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THERMODYNAMIC MULTICOMPONENT SILICATE EQUILIBRIUM PHASE CALCULATIONS

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ABSTRACT

Phase equilibria of solution phase—solution phase and pure phase—solution phase type in binary and ternary systems are calculated by computer assuming excess free energies are constant over the temperature ranges encountered. The multicomponent activities are calculated with a thermodynamically consistent equation from a general excess free energy model. Input data are heats of fusion and partial excess chemical potentials of mixing derived from binary phase diagrams. The system quartz-fayalite-leucite has a calculated internal immiscibility field at liquidus temperatures above 1100°C. The solid solution liquidus is calculated for the granite system and diopside-albite-anorthite with an accuracy of ±8°C, ±5 % composition of liquid and ±2% of crystal. Isocons of the coexisting solid solution phase (icophases) are contoured on the ternary liquidus. An empirical n-component correction free energy with n-independent parameters is suggested to adjust calculated results to experiments using one (eutectic minimum) or two (cotectic line) points. The calculations can be used to guide experiments.

INTRODUCTION

Modern authors have used a thermodynamic approach to calculate phase diagrams, guide experimentation, and to restrict the number of experiments necessary to define a system. This is especially valuable when experimentation times are long or equipment is expensive. More recently, Thompson and Waldbaum (1969b) and Green (1970) have used binary phase diagrams to obtain detailed thermodynamic data based on non-ideal solution models, while Levin (1962), Olson (1965), Blander (1968), and Thompson and Waldbaum (1969a) have used thermodynamic data to calculate binary and some ternary phase diagrams. These calculations assumed a statistical fit of only one or two parameters to binary excess free energy data; if more parameters are added, the necessary formulation of the corresponding n-component excess chemical potentials rapidly becomes difficult. To complicate matters further, Lumsden (1966) and Green (1970) have shown that although the regular and subregular solution models may adequately fit binary excess free energy values at one temperature, the resulting excess entropies often do not agree with those determined by calorimetry. One solution to this problem is to use a *general* excess free

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energy and excess entropy model but this requires much more primary data than is usually available. The three purposes of this paper are to:

(a) Develop an easily computerised n-component general excess free energy model that permits the use of *precise* binary excess free energies *as opposed to* a fitted one or two parameter model. Excess entropies of mixing are not considered separately and G^x is assumed to be constant over the temperature ranges encountered.

(b) Combine this approach with standard equations of phase equilibria to calculate some ternary phase diagrams from binary data only.

(c) Suggest how the scheme may be extended to higher order systems and how it may be improved with a correction factor based on a few experimental points.

SYMBOLS: Throughout this paper all extensive functions are molar quantities

V^x	superscript x for excess thermodynamic function V
V^k	superscript k for correction thermodynamic function V
V_A	subscripts (A, B, crystal, liquid) for function V of phases A, B, etc.
V_i	subscripts (i, j, 1, 2) for function V of components i, j, 1, 2
V_{iA}	function V for component i in phase A
n	number of components in the system
R	gas constant
μ	chemical potential
G	Gibbs free energy
T	absolute temperature
N	mole fraction
a	activity
γ	activity coefficient
T°_i	temperature of fusion of pure crystalline component i
ΔH°_i	heat of fusion of pure crystalline component i at T°_i
ΔH°_{iBA}	heat of transformation of phase B to phase A, both phases pure in i
W_{ijA}	regular or subregular solution model interaction energy parameter between components i and j in phase A
G^x_{ij}	values of excess free energy of mixing across the binary ij
Z_{ij}	normalized mole fraction of component i in binary ij, from an n-component system
θ_{ij}	slope of G^x_{ij} at Z_{ij}

PARTIAL AND TOTAL EXCESS FREE ENERGY AND THE ASYMMETRIC SOLUTION MODEL

The original definition of the excess quantities can be extended to chemical potentials (*e.g.*, Thompson 1967) so that for any component i, $\mu_i(real) = \mu_i(ideal) + \mu_i^x(excess)$ where the superscript ^{x} indicates an excess quantity. However, $\mu_i(real) = \mu_i^\circ + RT \ln a_i = \mu_i^\circ + RT \ln N_i + RT \ln \gamma_i$ where γ_i is an activity coefficient. Since $\mu_i(ideal) = \mu_i^\circ + RT \ln \mathrm{N}_i$ it follows that $\mu_i^x = RT \ln \gamma_i$. Like other partial molar quantities, μ_i^x satisfies Moore (1963), so

$$\mu_i^x = G^x + (1 - N_i)\frac{\partial(G^x)}{\partial(N_i)} \tag{1}$$

where the differential[1] is taken *directly towards* $N_i = 1$ and

$$G^x = \sum_{i=1}^{n} \mu_i^x N_i \tag{2}$$

Consider the n-component regular solution model (Kern and Weisbrod 1967)

$$G^x = \sum_{i=1}^{n} \sum_{j>i}^{n} N_i N_j W_{ij} \tag{3}$$

where W_{ij} is the interaction energy constant between components i and j. Each binary pair ij contributes to the total G^x. This can be interpreted as

$$\left[\left(\frac{N_i}{N_i + N_j}\right)\left(\frac{N_j}{N_i + N_j}\right)W_{ij}\right](N_i + N_j)^2.$$

The term in square brackets is the value of excess free energy in the binary ij at composition $Z_{ij} = (N_i/N_i + N_j)$ and the term in heavy parentheses is the *dilution factor* which the binary excess free energy value is multiplied by to take its contribution into the n-component system. Making G_{ij}^x the value to the excess free energy in the binary ij at Z_{ij}, then G_{ij}^x becomes

$$G^x = \sum_{i=1}^{n} \sum_{j>i}^{n} G_{ij}^x (N_i + N_j)^2. \tag{4}$$

This is an asymmetric model and makes use of the actual values of G_{ij}^x that occur in the binaries. The corresponding n-component formula for μ_i^x must be derived by the application of (1) on (4). With respect

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[1] All partial derivatives in this paper are understood to be obtained at constant temperature.

to component *1*, a transformation, with constants $C_j = N_j/N_2$, $2 \leq j \leq n$, allows the differential in (1) to be taken directly towards $N_1 = 1$. The resulting general expression for μ_i^x is

$$\mu_i^x = 2 \sum_{j \neq i}^{n} (N_i + N_j) G_{ij}^x + \sum_{j \neq i}^{n} N_j \theta_{ij} - G^x \tag{5}$$

where

$$\theta_{ij} \equiv \frac{d(G_{ij}^x)}{d(Z_{ij})},$$

that is, the slope of G_{ij}^x in the binary *ij* at Z_{ij}. Applying the general formula (5) for three components

$$\begin{aligned}
\mu_1^x &= 2[(N_1 + N_2)G_{12}^x + (N_1 + N_3)G_{13}^x] + N_2\theta_{12} + N_3\theta_{13} - G^x \\
\mu_2^x &= 2[(N_1 + N_2)G_{12}^x + (N_2 + N_3)G_{23}^x] + N_3\theta_{23} + N_1\theta_{21} - G^x \\
\mu_3^x &= 2[(N_1 + N_3)G_{13}^x + (N_2 + N_3)G_{23}^x] + N_2\theta_{32} + N_1\theta_{31} - G^x
\end{aligned} \tag{6}$$

where

$$G^x = (N_1 + N_2)^2 G_{12}^x + (N_1 + N_3)^2 G_{13}^x + (N_2 + N_3)^2 G_{23}^x$$

The form of G_{ij}^x and θ_{ij} in (5) is completely unspecified. This is an advantage, for now if we wish to specify a certain model, say an *n*-component regular solution model, then (5) may be used to generate the corresponding explicit equations for μ_i^x: with $G_{ij}^x = [N_i N_j W_{ij}/(N_i + N_j)^2]$ and $\theta_{ij} = [(N_j - N_i)/(N_i + N_j)]W_{ij}$ then by (5) we have

$$\begin{aligned}
\mu_i^x &= 2 \sum_{j \neq i}^{n} \frac{N_i N_j W_{ij}}{(N_i + N_j)} + \sum_{j \neq i}^{n} \frac{N_j (N_j - N_i) W_{ij}}{(N_j + N_i)} - G^x \\
&= \sum_{j \neq i}^{n} N_j W_{ij} - G^x
\end{aligned} \tag{7}$$

For a complex type of G_{ij}^x, μ_i^x may be analytically calculated by a short fifteen card general computer routine which uses (5) with the appropriate substitutions for G_{ij}^x and θ_{ij}.

Non-ideality in every binary system influences the activity of component *i* since G^x in (5) and (7) has contributions from every binary. Conversely, if another component is added to an *n*-component system, data must be available from the *n* new binary systems introduced before G^x, μ_i^x and phase relations can be calculated. For a large number of components then such calculations should be combined with experimentally determined multicomponent equilibria or else the amount of required primary data is enormous and often not available.

Equations of Phase Equilibria and Derivation of μ_i^x Curves from Binary Phase Diagrams

The cryoscopic equation for simple eutectic liquids, used by Bowen (1928), is

$$\ln a_i = \frac{\Delta H_i^o}{R}\left(\frac{1}{T_i^o} - \frac{1}{T}\right) \tag{8}$$

where a_i is the activity of component i in the liquid phase at T, with reference state pure crystalline i at T. Rearranging yields

$$\mu_i^x \equiv RT \ln \gamma_i = \Delta H_i^o\left(\frac{T}{T_i^o} - 1\right) - RT \ln N_i \tag{9}$$

where γ_i is the activity coefficient of i at *Ni* and T. Using (9) and liquidus data from a simple binary phase diagram, a μ_i^x curve for component i in the liquid phase may be calculated for the composition range between *Ni* = 1 and the simple eutectic composition, but not on the other side of the eutectic. A modified Gibbs–Duhem integration was used to complete the μ_i^x curve on *j*'s side of the eutectic. The fact that μ_i^x curves must be continuous in general, more specifically at the eutectic, permits the estimation of some metastable eutectics. The position of the predicted eutectic temperature and composition may be varied until the μ_i^x curves are smooth and continuous at the eutectic composition after the Gibbs–Duhem integration is used. Using the existing liquidus data and this technique, the metastable eutectic in the system anorthite-orthoclase is estimated to be at 1186 ± 5°C at 94.5 ± 1 mole percent orthoclase.

For the case of solution phase A in equilibrium with solution phase B, Kern and Weisbrod (1967) have shown, using $\mu_{1A} = \mu_{1A}^o + RT \ln a_{1A}$, and $\mu_{1B} = \mu_{1B}^o + RT \ln a_{1B}$ with standard states of the end members of phases A and B being pure in component *1* at T, then for the reaction $B \rightarrow A$

$$\mu_{1B}^x - \mu_{1A}^x = RT \ln\left(\frac{N_{1A}}{N_{1B}}\right) + \Delta H_{1BA}^o\left(1 - \frac{T}{T_1^o}\right) \tag{10}$$

Similarly, with standard states of end members of phases A and B being pure in component *2* at T,

$$\mu_{2B}^x - \mu_{2A}^x = RT \ln\left[\frac{(1 - N_{1A})}{(1 - N_{1B})}\right] + \Delta H_{2BA}^o\left(1 - \frac{T}{T_2^o}\right) \tag{10}$$

where the temperature dependence of ΔH_{iBA}^o is taken to be zero. Using the concept of a *moving* first or second order approximation to a general

G^x, curves of μ_i^x may be obtained from binary phase diagrams of two coexisting solution phases by substituting the regular solution model, $G^x = N_1N_2W_{12}$, or the subregular solution model, $G^x = N_1N_2(N_1W_{21} + N_2W_{12})$ into equations (10). Minimum and maximum values for the error envelope about μ_i^x are obtained by combination of reasonable errors in reading points of the phase diagram. A technique of curve smoothing within the error envelope in $N_i \geq .5$, combined with a Gibbs–Duhem integration in $N_i \leq .5$ results in curves for μ_i^x that are smooth and continuous in $0 \leq N_i \leq 1$ but the curves are not constrained to the shapes of regular solution or subregular solution model μ_i^x curves. When two phases A and B form by unmixing of a single phase, the above scheme can again be used with the additional restrictions of

$$\mu_{iA}^o = \mu_{iB}^o, \qquad a_{iA} = a_{iB} \tag{11}$$

(Kern and Weisbrod 1967) and $\Delta H_{iBA}^o = 0$ for $T_i^o \neq 0$. One additional assumption that may be made with two immiscible phases is that W_{ij} is the same for both phases, and the equations that result for generating μ_i^x curves for both models have already been developed (Kern and Weisbrod 1967; Thompson 1967; Thompson and Waldbaum 1969b).

COMPUTER CALCULATION OF PHASE EQUILIBRIA

A Fortran IV computer program GAPMIS has been designed, at a specified temperature, to find by elimination, two areas A and B in a ternary such that there *exists* activities a_i so that

$$a_i \text{ (in area } A) = a_i \text{ (in area } B)$$

$$\text{for components } i = 1, 2, 3.$$

These two areas are then reduced in size until activity matching has been demonstrated for two parallelograms of .005 mole fraction size, with the resulting tie-line joining them. Isotherms are mapped out by moving the initial search areas A and B at each specified temperature. The data for calculating the ternary activities in the areas are derived using G_{ij}^x data for the appropriate phase from the associated binary phase diagrams, combined with (6) and $a_i = N_i \exp(\mu_i^x/RT)$. The actual input format of the G_{ij}^x data used by GAPMIS is the two curves, μ_i^x, μ_j^x, fitted in several parabolic segments. It is necessary, for calculations of solution crystal-liquid type equilibria, to refer activities in the crystal to a fused state at the same composition and temperature using (10), before activities may be matched with the coexisting liquid phase at the same temperature. Strictly binary solid solution phases require activity matching for only the two components in the crystalline phase. Equilibria involving two immiscible phases, either solid or liquid, are governed by (11) and activity matching of the necessary components. Simple eutectic liquidus temperatures are calculated using a rearrangement of (8)

$$T = -T_i^{\circ} \frac{(u_i^x + \Delta H_i^{\circ})}{(RT_i^{\circ} \ln N_i - \Delta H_i^{\circ})} \tag{12}$$

with isotherms being hand contoured. The general procedures may be extended to quaternary systems with activity matching in parallelpiped volumes. Isotherms for a simple eutectic liquidus would better be determined by activity matching between liquid and fused pure crystal than by (12) with hand contouring.

GENERAL TERNARY RESULTS AND SUGGESTIONS

Repeatedly it was found that the predominant sign of the three binary G_{ij}^x's was the same as the predominant sign of calculated minus experimental liquidus temperatures. This is consistent with a three-component matrix reducing the strength of two-component interactions, the result being that the calculated *absolute* values of an n-component G^x are too large. Since the sign of excess entropy need not be the same as the sign of G^x, this consistency of sign also suggests that excess entropy considerations (outside of the general G^x model used here) are of secondary importance to the three component matrix effect. Corrections to *ideality* assume the form of $G(real) = G(ideal) + G^x(excess)$ and $\mu_i(real) = \mu_i(ideal) + \mu_i^x(excess)$, so that an empirical correction to a predicted n-component *non-ideality* should take the form of

$$G(real) = G(ideal) + G^x(excess) + G^k(correction) \text{ and}$$

$$\mu_i(real) = \mu_i(ideal) + \mu_i^x(excess) + \mu_i^k(correction). \tag{13}$$

There are several constraints which μ_i^k and G_i^k must satisfy, such as

(a) both G^k and μ^k must approach zero towards any binary,
(b) G^k should have at least n-independent parameters so that in the case of an $(n + 1)$ phase point, the n-liquidus surfaces may be adjusted independently to the experimental eutectic temperature and composition,
(c) the sign of the parameters should reflect the sign of the correction due to the n-component matrix effect mentioned above.

One empirical model for G^k which satisfies these restrictions is

$$G^k = \left[\prod_{i=1}^{n}\prod_{j>i}^{n}(1 - N_i - N_j)\right]\sum_{i=1}^{n} N_iK_i \qquad (14)$$

with the resulting expression for μ_i^k, linear in K_i,

$$\mu_i^k = L\left[(xs - xs_i)\sum_{j=1}^{n} N_jK_j + K_iN_i\right] \qquad (15)$$

where

$$L = \prod_{k=1}^{n}\prod_{j>k}^{n}(1 - N_k - N_j), \qquad xs = \sum_{k=1}^{n}\sum_{j>k}^{n}\frac{(N_k + N_j)}{(1 - N_k - N_j)}$$

both independent of choice of component i, and

$$xs_i = (N_i + 1)\sum_{j\neq i}^{n}\frac{1}{(1 - N_i - N_j)},$$

dependent on choice of component i. The points used in calculating K_i are arbitrarily chosen as invariant points or points on univariant curves: the data required are temperature, composition of liquid and the composition of the coexisting solid solution phase, and these are used in conjunction with equations (15), (13), and (9). Since compositions of small crystals are difficult to determine, melting experiments are more suitable than crystallization experiments. The preliminary calculated results can be used to guide the placing of the few required experimental runs. If the compositions of the solid solution phases are not known then more liquidus points on the cotectic are required and it becomes difficult to solve for K_i.

CONCLUSIONS

The calculated systems quartz-fayalite-leucite, diopside-albite-anorthite, and quartz-albite-orthoclase are shown in Figures 1, 2, and 4. The sources of liquidus-solidus data for these systems are presented in Table 1. Molecular weights and heats of fusion are from Waldbaum and Robie (1968), except the heat of fusion of leucite which was estimated to be 6770 cals/mole from the systems leucite-quartz and leucite-forsterite.

In the system quartz-fayalite-leucite, Figure 1, the calculated immiscibility fields are considerably larger than the experimental ones, a reflection of the three-component matrix effect mentioned previously. The minimum temperature of the internal immiscibility field is about 1090 ± 10°C in both cases. The calculated internal immiscibility field completely cuts across the field of crystallization of fayalite and

TABLE 1

SOURCES OF THERMODYNAMIC DATA

SYSTEM	SOURCE
quartz-fayalite-leucite	Roedder (1951)
diopside-albite-anorthite	Bowen (1928)
quartz-albite-orthoclase	J. Schairer in Levin et al. (1964) Fig. 786, Krauskopf (1967) fig. 14.1.
quartz-fayalite	Levin et al. (1964) 586, 682, 696
quartz-forsterite	Levin et al. (1964) fig. 598, 683, 803, Turner and Verhoogen (1960) page 126.
forsterite-leucite	Levin et al. (1964) fig. 803, 811
fayalite-leucite	μ_i^x from forsterite-leucite
leucite-quartz	Levin et al. (1964) fig. 412, 795, 803, Turner and Verhoogen (1960) page 107.
quartz-albite	Luth (1966-67)
quartz-orthoclase	Luth (1966-67)
orthoclase-anorthite	Levin et al. (1964) fig. 795, 799.
diopside-albite	Bowen (1928)
diopside-anorthite	Bowen (1928)
albite-orthoclase	Waldbaum and Thompson (1969) part IV
albite-anorthite	Deer et al. (1966)

encroaches 250°C into the field of leucite. Actually, the line orthoclase-fayalite crosses the immiscibility field between 1290 and 1320°C and is cut by the immiscibility tie-lines in this area. This means that a critically undersaturated liquid below the line orthoclase-fayalite could exsolve a liquid above the line which would eventually fractionate to free quartz, orthoclase and fayalite. If a few more components were added it is entirely possible that this trend of immiscibility could occur in systems close to natural rock systems. Philpotts (1970) has recently found field evidence that liquids of quartz syenite composition show immiscibility phenomena with liquids of feldspathoidal basalt composition in the Monteregian province of Quebec.

The shape of the calculated internal immiscibility field is quite irregular although smooth. Now it is reasonable that an immiscibility field should be elongated or stretched towards binary compositions that support the liquid structures causing immiscibility, and if there are three such structures then an irregular immiscibility field would

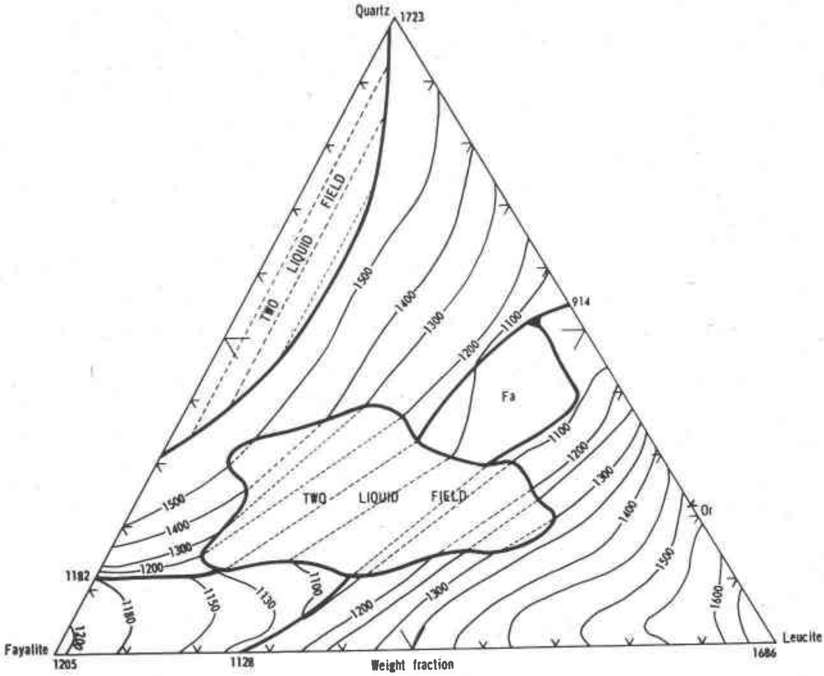

FIG. 1. Low temperature liquid immiscibility field calculated in quartz-fayalite-leucite

result, with the additional possibility of a three liquid field occurring if the non-ideality is large enough. There are at least three common well defined crystalline silicate structures, and the evidence suggests that upon melting these structures locally persist up to high temperatures (Porai-Koshits, 1953–1963). Ternary immiscibility fields are inevitably shown with smooth regular isotherms and liquidus intersections but perhaps this is assumed rather than proven experimentally (see McTaggart in Levin *et al.*, 1964, Figure 783).

Alkemade's rule (Levin *et al.*, 1964) of maximum temperatures along a binary join is violated by the liquidus surfaces of fayalite and leucite as they approach the binary fayalite-leucite. Consider the sources of the data for this binary: ΔH°_{leu} is estimated from the liquidus surfaces in quartz-leucite and forsterite-leucite, and μ^{x}_{leu}, μ^{x}_{Fa} for fayalite-leucite are assumed to be the same as for μ^{x}_{Fo}, μ^{x}_{leu} from forsterite-leucite. Both of these sources are open to question, but as there is no published data on ΔH°_{leu} or the binary liquidus in fayalite-leucite, the assumptions

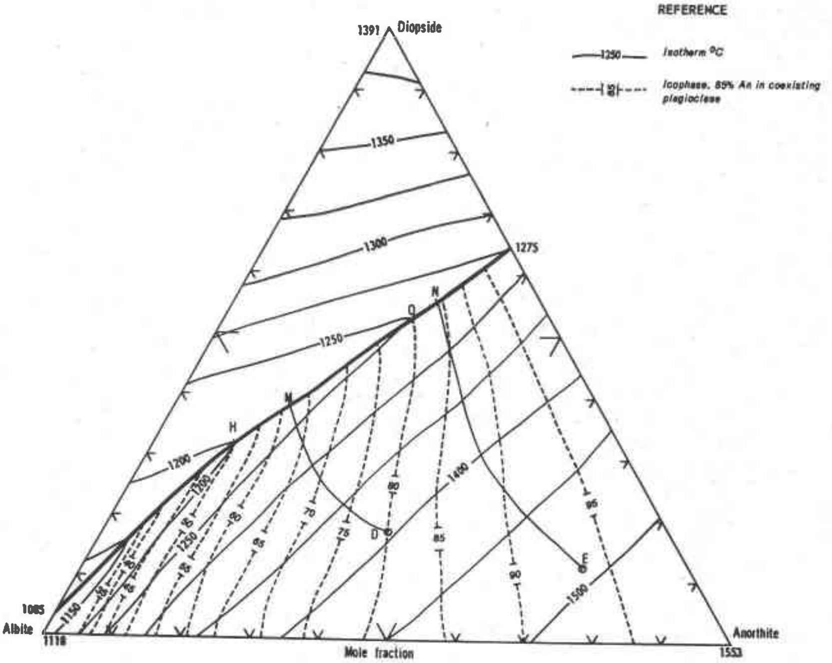

FIG. 2. Liquidus surfaces and plagioclase icophases calculated in diopside-albite-anorthite

are necessary, and the calculated results must be of a preliminary nature.

The calculated system diopside-albite-anorthite, Figure 2, compares very well with Bowen's (1928) experimental results, Figure 3. In general the ternary liquidus calculated is high by 2–15°C with an average of 8°C. Bowen's paths for the equilibrium crystallization of liquids D and E permit the checking of temperatures and crystal compositions calculated from a similar path mapped out using Figure 2. Table 2 shows the correspondence, with data source 3 resulting from carefully plotting Bowen's quoted compositions on his diagram and interpolating temperatures using the isotherms. In four cases this changed temperatures by as much as 4–5°C. The compositions of crystals at H and O are fixed by the bulk composition only, so here the temperatures are the things to compare. The exercise in working out a crystallizing path using the isocons of the coexisting plagioclase immediately indicates the usefulness of the isocons. Further details are provided in another paper to be published, but in general it can be stated that any type of crystallization path may be constructed easily and quickly using the isocons. Much important information can be obtained from these paths, but they can only be defined by extensive crystallization experimentation or by the simpler use of the isocons. Therefore a new term for this type of contour is proposed. The contours are lines on the liquidus of constant composition of the coexisting solid solution phase. The term suggested is *icophase,* short for isocophase, with *i* for equal composition and *cophase* for the coexisting phase. As a suggestion it would be worthwhile if simplified systems of geological importance were redone experimentally with the purpose of obtaining icophases of the main minerals that are solid solutions. The solvus of feldspars in An-Or-Ab would require two sets of icophases as the solid solution is ternary. Graphical construction of crystallization paths may be replaced by computer if the information contained in the icophases is fitted to an analytical function of the liquid composition.

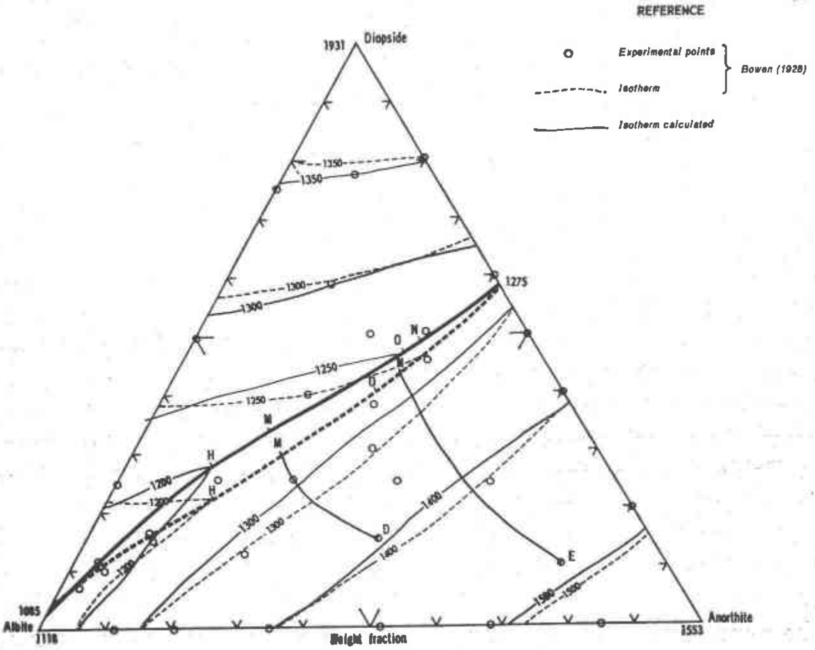

Fig. 3. Comparison of calculated and experimental liquids surfaces and cooling paths in diopside-albite-anorthite

The calculations done on the granite system, Figure 4, yield slightly higher temperatures than the experimental results. Table 3 shows the results at the ternary minimum. The quoted accuracy of the binary eutectic in quartz-orthoclase is 990 ± 20°C so that the ternary minimum might only be depressed one or two degrees below the eutectic in quartz-orthoclase. If the experimental ternary minimum is accurate, the calculations would suggest that the eutectic in quartz-orthoclase is near 982°C. One important fact shown by the calculated icophases in Figure 4 is that the compositions of the coexisting alkali feldspars change quite rapidly in the region of the minimum, especially on the cotectic line towards albite. A change along the cotectic of 10 percent Ab in the liquid changes the composition of the coexisting feldspar by as much as 25 percent Or. A strange thing also happens if liquids close to Or are fractionally crystallized, for it appears to be possible for the coexisting crystal to first get poorer in Or, but then as the liquid swings and approaches the minimum from Ab, the crystal will then increase in Or: the same composition of alkali feldspar can crystallize at two different temperatures along the same crystallization path. It would be interesting to see if this could be demonstrated in the field.

TABLE 2

EQUILIBRIUM CRYSTALLIZATION IN

DIOPSIDE-ALBITE-ANORTHITE

MOLE PERCENT VARIATION IN PLAGIOCLASE

source data	liquid	mole % Dio/Ab/An	first crystal		first diopside		last liquid	
			T	X	T	X	T	X
1	D	18	D 1375	80	M 1216	66	H 1200	50
2	D	41	D 1385	80	M 1215	62	H 1200	50
3	D	41	D 1380	80	M 1220	66	H 1200	50
1	E	13	E 1480	95	N 1245	85	O 1237	82
2	E	16	E 1480	94	N 1255	84	O 1251	82
3	E	71	E 1480	95	N 1249	85	O 1241	82

SOURCES 1: Bowen (1928), 2: calculated, 3: Bowen (1928)

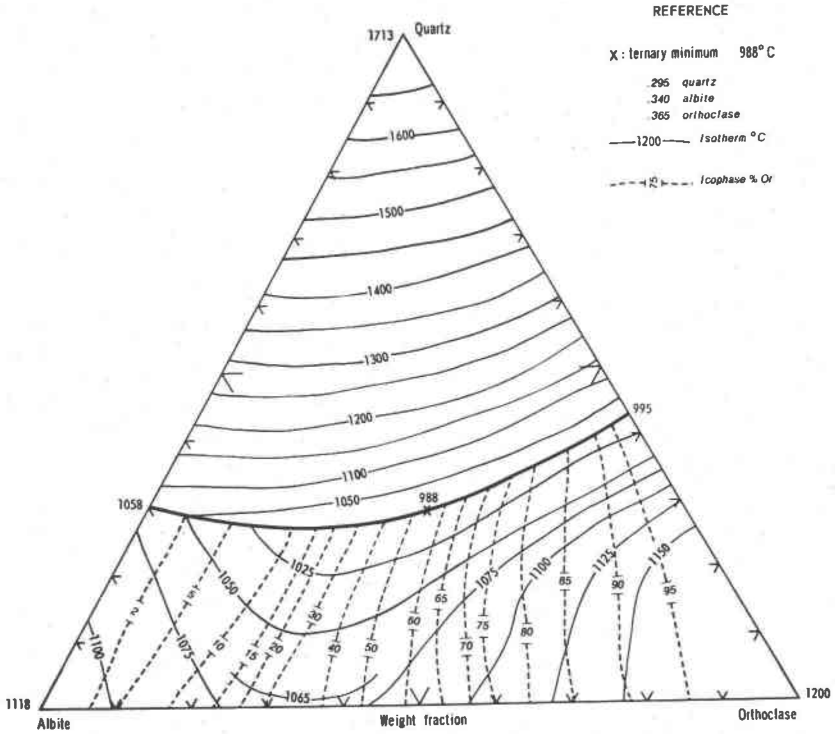

FIG. 4. Liquidus surfaces and alkali-feldspar icophases calculated in the granite system.

TABLE 3

TERNARY MINIMUM IN THE GRANITE SYSTEM

Source	Composition Weight Percent Qtz	 Ab	 Or	Temperature °cent
Calculated	29.5	34.0	36.5	988
Experiment	35.0	27.0	38.0	975 *

* Krauskopf (1967)

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