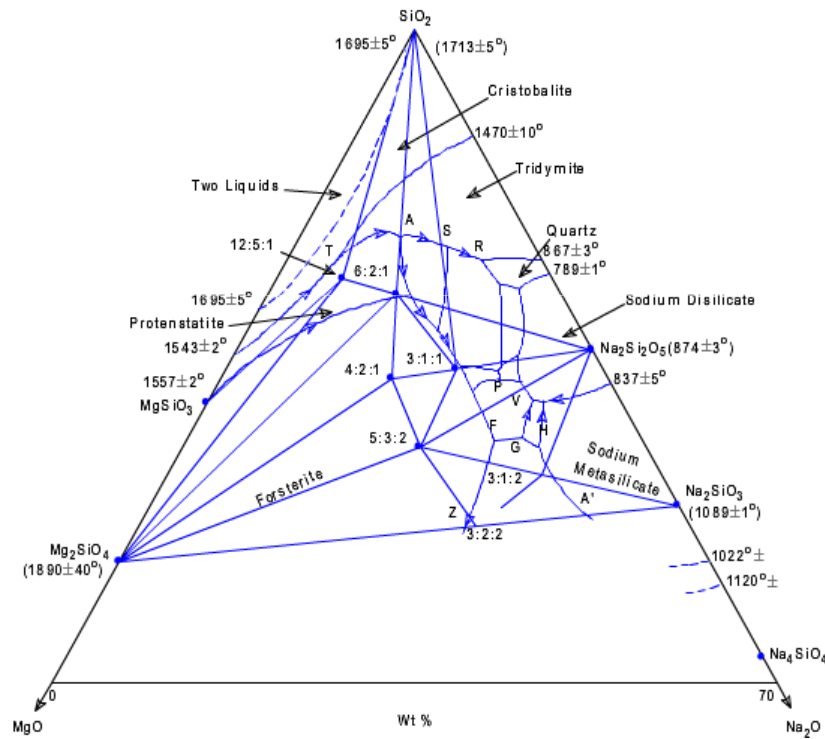
I. E. Grey and C. Li, *J. Solid State Chem.*, 69 [1] 116-125 (1987).



# Liquidus surface in MgO-Na<sub>2</sub>O-SiO<sub>2</sub>

GTT-Technologies

J. F. Schairer, J. Am. Ceram. Soc., 40 [7] 215-235 (1957).



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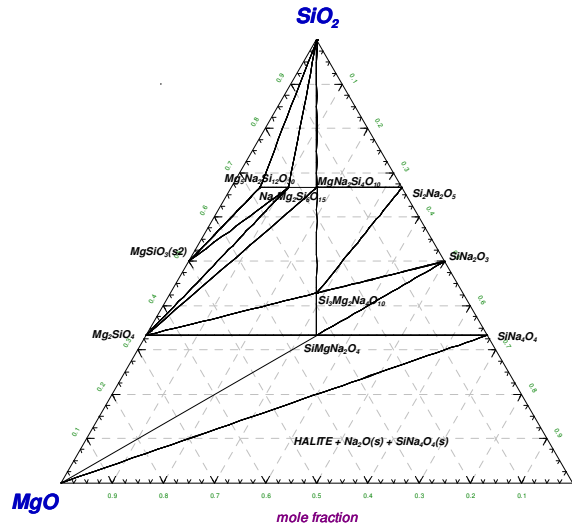


# Predicted isothermal sections in MgO-Na<sub>2</sub>O-SiO<sub>2</sub>

GTT-Technologies

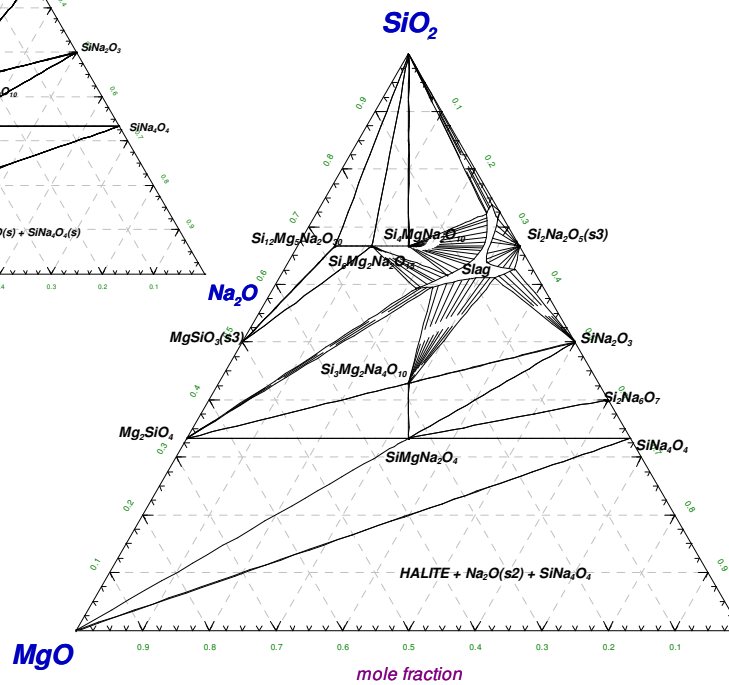
Na<sub>2</sub>O - SiO<sub>2</sub> - MgO  
600°C

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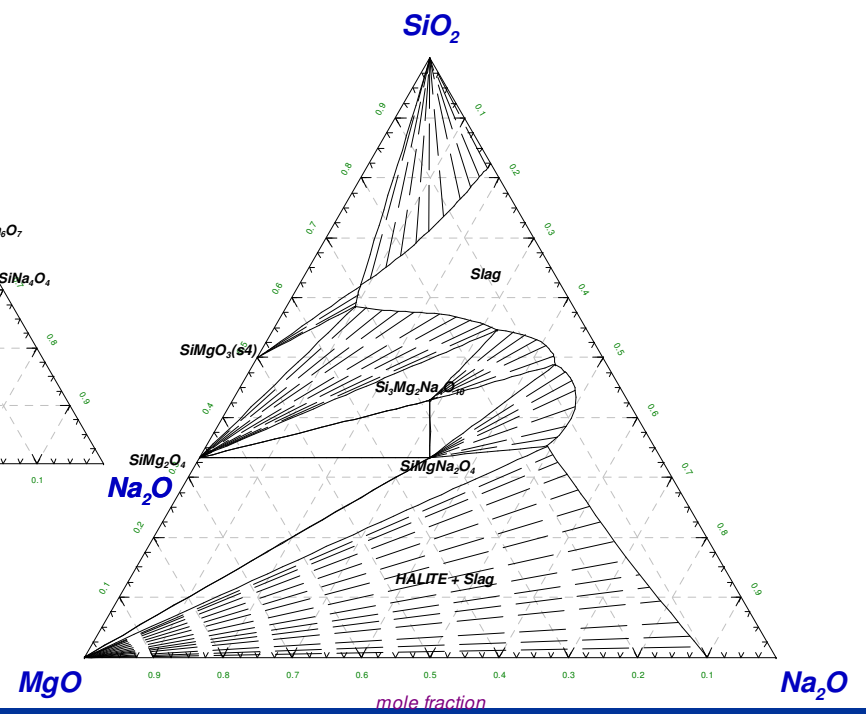


Na<sub>2</sub>O - SiO<sub>2</sub> - MgO  
800°C

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Na<sub>2</sub>O - SiO<sub>2</sub> - MgO  
1200°C

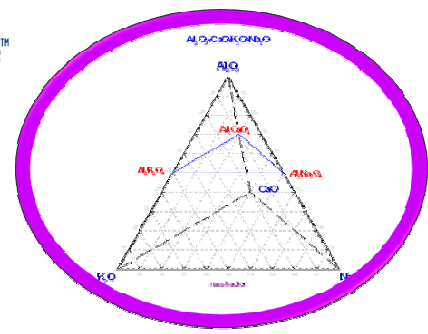




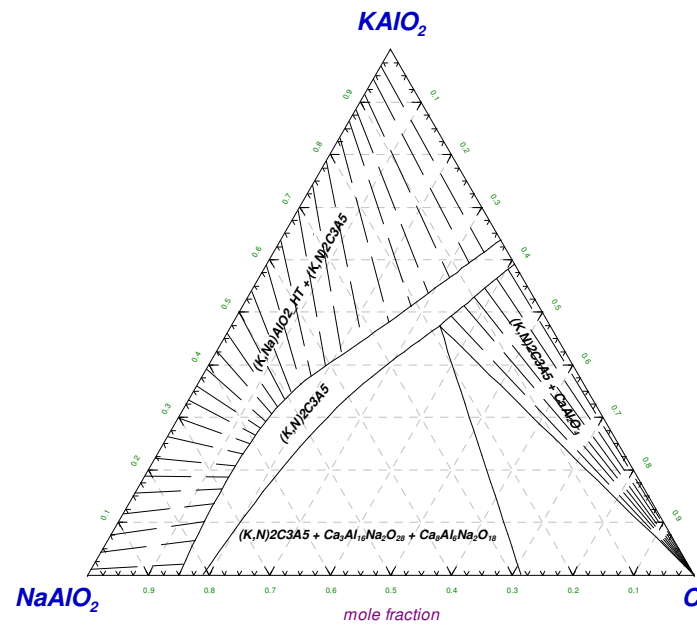
# Proposed isothermal sections in $\text{Al}_2\text{O}_3$ - $\text{CaO}$ - $\text{K}_2\text{O}$ - $\text{Na}_2\text{O}$

GTT-Technologies

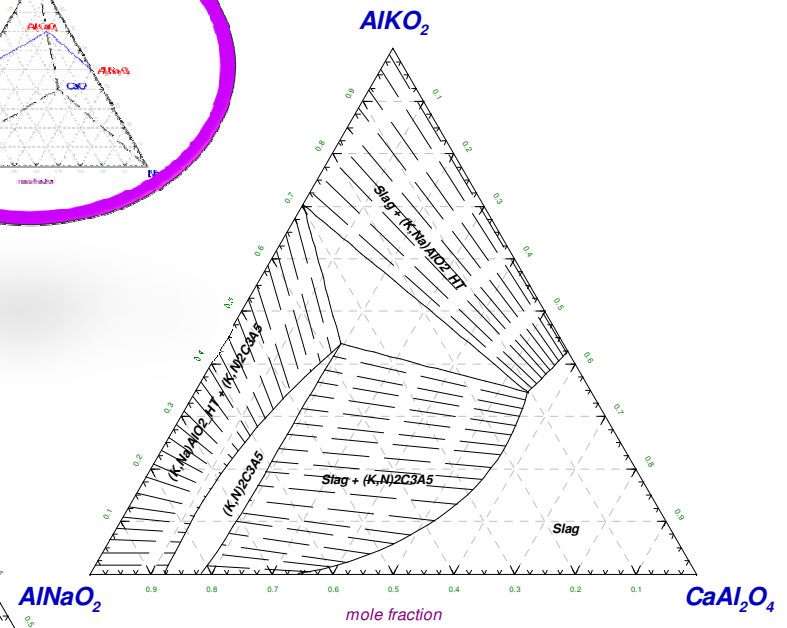
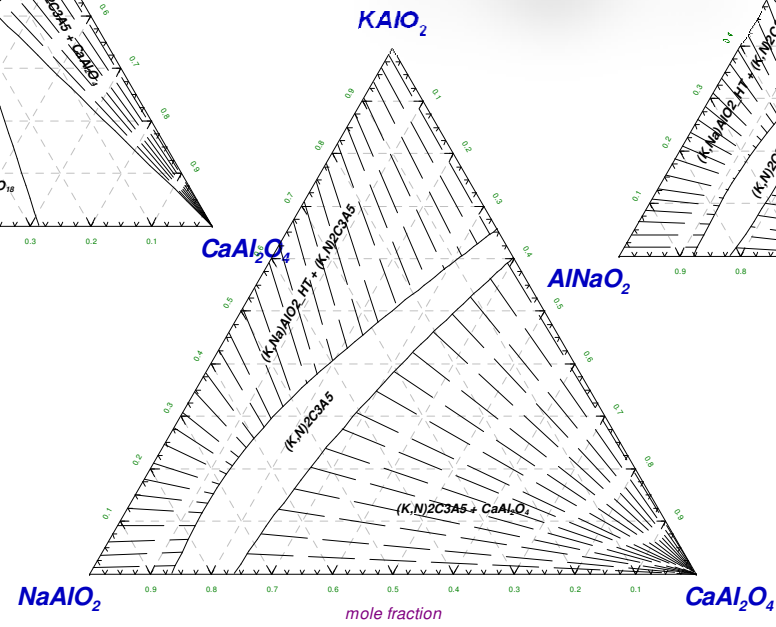
$\text{KAIO}_2$  -  $\text{NaAlO}_2$  -  $\text{CaAl}_2\text{O}_4$   
600°C



$\text{AlNaO}_2$  -  $\text{AlKO}_2$  -  $\text{CaAl}_2\text{O}_4$   
1700°C



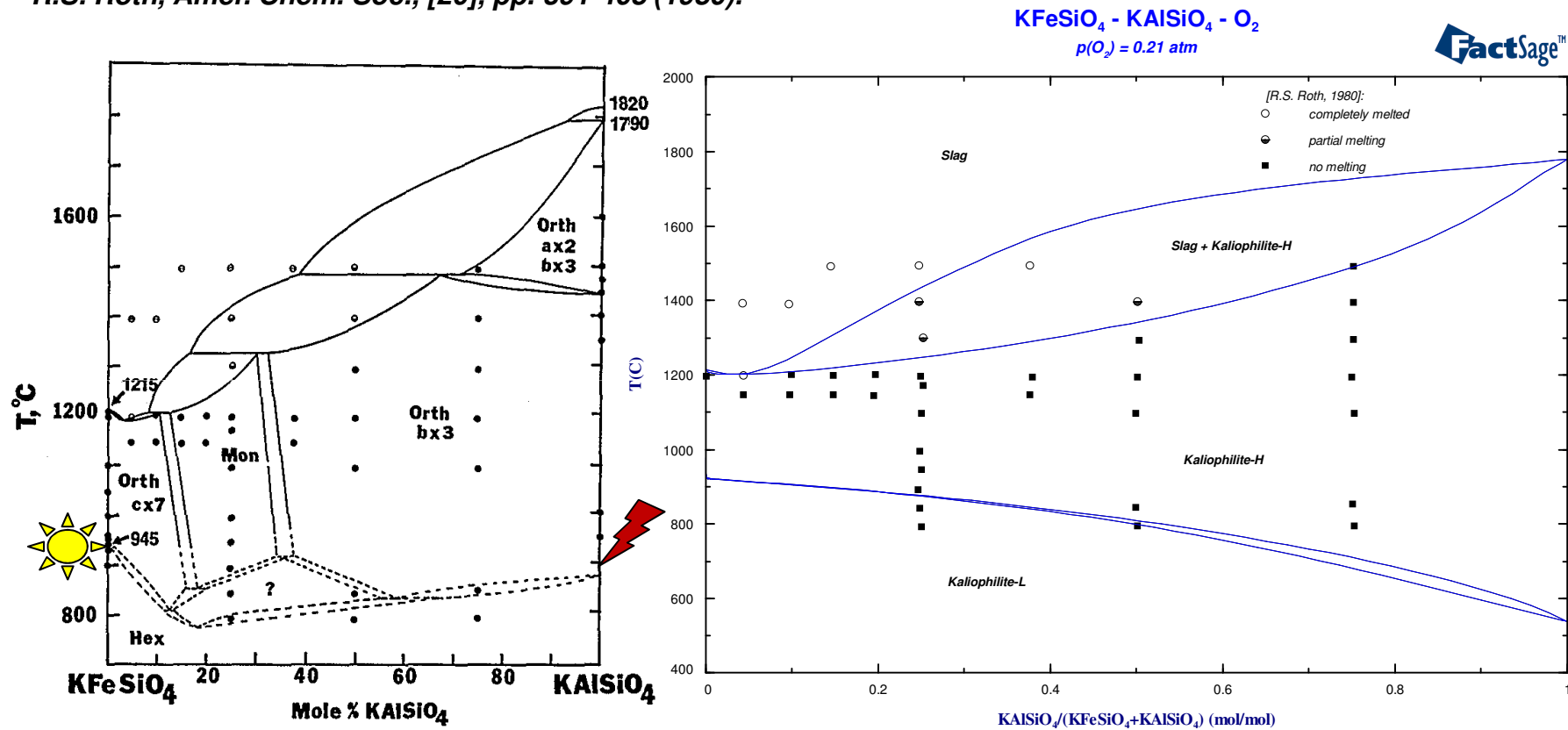
$\text{KAIO}_2$  -  $\text{NaAlO}_2$  -  $\text{CaAl}_2\text{O}_4$   
1100°C



# Phase equilibria diagram of the system $\text{KFeSiO}_4$ - $\text{KAlSiO}_4$

GTT-Technologies

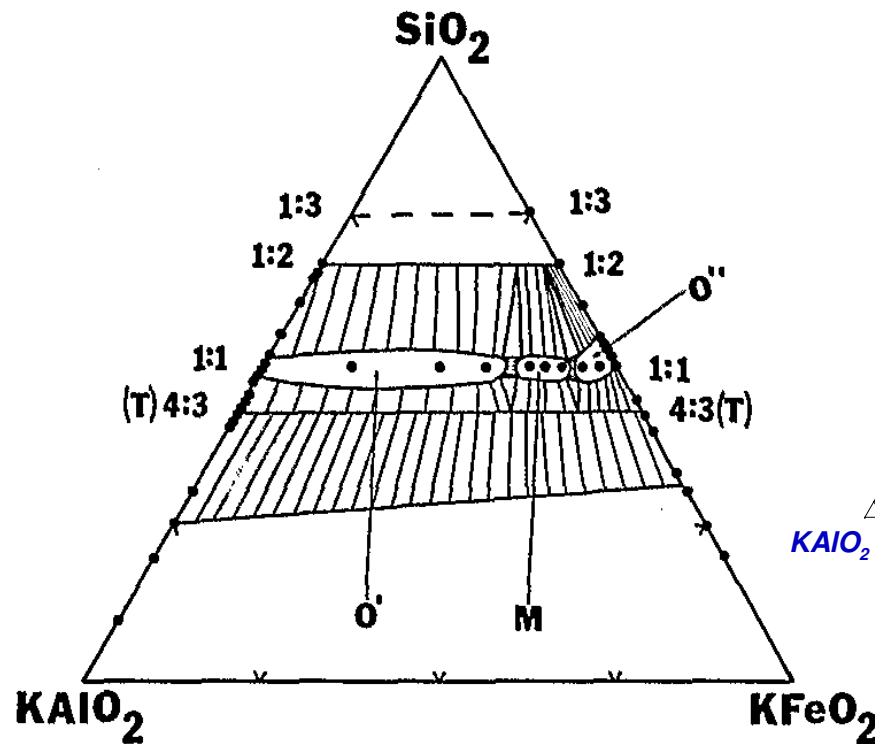
R.S. Roth, Amer. Chem. Soc., [20], pp. 391-408 (1980).



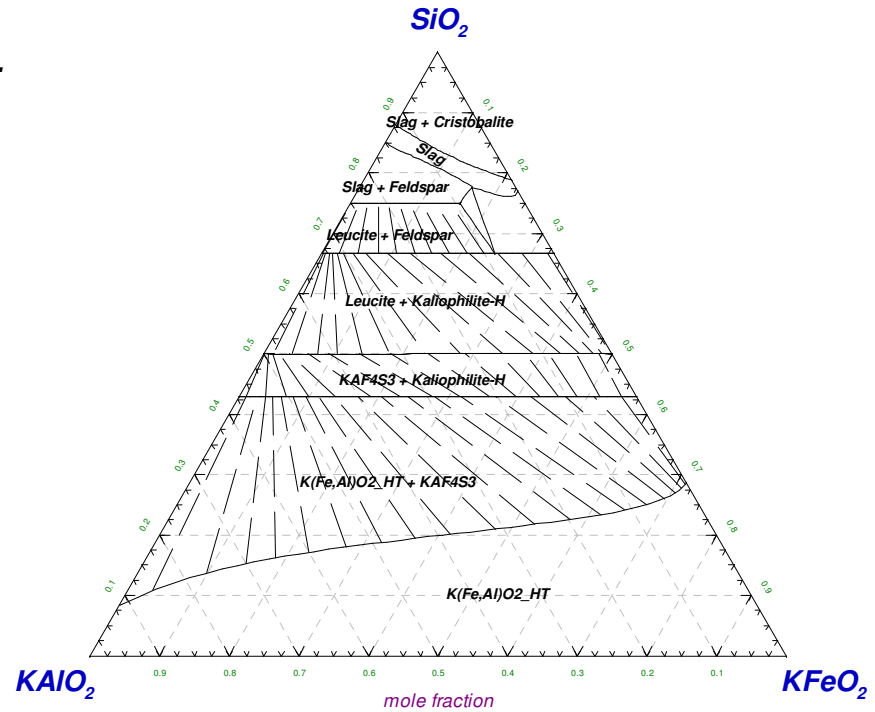
# Phase equilibria diagram of the system $\text{KFeSiO}_4\text{-KAlSiO}_4$

GTT-Technologies

R.S. Roth, Amer. Chem. Soc., [20], pp. 391-408 (1980).



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# Conclusions

- The database for the  $\text{Al}_2\text{O}_3\text{-CaO-FeO-Fe}_2\text{O}_3\text{-K}_2\text{O-Na}_2\text{O-MgO-SiO}_2$  system was created combining the following databases:  
 $\text{Al}_2\text{O}_3\text{-CaO-FeO-Fe}_2\text{O}_3\text{-MgO-SiO}_2$  (GTT) and  
 $\text{Al}_2\text{O}_3\text{-Na}_2\text{O-K}_2\text{O-SiO}_2$  (FZ Jülich)
- The 3 binary systems, 11 ternary and 4 quaternary subsystems were assessed using available experimental information.
- The liquid phase in all subsystems was evaluated using associate species model (two cations per species).
- In order to get a compatibility the solubility ranges for iron were introduced into existing thermodynamic description for three solid solution phases.
- The solubility ranges of nine new solid solution phases were described using sublattice model. The missing Gibbs functions for these phases were estimated using appropriate reciprocal equations.
- The 29 stoichiometric phases were incorporated.

All phase diagrams incorporated in *New Slag Atlas*



# Future developments

- Expansion of the entire database by addition of such oxides as MnO and NiO as well as  $\text{CrO}_x$  and  $\text{P}_2\text{O}_5$ .
- Addition of PbO, ZnO and  $\text{V}_x\text{O}_y$  in co-operative projects.
- Addition of non-oxidic components such as CaS, FeS and MnS is in planning.



Thanks for your  
attention!

