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Thermochemical assessments

of alkali oxide - Al_2O_3 - SiO_2 systems

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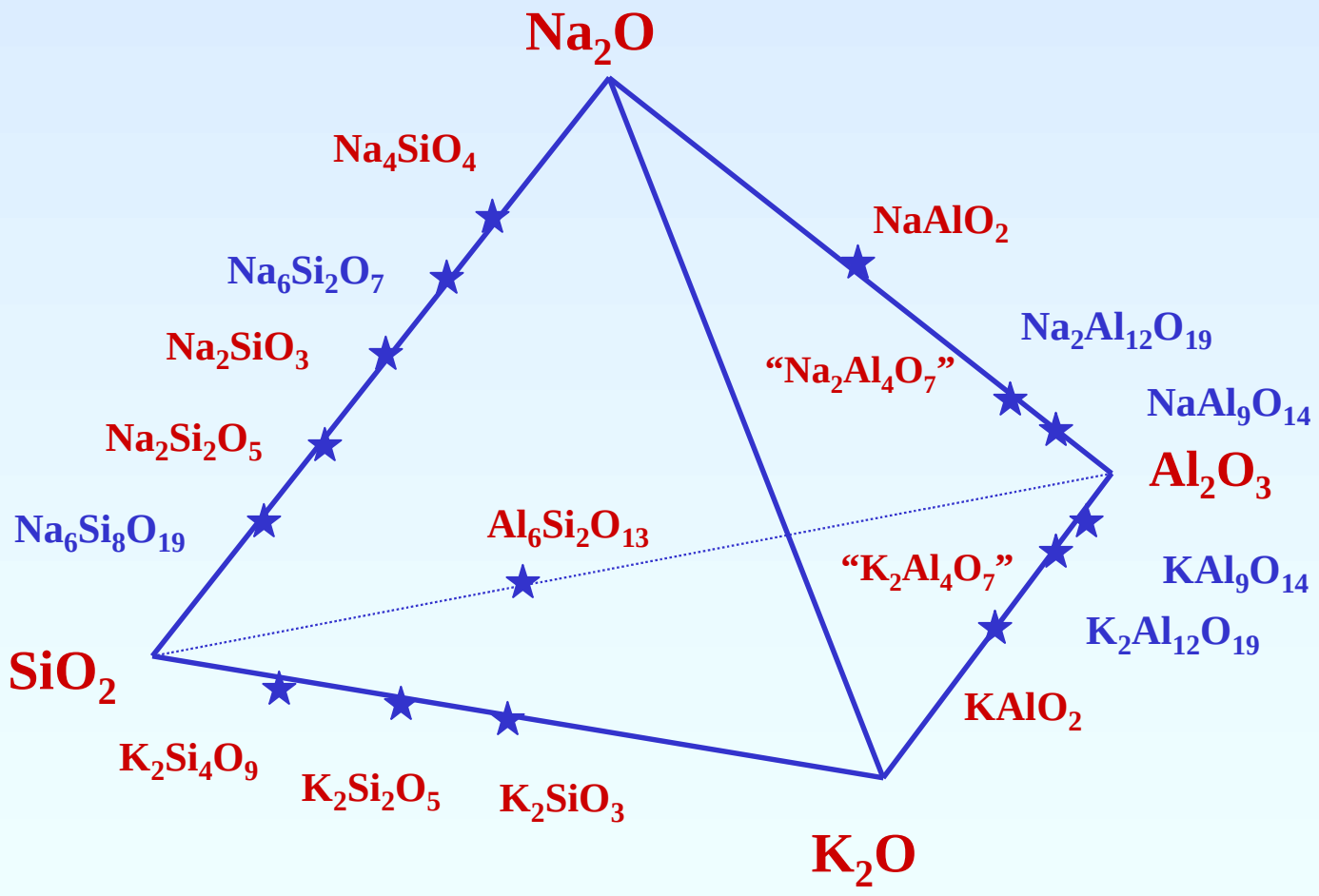
Na_2O-K_2O-Al_2O_3-SiO_2



Contents

- ✓ Model and optimisation
- ✓ Application of a new data base for binary subsystems
- ✓ Application of a new data base for ternary subsystems
- ✓ Conclusions and outlook

Associate species model

Liquid (slag), solid solutions, mullite

Binary liquid

Pure liquid oxide:
Na_2O, K_2O, Al_2O_3, $SiO_2 \cdot 2/5$

+

Congruent melting compounds	Associate species
Na_4SiO_4	$Na_4SiO_4 \cdot 2/5$
Na_2SiO_3	$Na_2SiO3 \cdot 2/3$
$Na_2Si_2O_5$	$Na2Si2O5 \cdot 1/2$
K_2SiO_3	$K_2SiO_3 \cdot 2/3$
$K_2Si_2O_5$	$K_2Si_2O_5 \cdot 1/2$
K2Si4O9	$K_2Si_4O_9 \cdot 1/3$
$NaAlO_2$	$NaAlO_2$
	$Na_2Al_4O_7 \cdot 1/3$
$KAlO_2$	$KAlO_2$
	$Na_2Al_4O_7 \cdot 1/3$
$Al_6Si_2O_{13}$	$Al_6Si_2O_{13} \cdot 1/4$

+

Interaction parameters between species

Solution components
(Spear et al.)

Associate species model

Liquid (slag), **solid solutions, mullite**

Solid solutions:

Solution components:
Solid "boundary" compounds

Nepheline
$NaAlSiO_4$ (nepheline)
$NaAlSi_2O_6$ (jadeite)

Carnegieite
$NaAlSiO_4$ (carnegieite)
$NaAlSi_2O_6$ (jadeite)

$KAl_{1-x}Si_xO_4$
$KAlO_2$
$KAlSiO_4$

\+ **Interaction parameters between species (by request)**

Mullite

Associate species model
$Al_6Si_2O_{13}\cdot 1/4$, Al_2O_3, $SiO_2\cdot 2$

four-sublattice model
(Hillert, Mao et al.)

Experimental data: phase diagram data, activity data (for binary systems)

Pure solid and liquid substances from the FACT database

Some solution species from database of Spear et al.

Optimisation

Adjustable parameters: $?H_f^{298}$ and S^{298} for the liquid and solid solution species, ΔH_f^{298} and S^{298} for the pure solid compounds (part.), interaction parameters between species

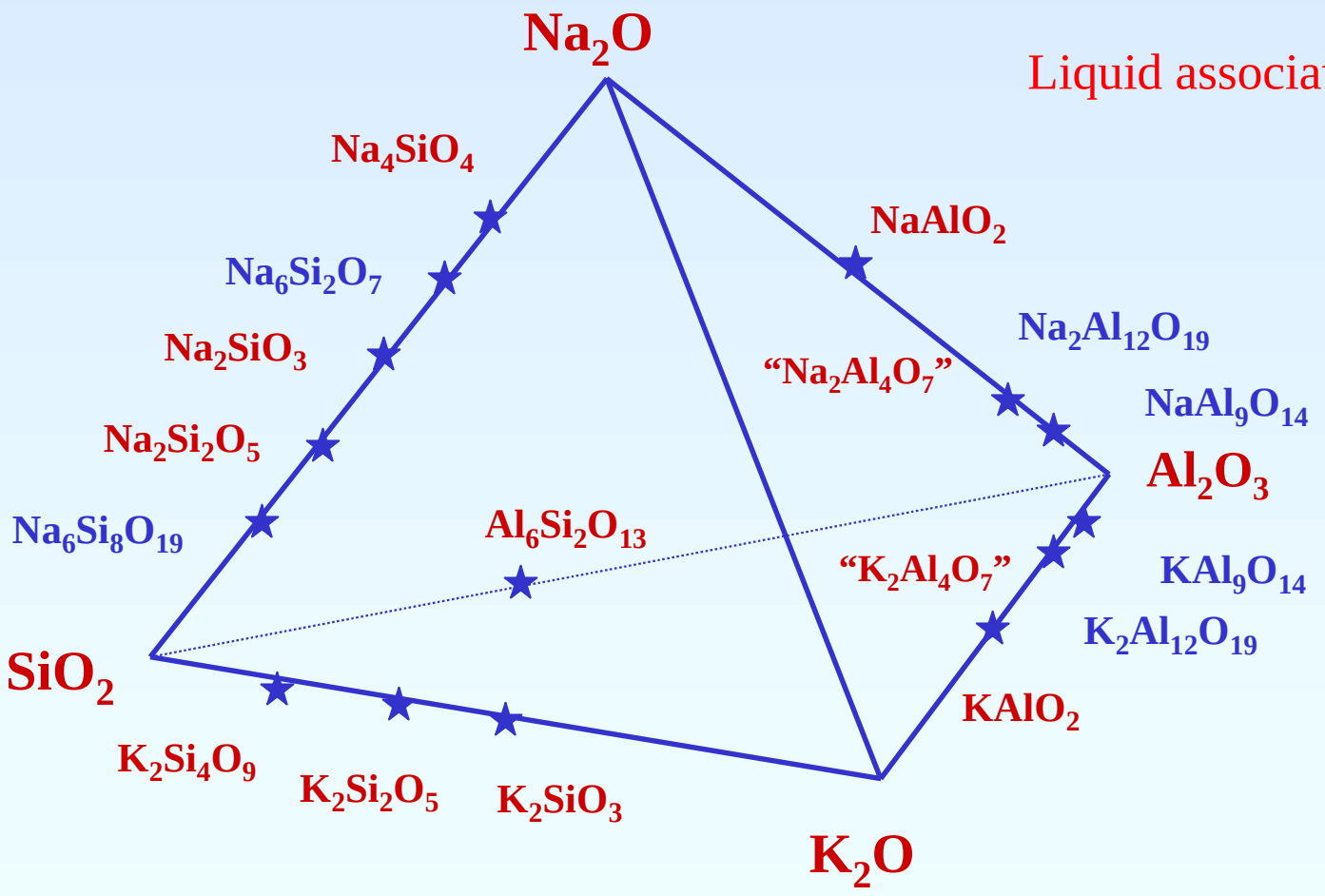
$$G_m = \sum x_i G_i^0 + RT \sum x_i \ln x_i + \sum_{i<j} \sum x_i x_j \sum_v L_{ij}^{(v)} (x_i - x_j)^v$$

$$L_{ij}^{(v)} = A_{ij}^{(v)} + B_{ij}^{(v)} \cdot T + C_{ij}^{(v)} \cdot T \cdot \ln T + D_{ij}^{(v)} \cdot T^2 + \ldots$$

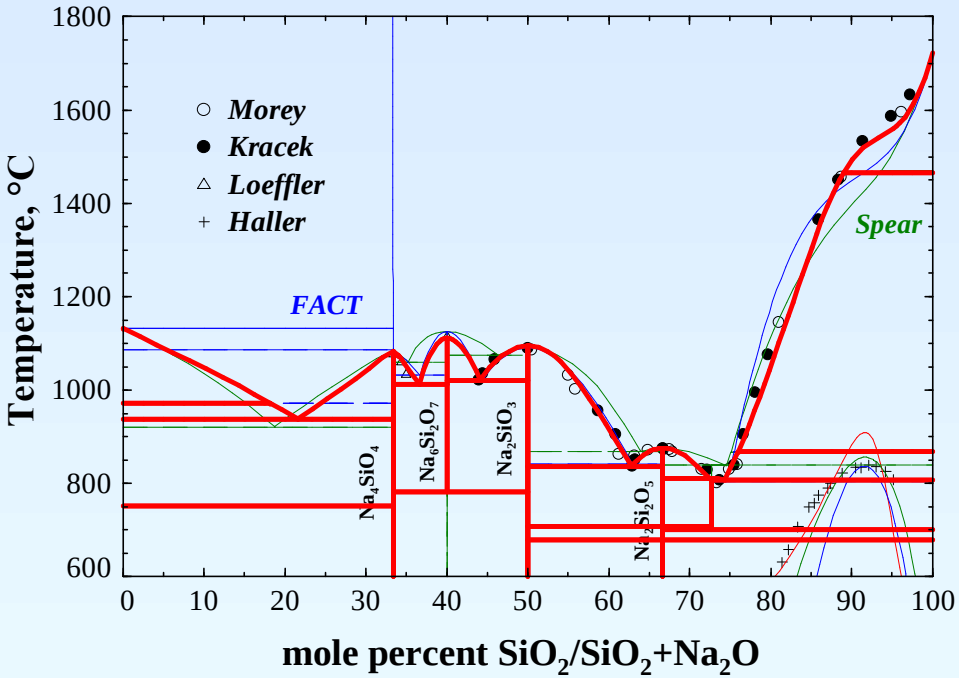
New database

Na_2O-K_2O-Al_2O_3-SiO_2 system

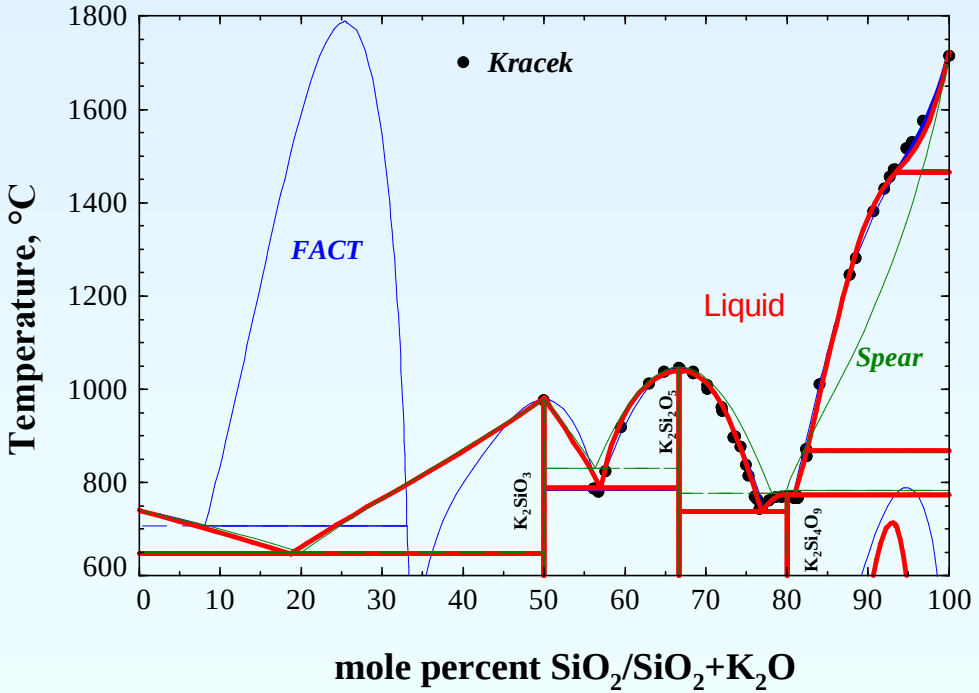
Liquid associate species



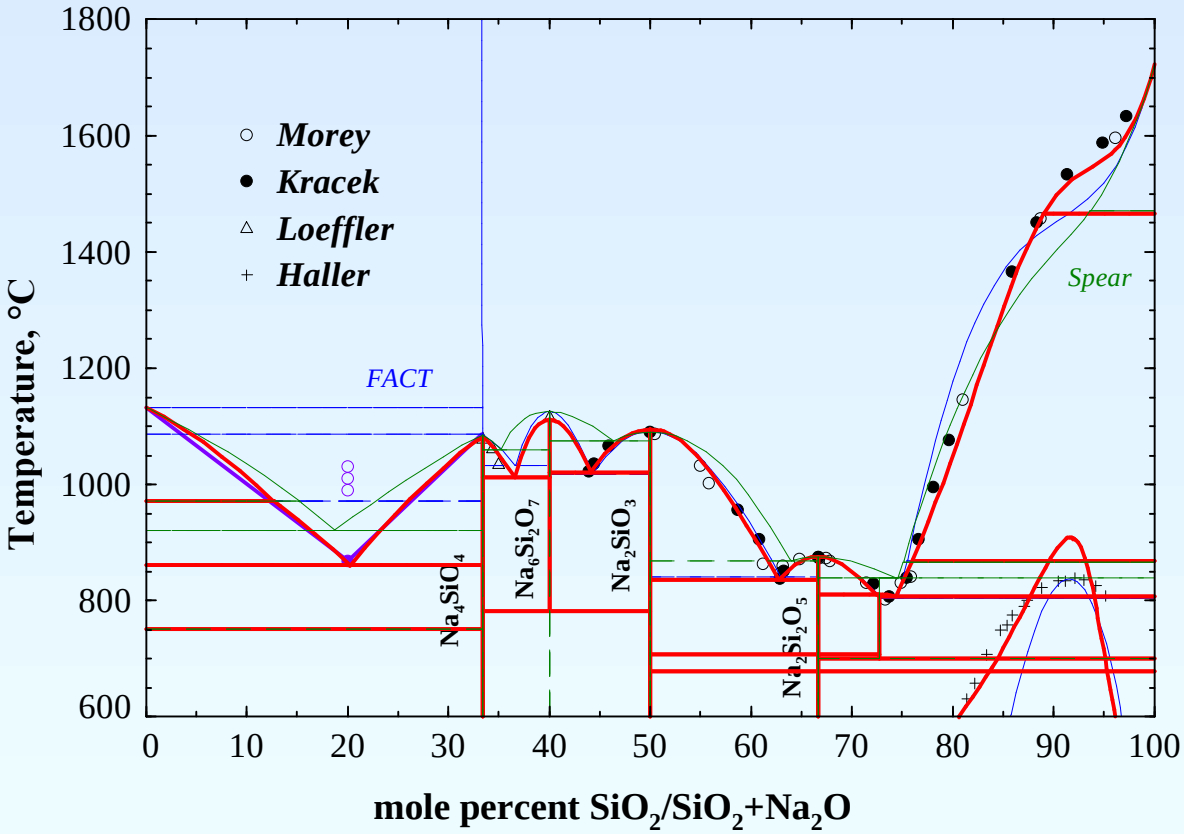
New database for the Me_2O-SiO_2 systems (Me=Na, K)



No solution using the FACT database in the Me_2O-rich region

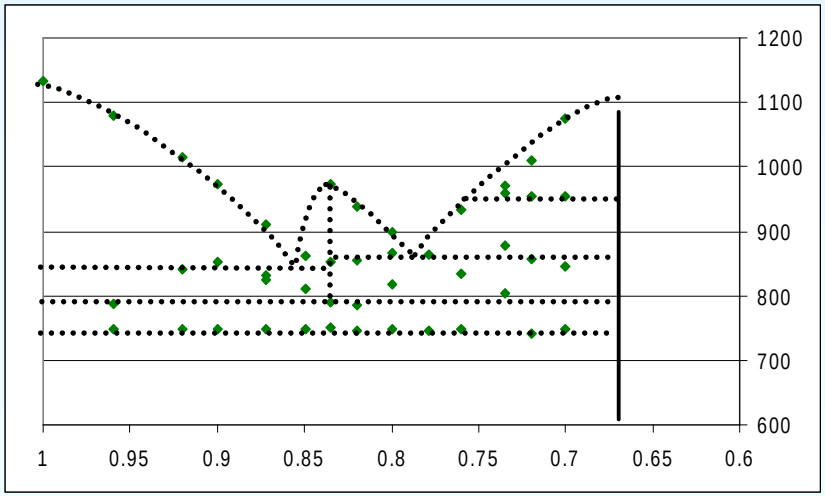


DTA measurements in the Na_2O-SiO_2 system



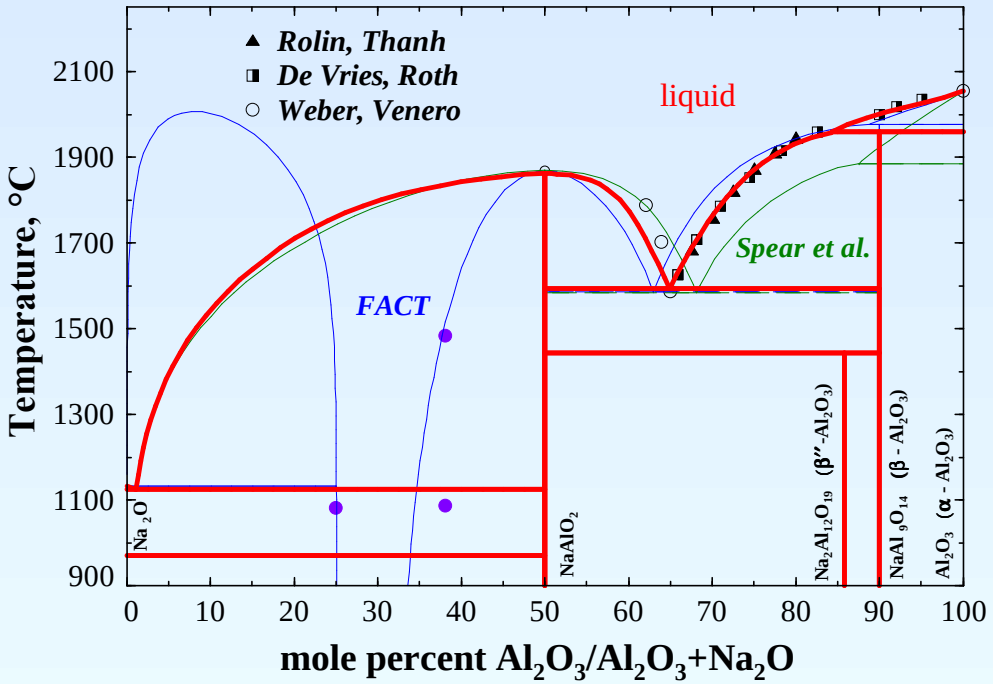
Experimental data

of M. Rys, IEF-2

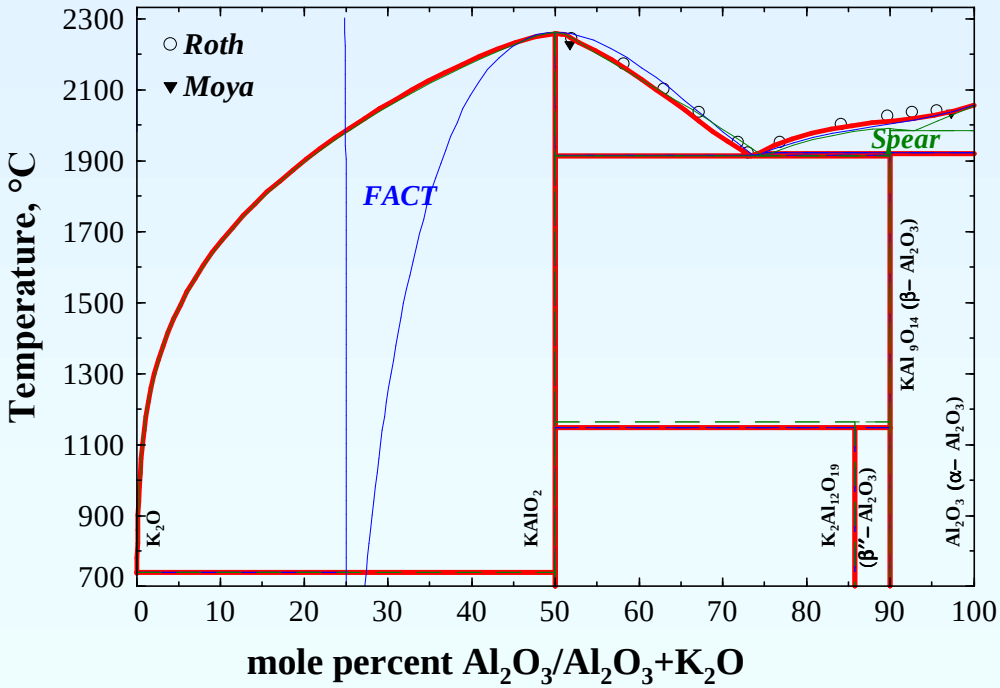


New eutectic point at 867 °C

New database for the Me_2O-Al_2O_3 systems (Me=Na, K)



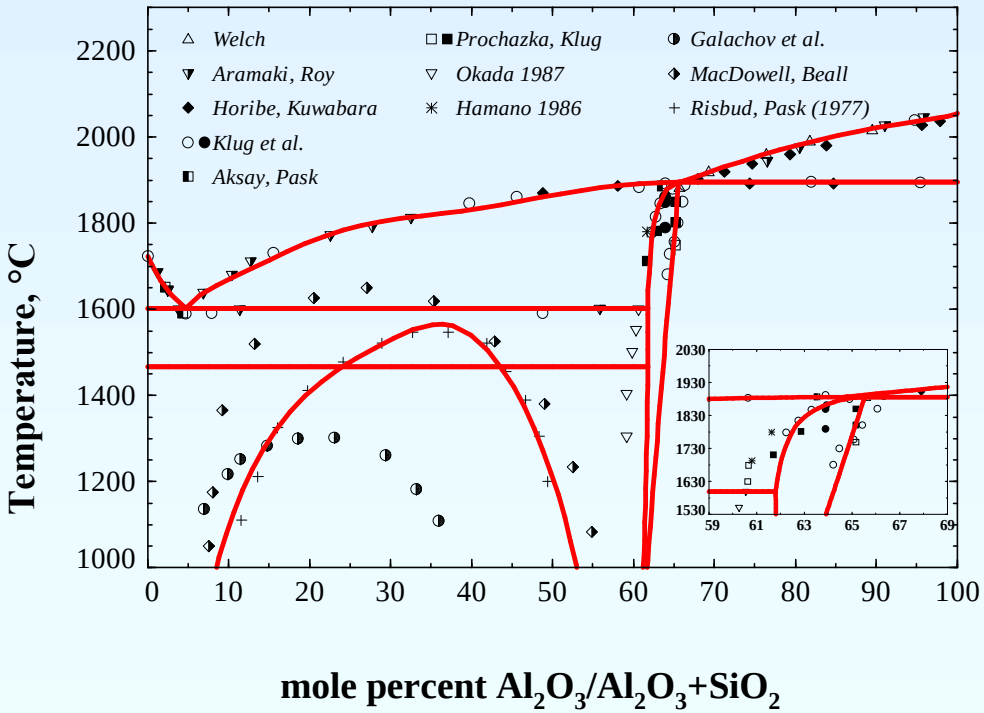
Thermodynamic data for the Na aluminates ($Na_2Al_{12}O_{19}$, $NaAl_9O_{14}$) were re-optimised



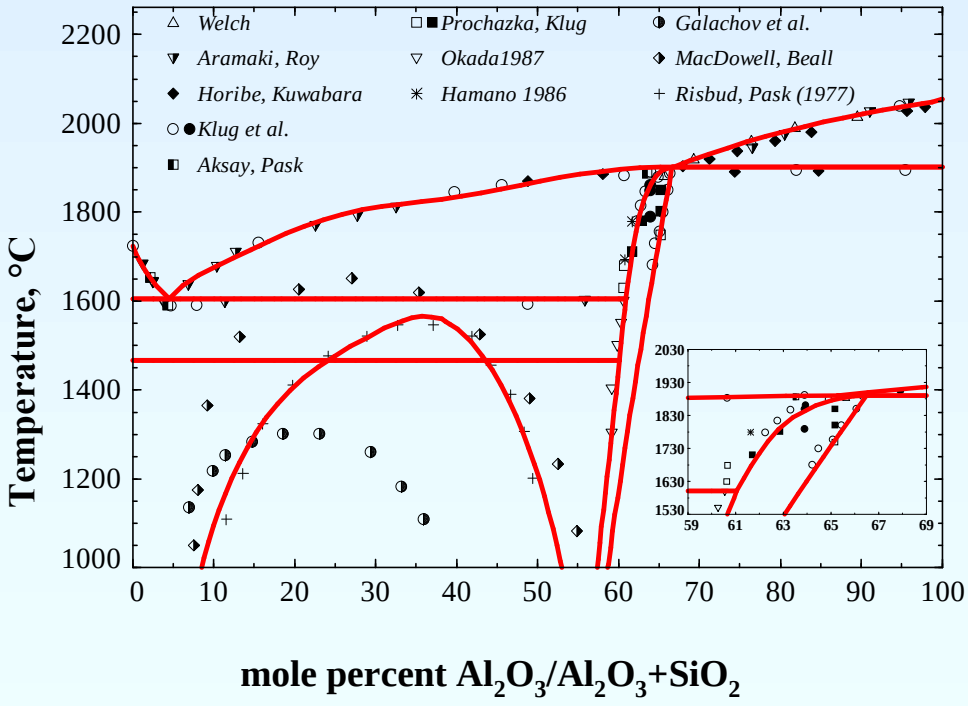
No solution using the FACT database in the Me_2O-rich region

Thermodynamic assessment of the Al_2O_3-SiO_2 system

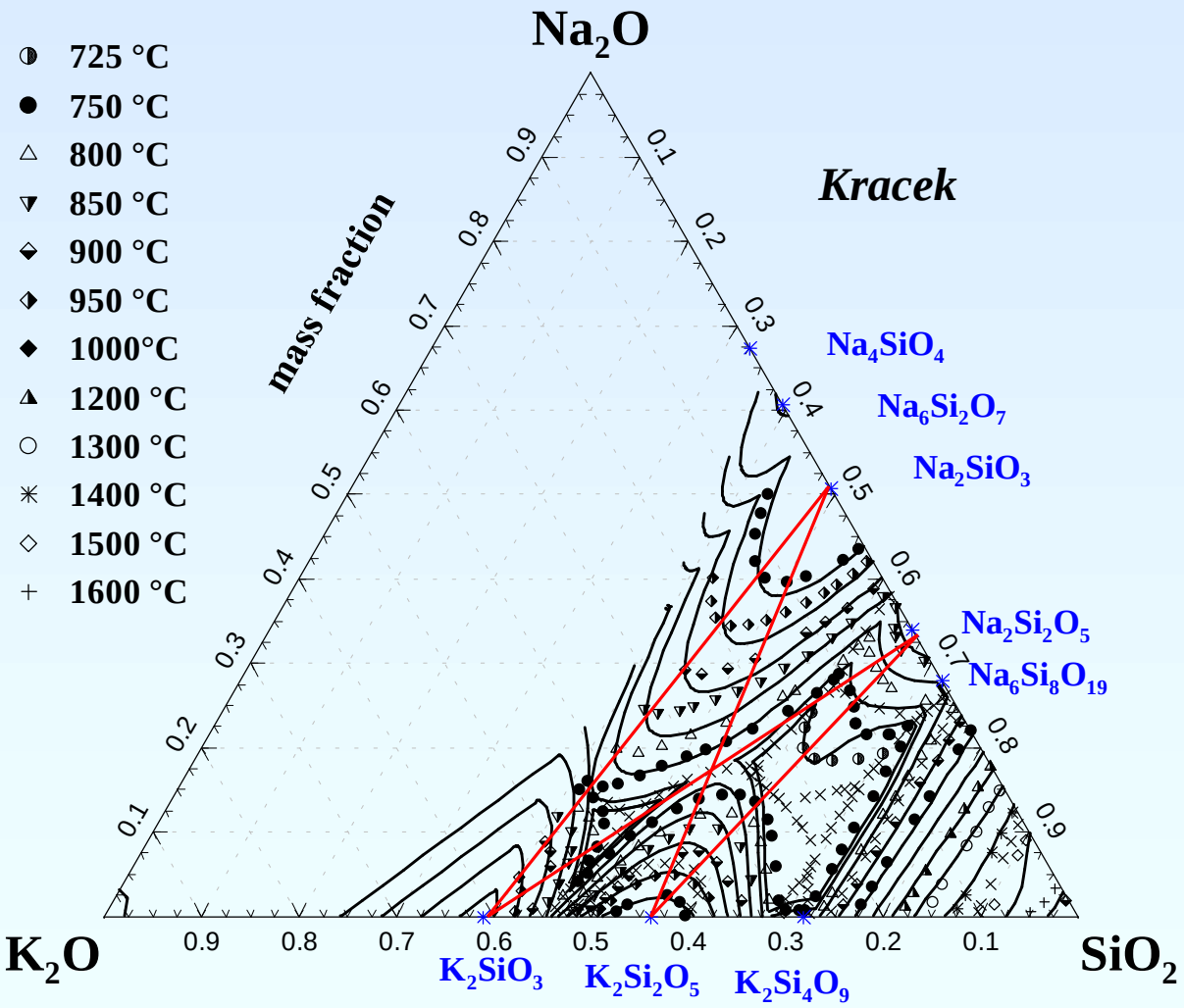
Associate model for mullite



Four-sublattice model for mullite



K_2O-Na_2O-SiO_2 system: comparison of the calculated isotherms with the experimental points



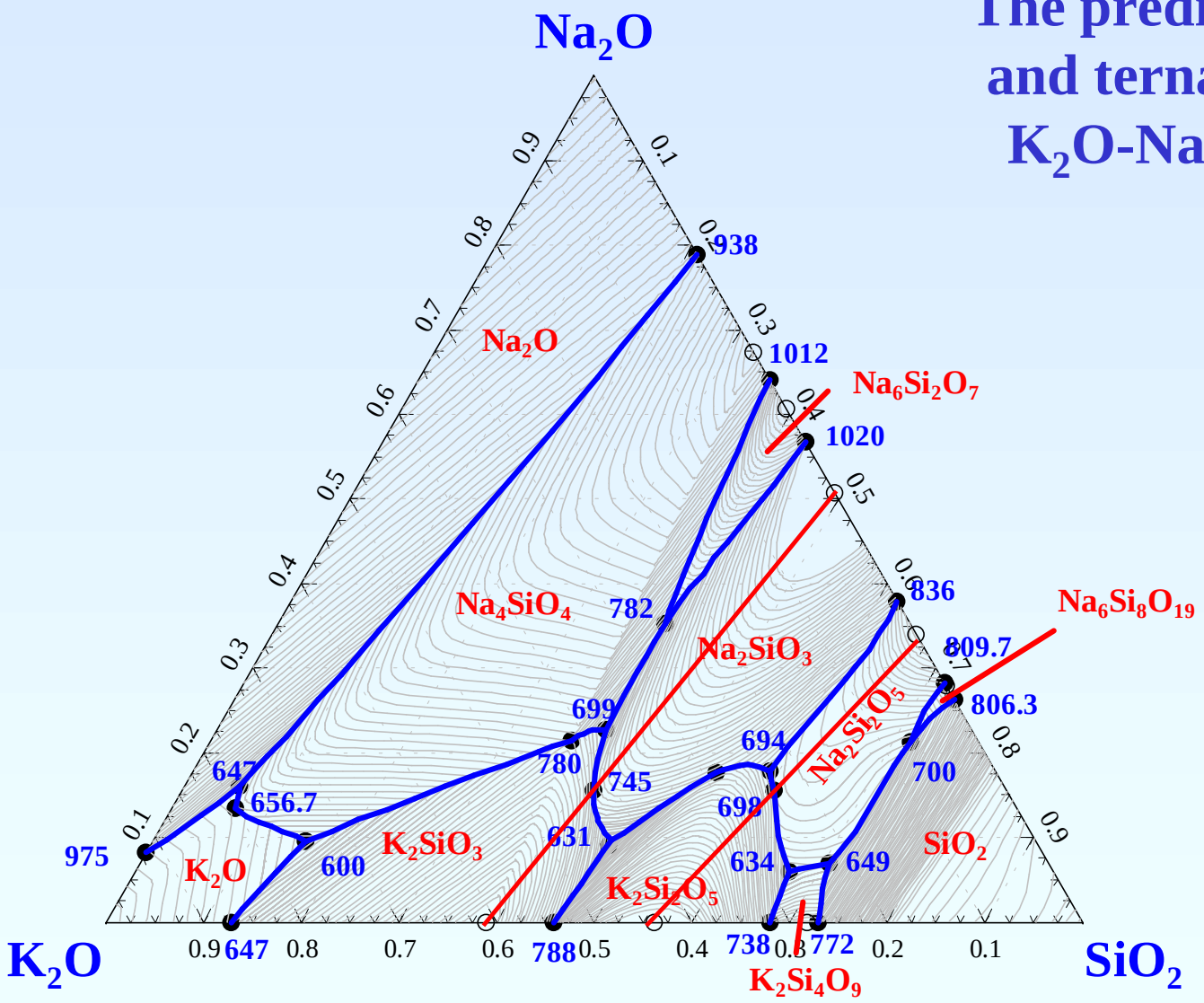
Solution species:

N414	Na_4SiO_4*2/5
N213	Na_2SiO_3*2/3
N225	$Na_2Si_2O_5$*1/2
K213	K_2SiO_3*2/3
K225	$K_2Si_2O_5$*1/2
K249	$K_2Si_4O_9$*1/3

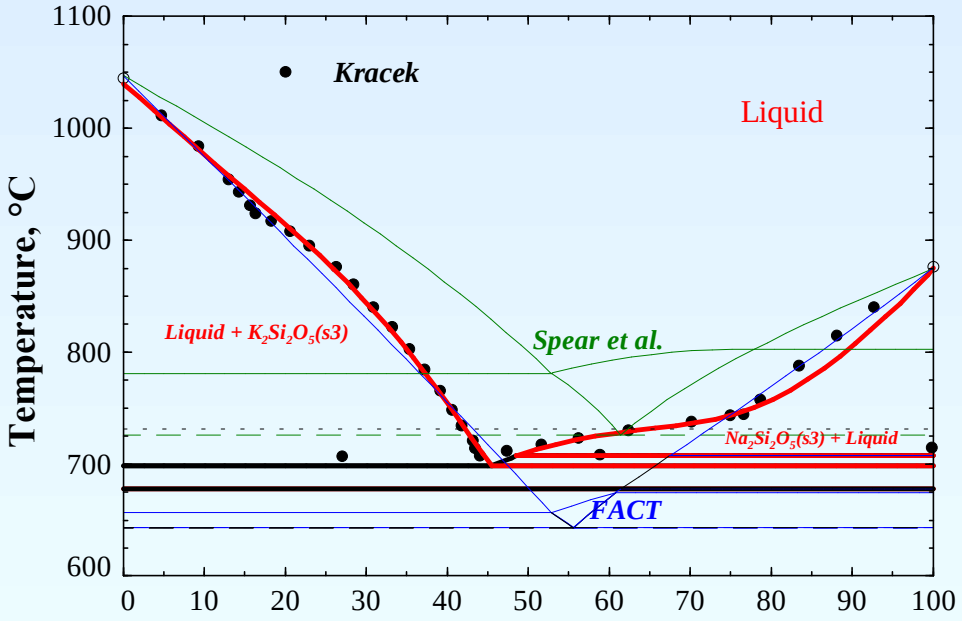
Interaction parameters:

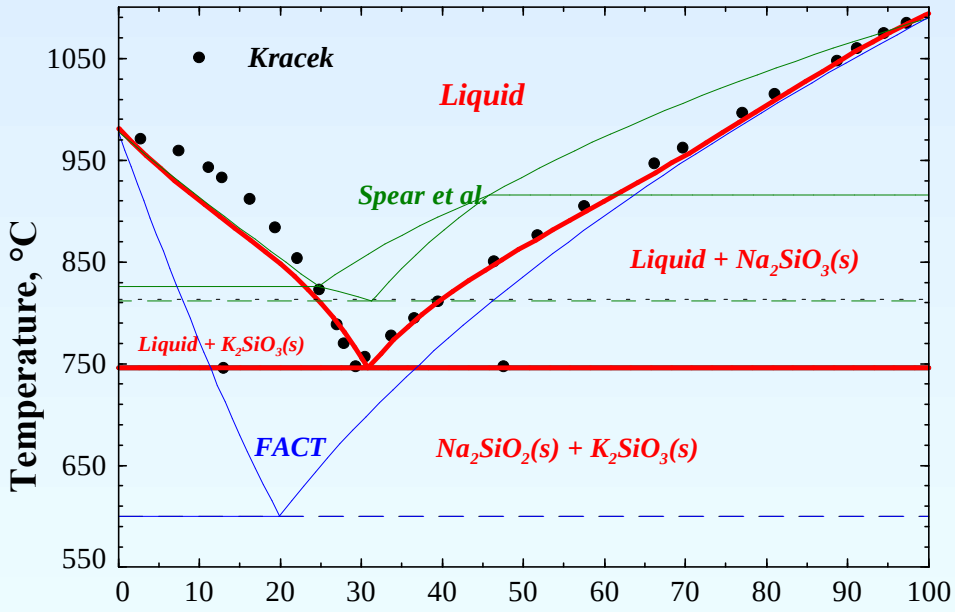
N213-K213
N225-K225
N213-K225
N225-K213

The predicted phase fields and ternary points in the K_2O-Na_2O-SiO_2 system

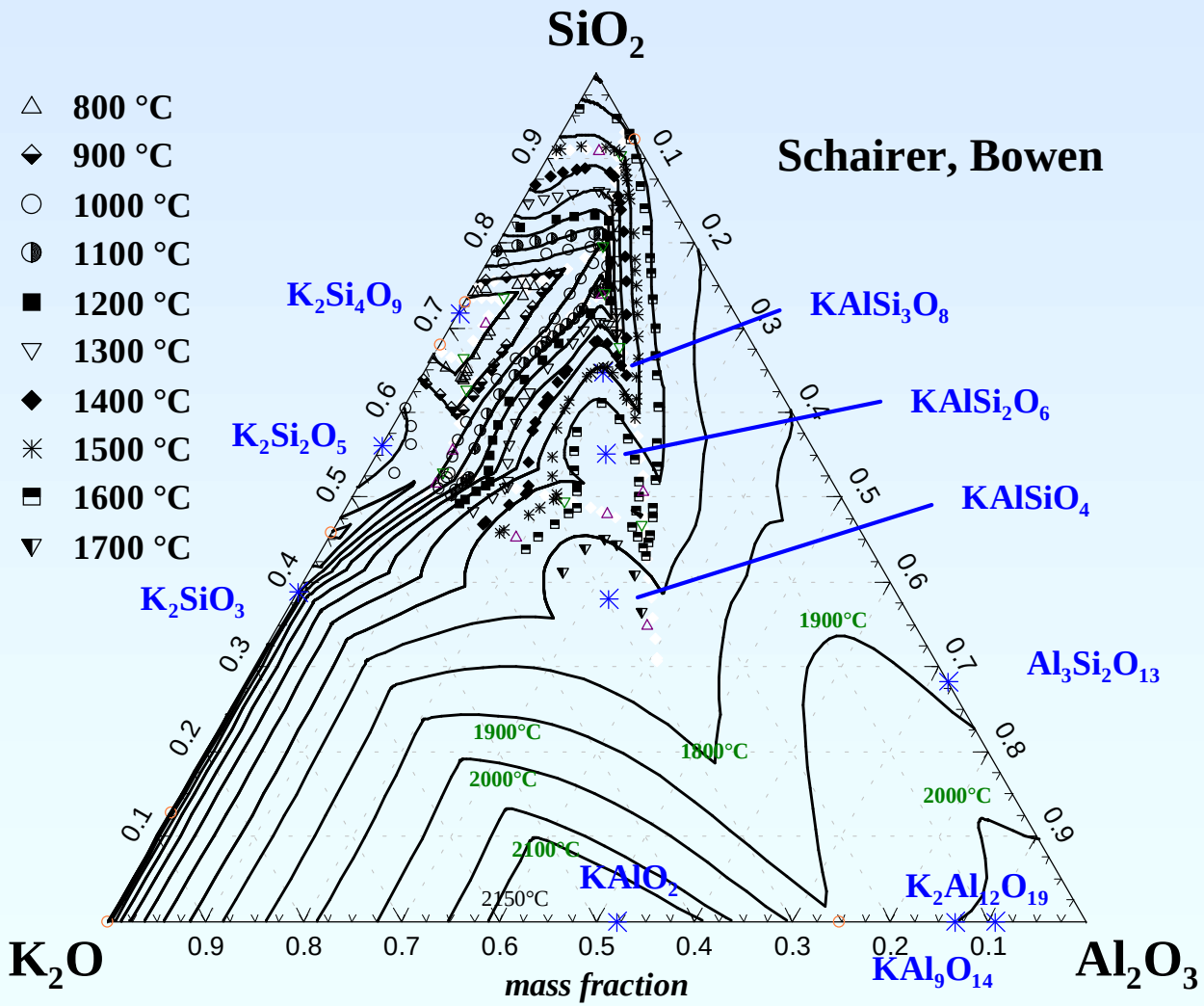


Quasi-binary section $Me_2Si_2O_5$ and Me_2SiO_3 (Me=Na, K)





K_2O-Al_2O_3-SiO_2 system: comparison of the calculated equlibria with the experimental points

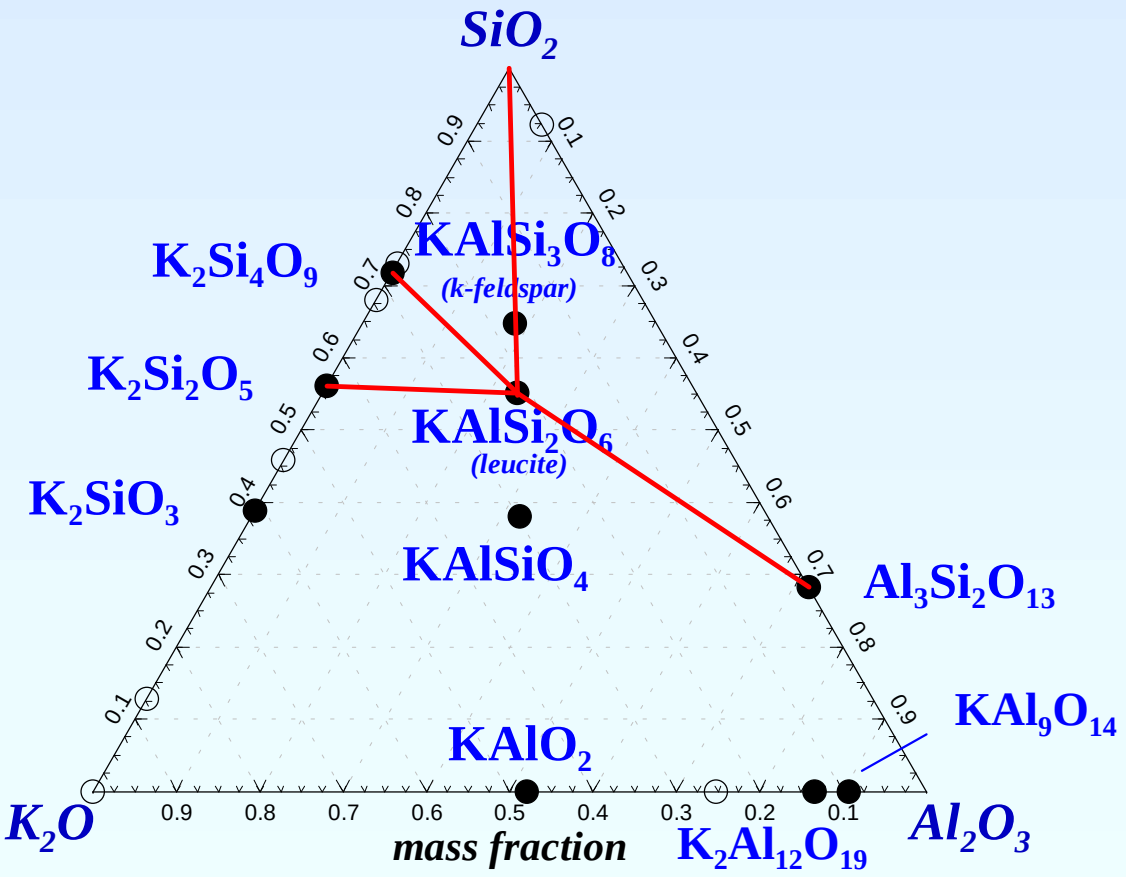


Liquid

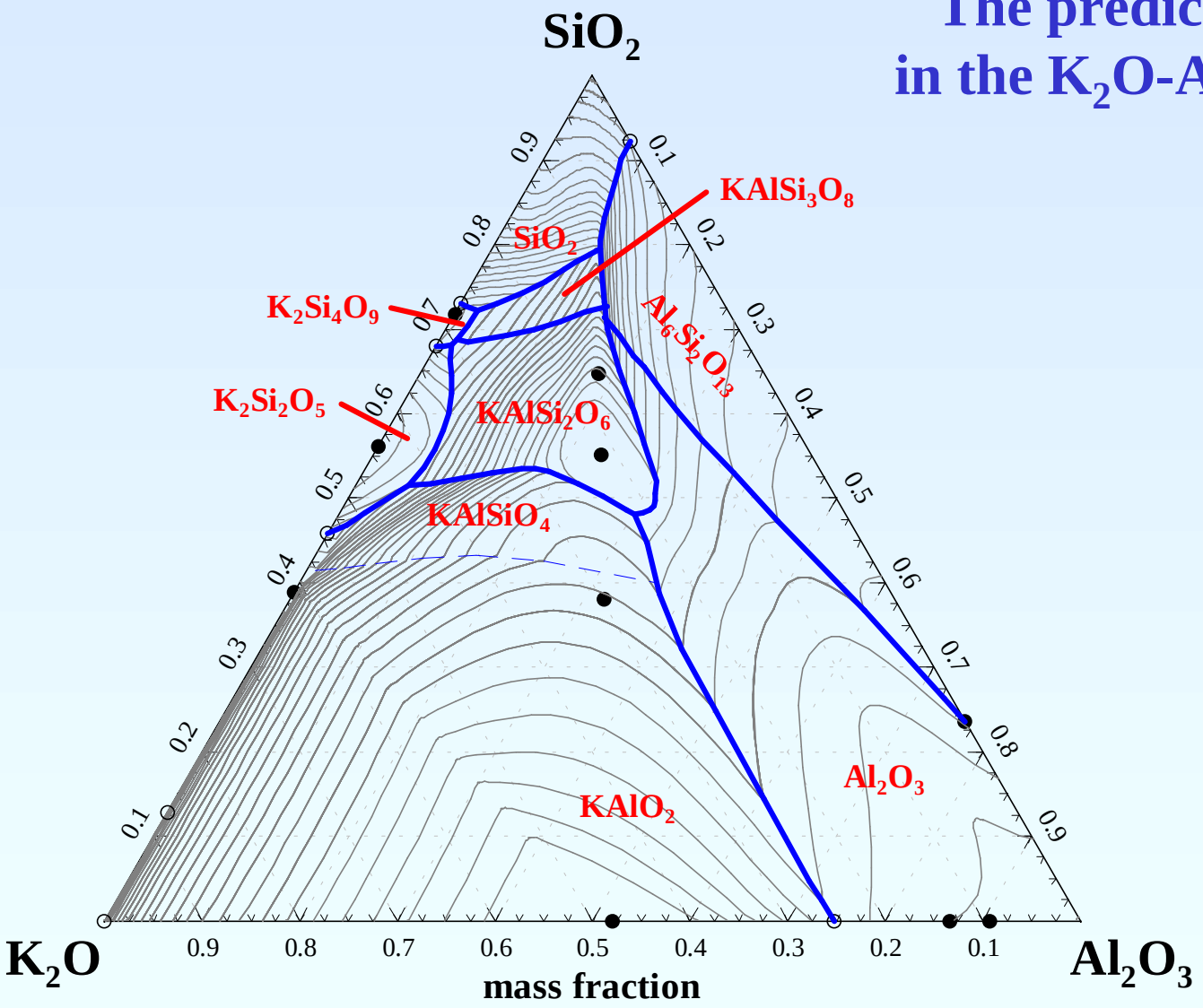
- **binary associate species**
- **ternary species: $KAlSi_2O_6 \cdot 1/2$ and $KAlSiO_4 \cdot 2/3$**

Solution species in the ternary liquid in the K_2O-Al_2O_3-SiO_2 system

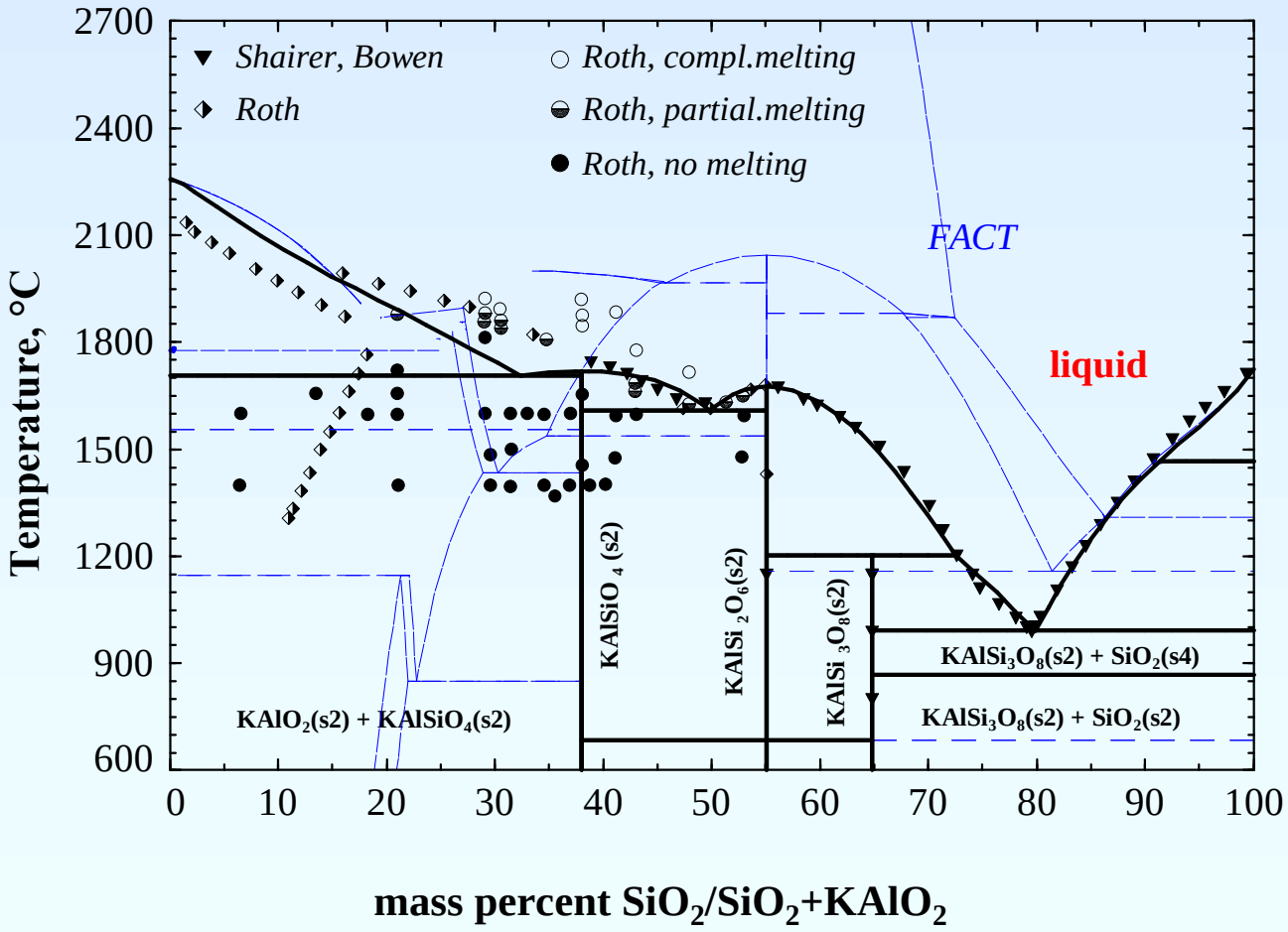
Interaction parameter between:	
Binary species	Ternary species
$K_2Si_4O_9$	$KAlSi_2O_6 \cdot 1/2$
$SiO_2 \cdot 1/2$	$KAlSi_2O_6 \cdot 1/2$
$K_2Si_2O_5$	$KAlSi_2O_6 \cdot 1/2$
$Al_6Si_2O_{13} \cdot 1/4$	$KAlSi_2O_6 \cdot 1/2$

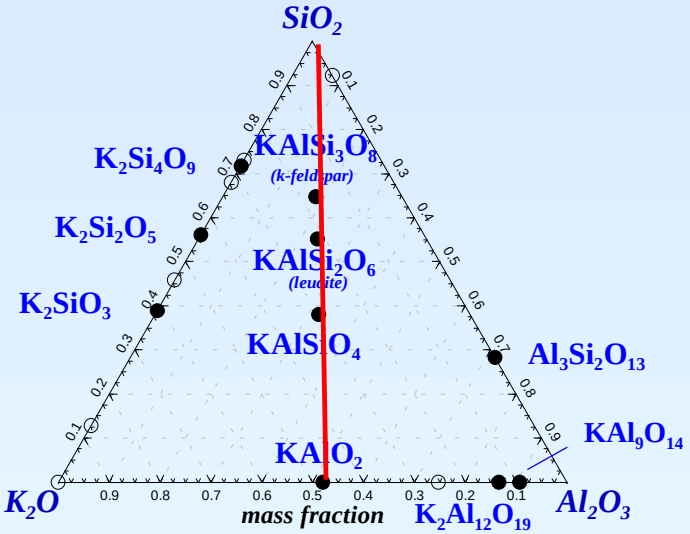


The predicted phase fields in the K_2O-Al_2O_3-SiO_2 system



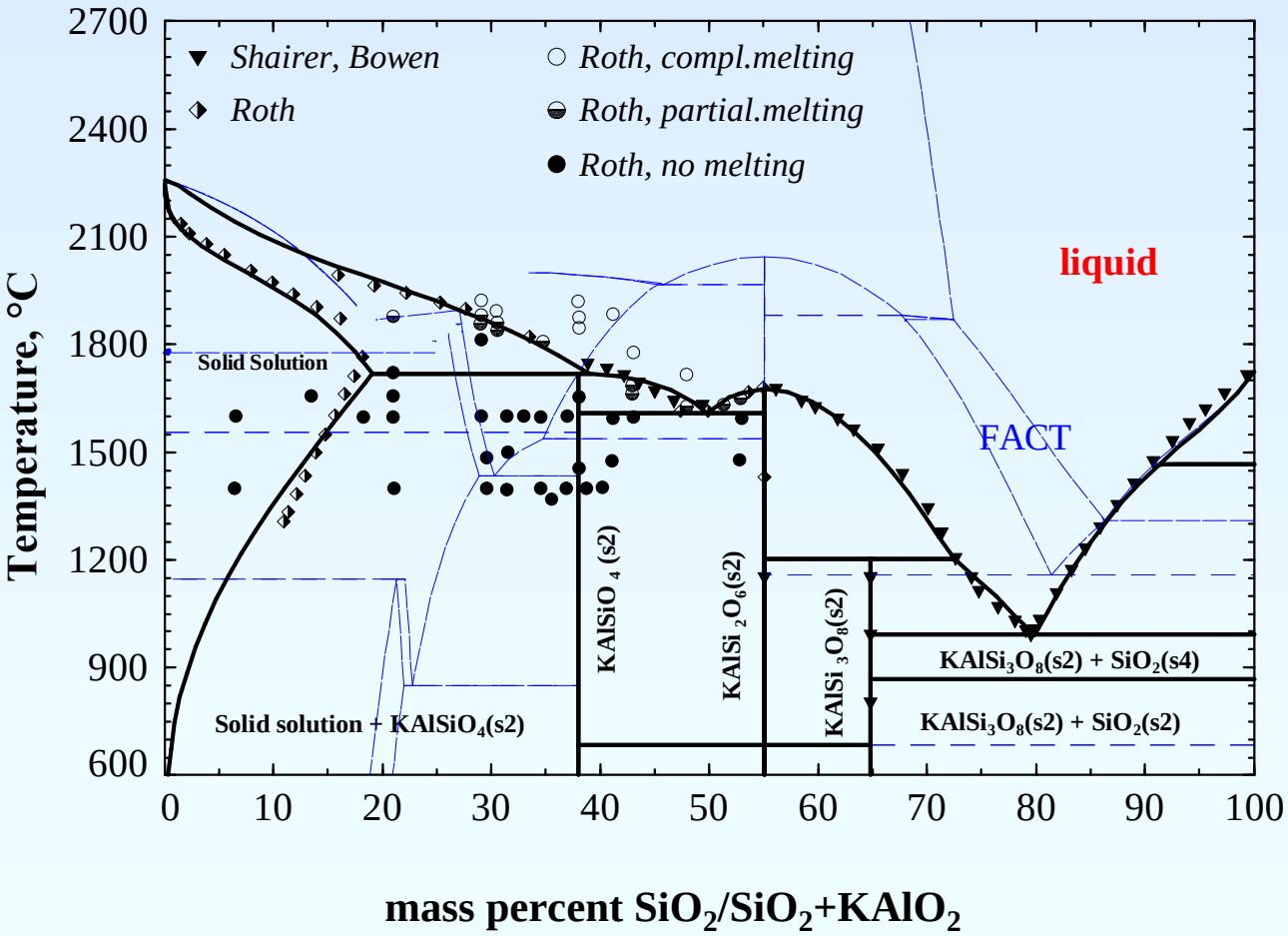
Quasi-binary section $KAlO_2$-SiO_2/ version I

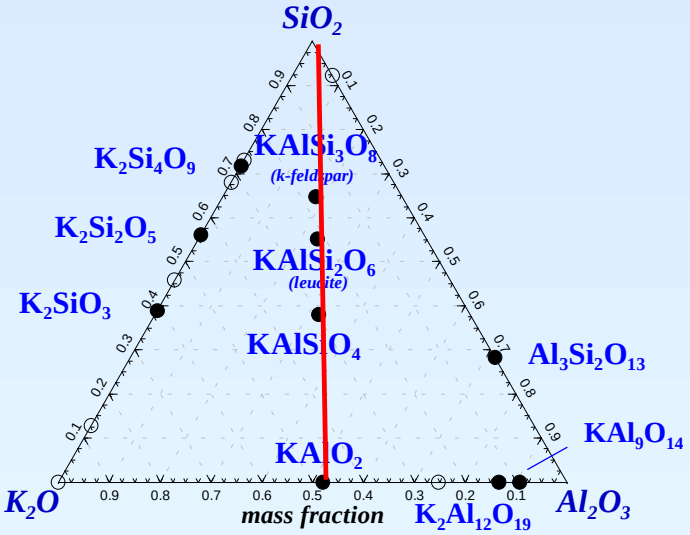




Thermodynamic data for $KAlSi_3O_8$ (K-feldspar) were re-optimised

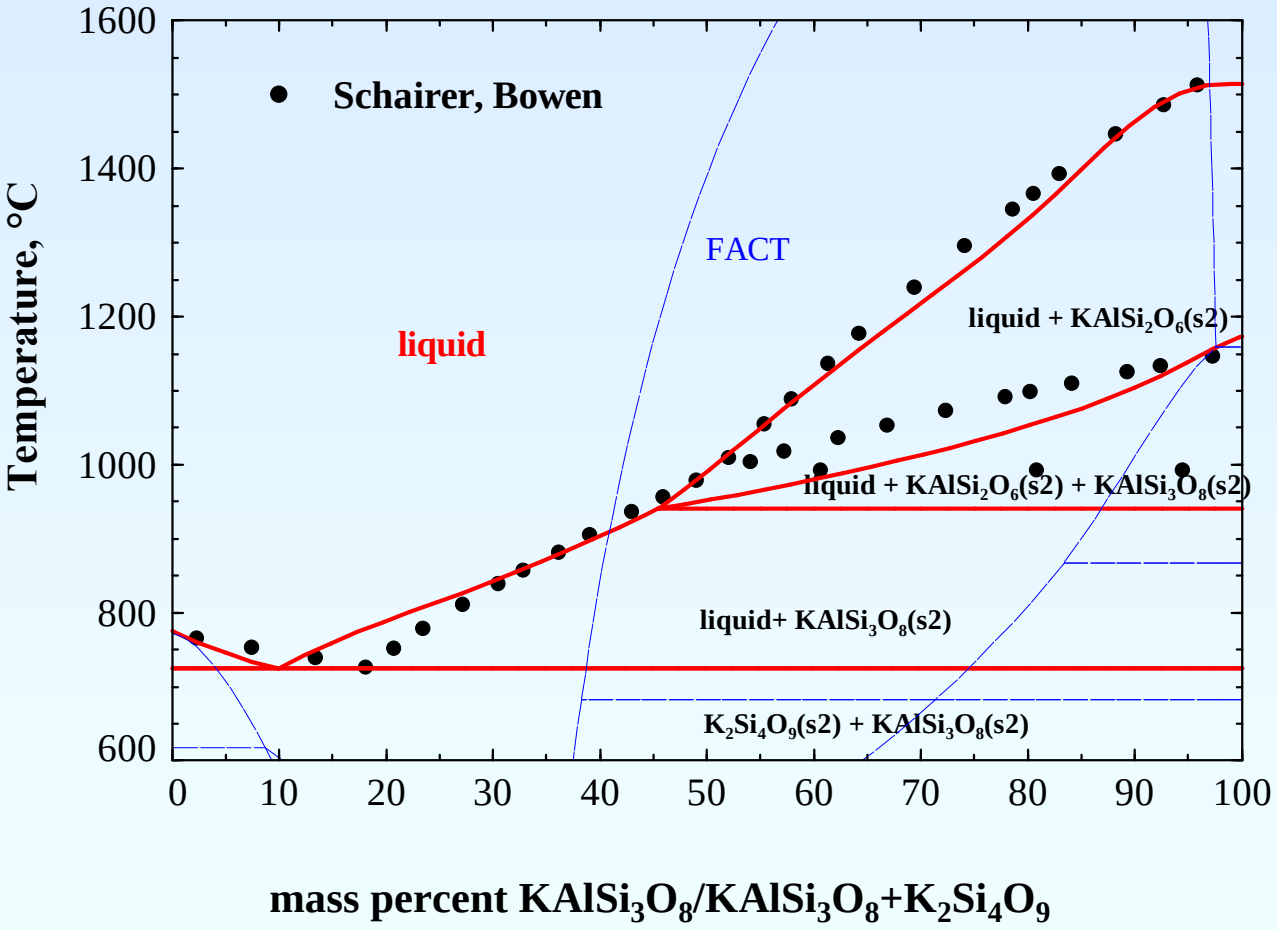
Quasi-binary section $KAlO_2$-SiO_2 / version II

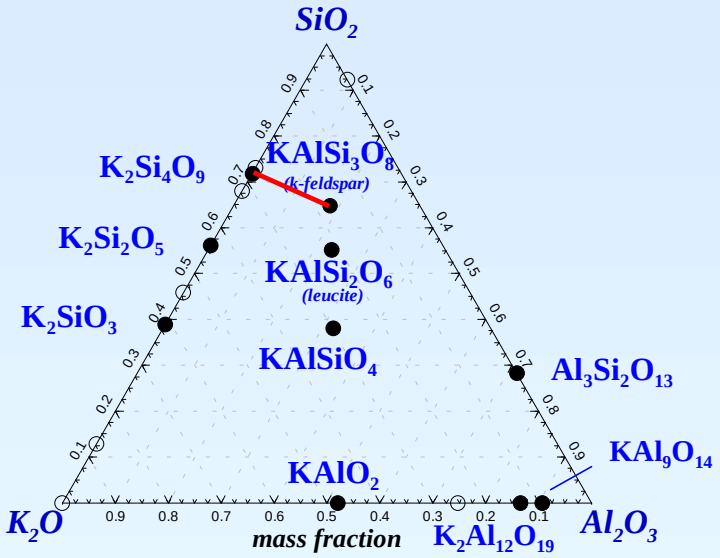




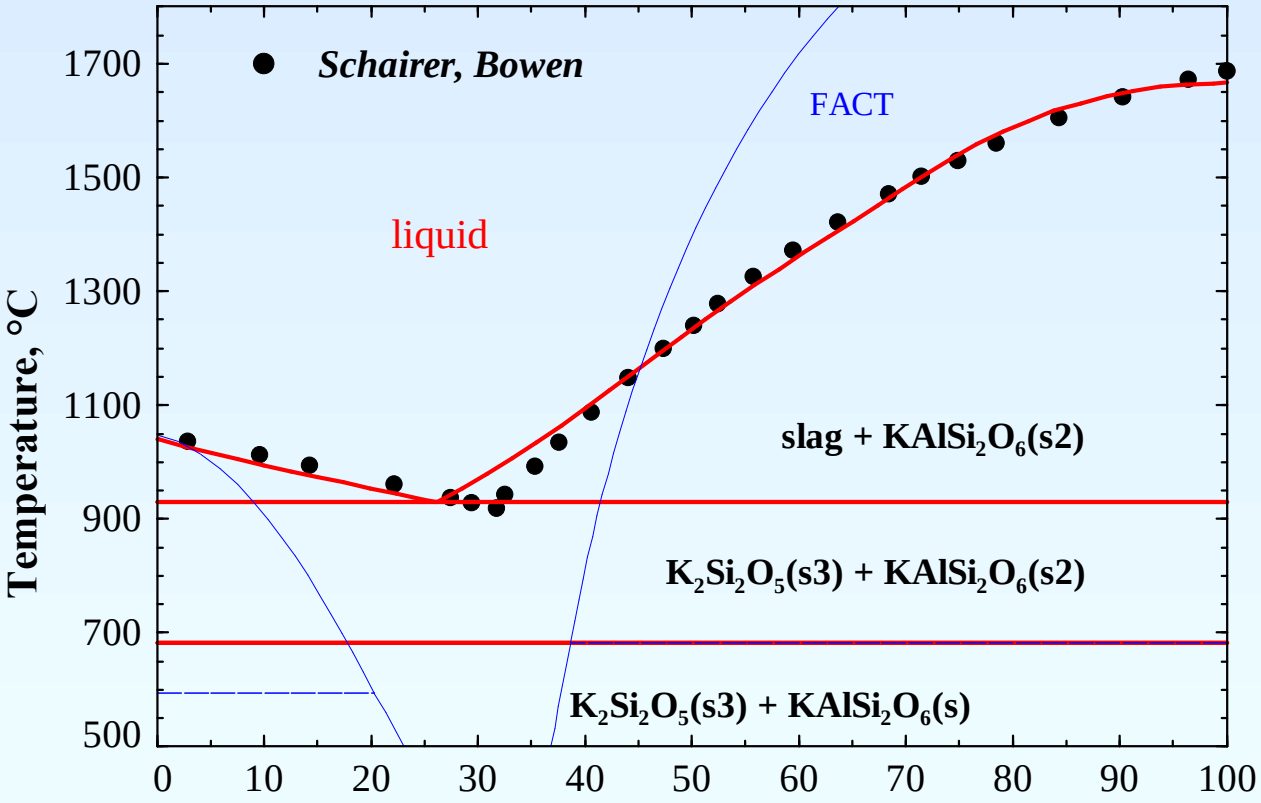
Solid solution components:
Associate species:
$KAlO_2$
$KAlSiO_4$

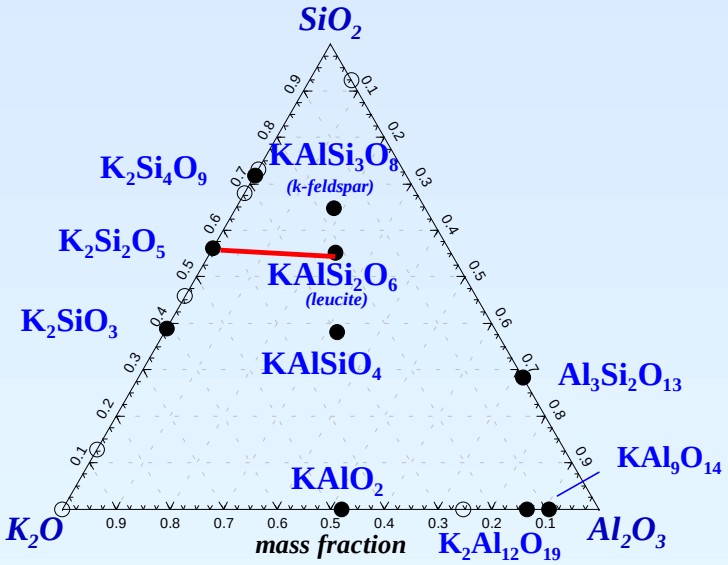
Quasi-binary section $K_2Si_4O_9$-$KAlSi_3O_8$ (k-feldspar)



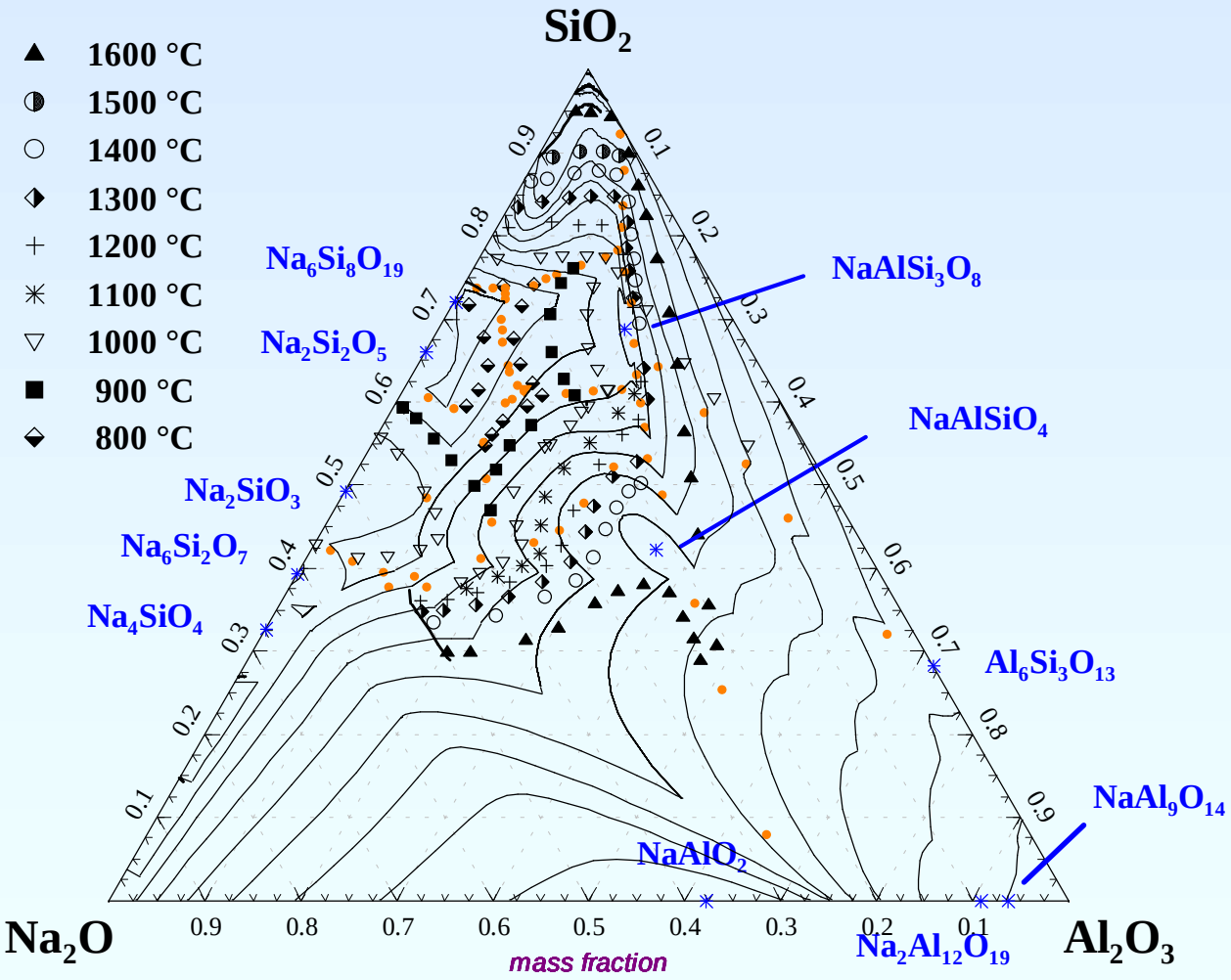


Quasi-binary section $K_2Si_2O_5$-$KAlSi_3O_8$ (leucite)





Current results: predicted phase equlibria in the Na_2O-Al_2O_3-SiO_2 system

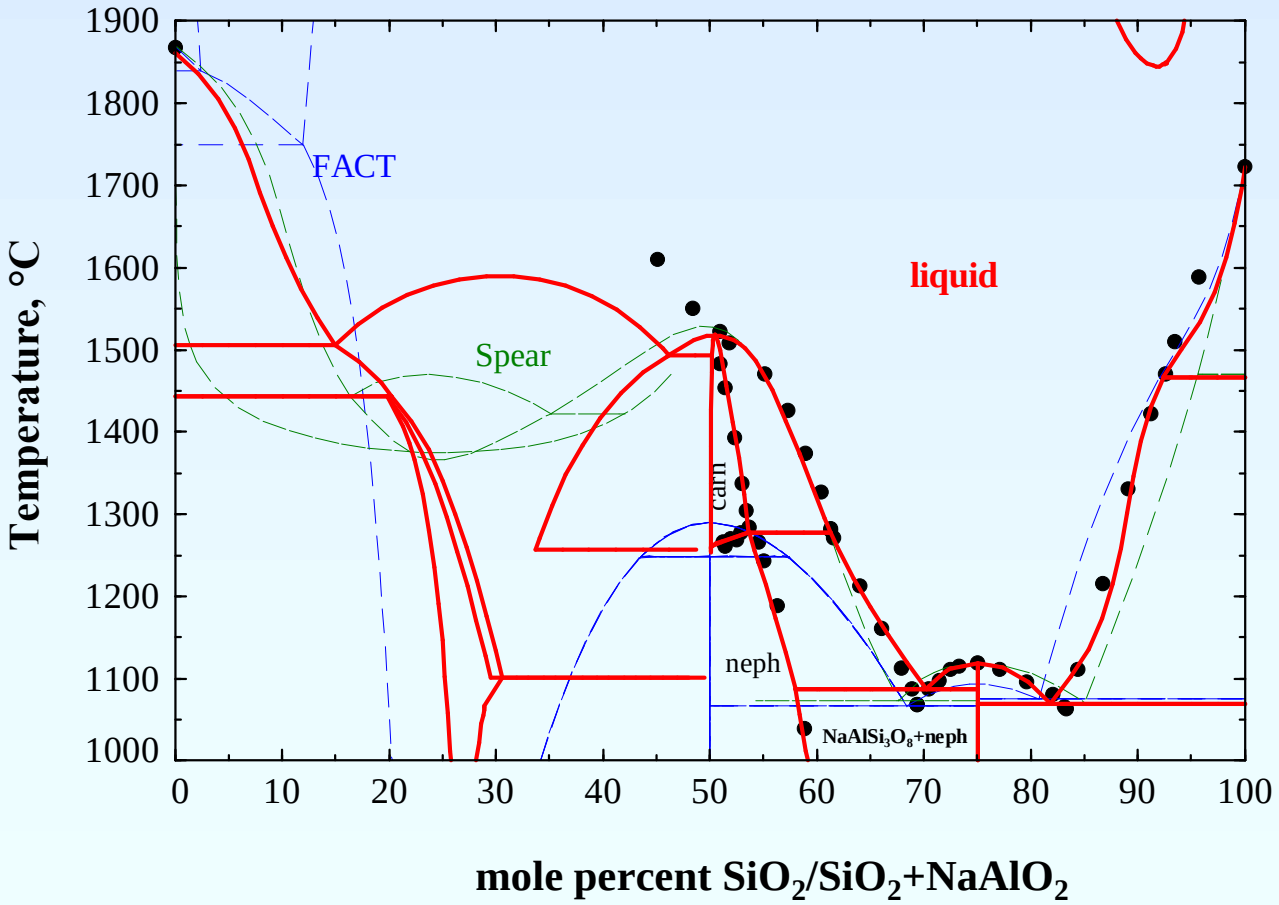


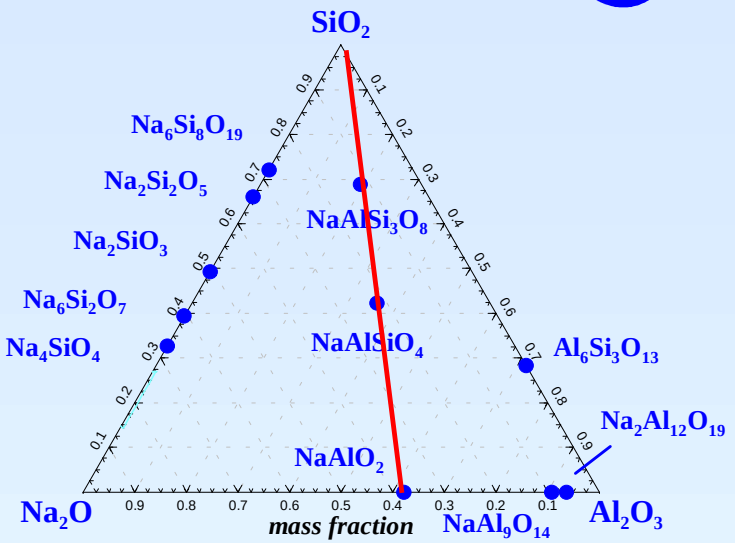
Thermodynamic data for $NaAlSi_3O_8$ (albite) were re-optimised

Liquid

- **binary associate species**
- **ternary species: $KAlSi_3O_8 \cdot 2/5$ and $KAlSiO_4 \cdot 2/3$**

Current results: quasi-binary section $NaAlO_2$-SiO_2





Solid solutions

Nepheline

$NaAlSiO4$ (neph, s3)

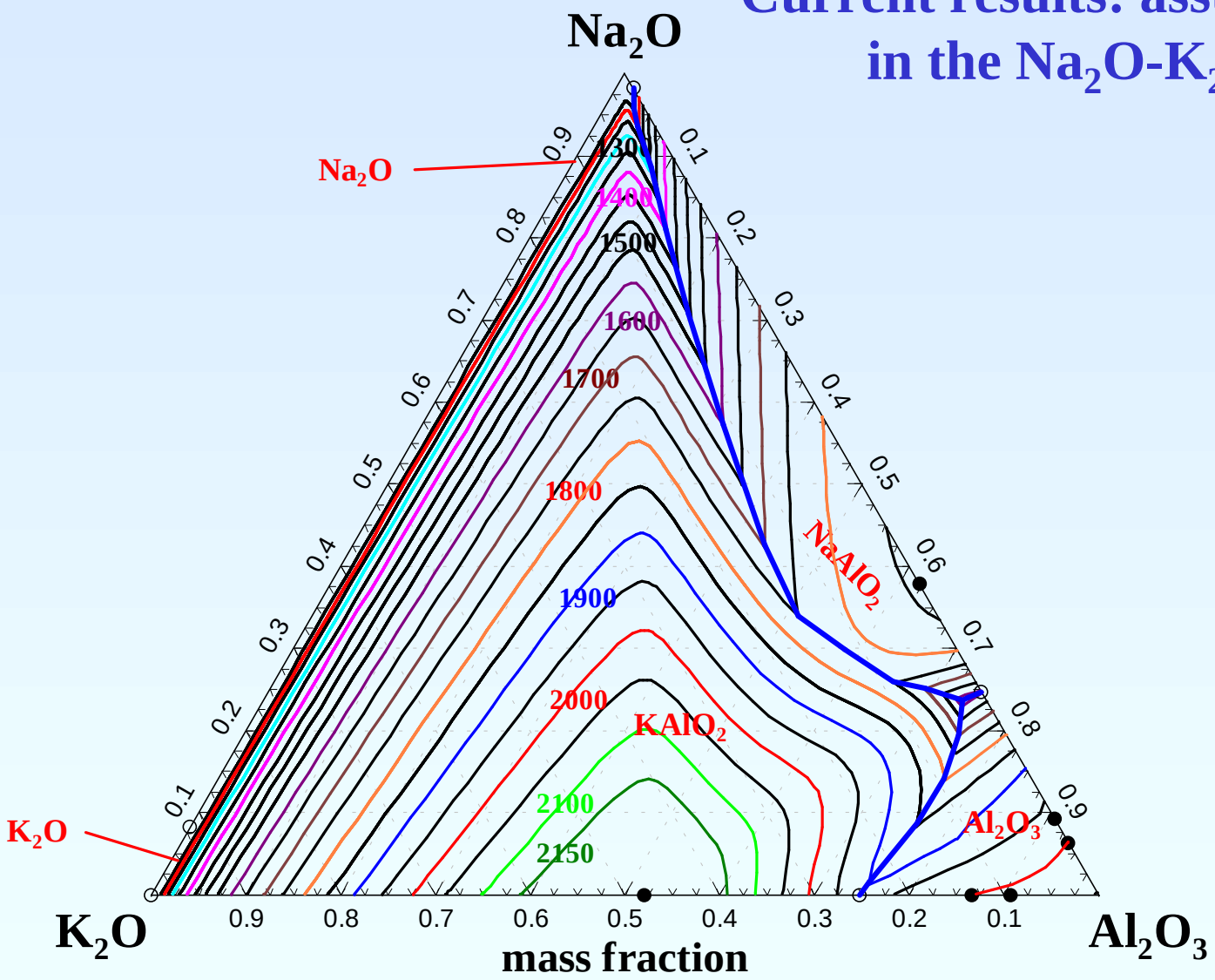
$NaAlSi_2O_6$ (jadeite)

Carnegieite

$NaAlSiO_4$ (carn, s4)

$NaAlSi_2O_6$ (jadeite)

Current results: assumed phase equlibria in the Na_2O-K_2O-Al_2O_3 system



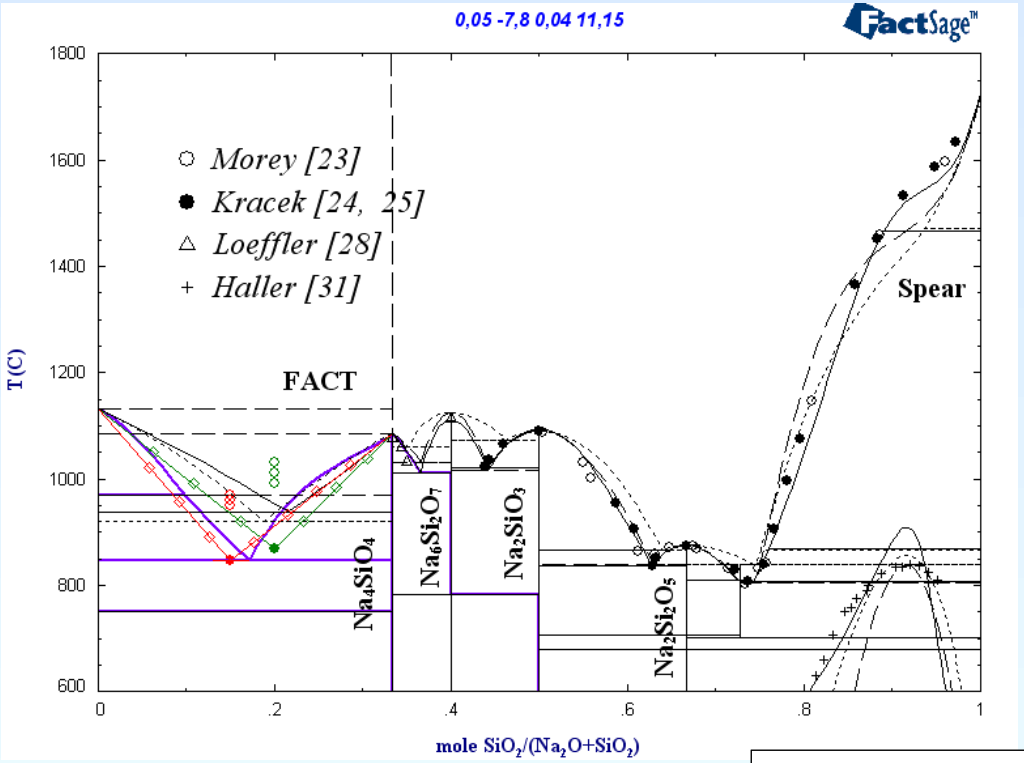
Conclusions

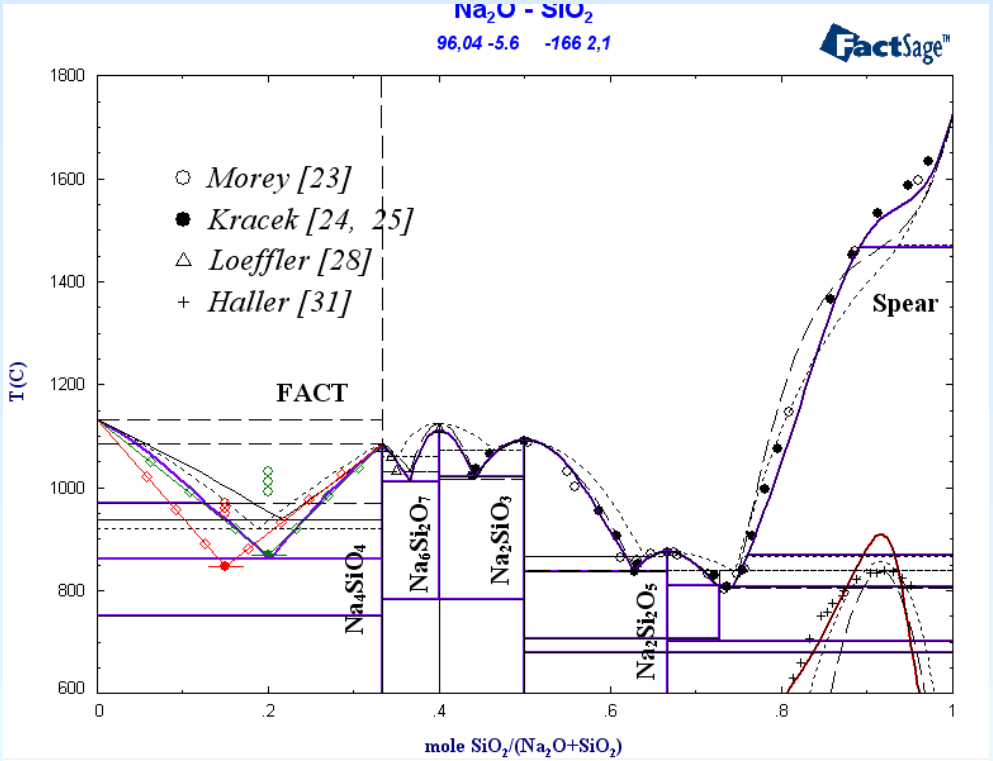
- **The solution data for the binary systems Me_2O-SiO_2, Me_2O-Al_2O_3 (Me=Na, K) and Al_2O_3-SiO_2 were improved to accurate description of the phase diagrams of the slag system**
- **Solid and liquid solutions in the ternary systems Na_2O-K_2O-SiO_2, K_2O-Al_2O_3-SiO_2 and Na_2O-Al_2O_3-SiO_2 (partly) were described using the new database**

In the future:

- **Assessment the further solution parameters in the Na_2O-Al_2O_3-SiO_2 system**
- **Consideration of the oxide systems containing CaO and MgO**

Thank you for your attention





New eutectic point at 845 °C

New eutectic point at 867 °C

Experimental data

of M. Rys, IEF-2