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MARKOVIAN GRAIN RELATIONSHIPS OF A GRENVILLE GRANULITE

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ABSTRACT. An exhaustive series of tests proves that the sequences of mineral-grain transitions along linear traverses across two mutually perpendicular sets of serial sections of a Grenville calc-silicate granulite possess the Markov property. The component amphibole, scapolite, and pyroxene are non-randomly spatially distributed, and grains of the same mineral are in contact less frequently than would be expected if randomly sited. Analogous relationships in granites were claimed by Vistelius and coworkers to reflect crystallization from a melt. The significance of the Markovian grain sequences in these metasedimentary rocks is assessed briefly.

INTRODUCTION

Vistelius and coworkers (for example, Vistelius, 1966, 1972; Vistelius and Faas, 1972; Vistelius and Romanova, 1972) made the important discovery that grain transitions along linear traverses of many granitic rocks possess the Markov property.[1] They assumed that "ideal" granite is a primary crystallization product of a melt and that Tuttle and Bowen's (1958) experimental studies permit prediction of the probable distribution of grains in natural granites. Their theoretical conclusion was that grain sequences along linear traverses through such "ideal" granites would be expected to form a Markov chain, and this contention was supported by finding that grain sequences in arbitrarily cut thin sections of most granitic rocks form Markov chains. Whitten and Dacey (1975) reviewed Vistelius and coworkers' published results and evaluated many of the characteristics, constraints, and complications of the Markov-chain model as applied to mineral-grain transitions of granitic rocks. Whitten and Dacey rejected Vistelius and coworkers' petrogenic justification of the Markov property and concluded that the property reflects petrologically important, but unidentified, factors. They speculated that the Markovian property may be shared by other igneous and metamorphic rocks, and that fundamental characteristics of the kinetics of nucleation and crystallization of silicates from magmas and in the solid state may dictate that the grain sequences have the Markovian property. Whitten and Dacey concluded that the subset of all igneous, metamorphic, and sedimentary rocks that have the Markov property should be identified as an aid in discerning the genetic significance of the attribute.

Numerous granites have been shown to have the Markovian property by Vistelius and coworkers and by Moore (ms); Sanderson (1974) also described the nonrandom distribution of magnetite in the felsic Melrose Stock, Nevada. For comparison, it seemed desirable to analyze a high-grade metamorphic rock. The spatial distribution of grains in meta-

[1] As originally defined, the Markov property referred to events that were controlled by earlier events, but, in the present context, it relates to observed mineral grains that are controlled by the composition of adjacent grains in a rock.

morphic rocks was studied by Kretz (1969) and Flinn (1969), but they drew strikingly different conclusions. Kretz made an extremely detailed statistical analysis of a single thin section of a Grenville calc-silicate granulite. He noted slight modal variations across the thin section but found that, within a homogeneous portion of it, crystals of pyroxene, scapolite, and sphene are randomly distributed; also, sphene crystals are not preferentially associated with pyroxene or scapolite grains. Kretz (1969, p. 39) concluded that ". . . each site of mineral nucleation was apparently located at random and with complete disregard for other crystals in the immediate vicinity." Flinn (1969) analyzed a quartz–oligoclase–biotite–muscovite permeation gneiss from the Colla Firth permeation belt of Shetland and some Siberian Archean granulites (from the Aldanski Shield, southern Yakutia) containing assemblages of plagioclase, K-feldspar, biotite, apatite, opaque ores, hornblende, quartz, and augitic clinopyroxene. He concluded that the grains are not distributed at random in these rocks. Flinn (1969, p. 363-364) also suggested that the thin section studied by Kretz ". . . is probably a non-random distribution but the test he used was not powerful enough to recognize this fact. . . . It is possible that the collection of more data (I noted four times as many grain contacts per section as Kretz did) would have led Kretz to the rejection of the null hypothesis."

Kretz (1969, p. 58-59) referred to the possibility of Markovian grain sequences, but neither he nor Flinn (1969) pursued the topic. The texture of the high-grade granulite studied by Kretz makes it an ideal subject for grain-transition probability studies. In this paper, it is demonstrated that new samples of this rock examined by us provide evidence favorable to the Markov-chain hypothesis. The implications of this discovery are assessed briefly.

MODE OF ANALYSIS

Professor Ralph Kretz kindly supplied us with a hand sample (specimen L12-57) of the calc-silicate granulite (from the Grenville terrain some 130 km northwest of Ottawa, Ontario, Canada) used for his paper (Kretz, 1969). The rock lacks any obvious schistosity and shows only very faint compositional banding in hand specimen, although such banding is more apparent in thin sections (pls. 1 and 2). The results discussed in this paper are based on analysis of nine of our sixteen thin sections. The major mineral phases are calcic pyroxene, scapolite, and calcic amphibole; accessory sphene, apatite, and zircon are easily recognized. Although Kretz's slide contained only some four percent amphibole, grains of the major phases are about equally abundant in most of our material.

A method described in detail by Vistelius and Romanova (1972) and Whitten and Dacey (1975) was used to develop, from the sequence of mineral grains along parallel linear traverses, a transition-probability matrix for each thin section. The important aspects of this construction are summarized:

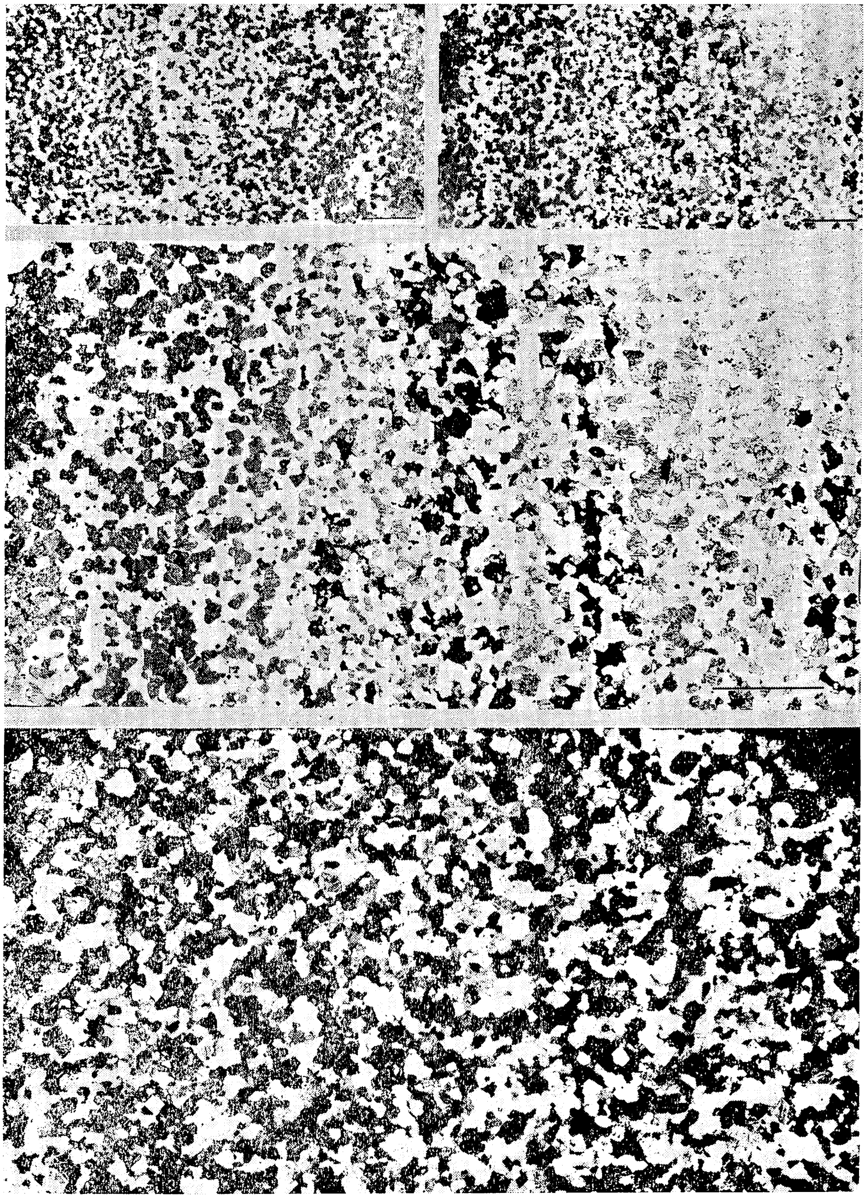
1. The parallel traverses are spaced, so that no grain is crossed by more than one traverse.

PLATE 1

A. B.

C.

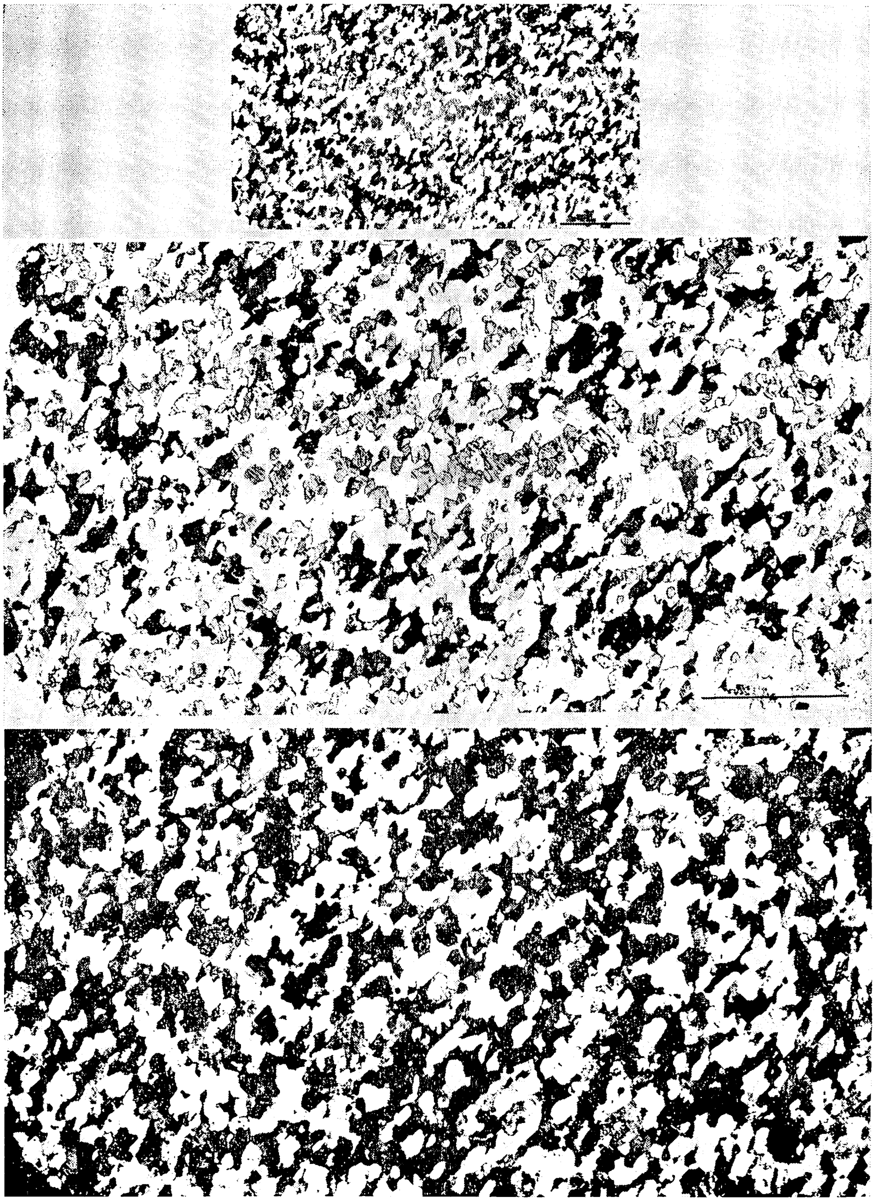
D.



Composition, texture, and grain-size variation of two slides in set A (Grenville calc-silicate granulite comprising calcic pyroxene, scapolite, and calcic amphibole); scale bar is 0.5 cm.

A: slide 1. B, C, and D: slide 2 (C and D are same field which is enlargement of B). A, B, and C photographed with polarizers at about 10 degrees from parallelism so that amphibole is mainly black, pyroxene gray, and scapolite colorless. D photographed with polarizers at about 10 degrees from perpendicularity.

PLATE 2



A.

B.

C.

Composition, texture, and grain-size variation of slide 6 (set B); scale bar is 0.5 cm. A and B photographed with polarizers at about 10 degrees from parallelism, and C with polarizers about 10 degrees from perpendicularity; each figure shows the same field.

2. A transition sequence of mineral grains along a traverse is terminated by accessory components, a hole, or the edge of the thin section. The length of a sequence is the number of mineral grains traversed.

3. A one-step transition-tally matrix T is constructed in which the (i, j) entry gives the number, $t\ (i, j)$, of times that a grain of type j immediately follows a grain of type i; for this purpose, both grains must belong to the same transition sequence.

4. A one-step transition-probability matrix P and a fixed probability vector Q are constructed from T. (Note, that, if there are m mineral grains labelled 1 through m, the (i, j) entry of P is

$$p(i, j) = t(i, j) \Big/ \sum_{i=1}^{m} t(i, j),$$

and the j-th entry of Q is

$$q(j) = \sum_{i=1}^{m} t(i, j) \Big/ \sum_{i=1}^{m} \sum_{j=1}^{m} t(i, j).$$

Moreover, the last double sum is the number N of one-step transitions obtained from all traverses.)

5. Additionally, tally matrices, probability matrices, and probability vectors may be constructed for two-step, three-step, and, more generally, r-step transitions, which for $r > 1$ are denoted by T_r, P_r, and Q_r. Procedures for these constructions were given by Whitten and Dacey (1975).

The data of P_r and Q_r are used to evaluate the hypothesis that the mineral-grain sequences form an r-th order Markov chain against the alternative hypothesis that they form an (r-1)-st order Markov chain. In an r-th order Markov chain with $r \geqslant 1$, the mineral phase of each grain on a traverse depends on the mineral phases of the preceding r grains and does not depend on the preceding grains. A 0-th order chain is a sequence of independent grains in which the mineral type of any n-th grain is not influenced in any way by some or all preceding mineral grains. A 0-th order chain is indicative of a random distribution of mineral types along the traverse in which each grain of the aggregate is of type j with probability $q(j)$.

The tally matrices were based on sequences of mineral grains comprising only amphibole, scapolite, and pyroxene. Whitten and Dacey (1975), following Vistelius and coworkers, recommended that the matrices be constructed from all sequences of length 10 or more. However, in the present work, because many sequences that satisfied this bound were too short to be used with statistical tests, tally matrices were constructed only from sequences of length 35 or more. This change facilitates statistical analysis, and, although the number of transitions is substantially reduced, it has only minor effects on the conclusions, as will be shown subsequently.

ANALYSES

Nine thin sections comprising two, mutually perpendicular sets (A and B) of serial sections were used for definitive analyses; each set was cut approximately normal to the faint compositional banding. Set A comprises slides 1 to 4, and set B comprises slides 5 to 9; slide labelling permitted the direction of tally counting to be controlled.

The observed sequences of mineral grains along traverses perpendicular to the mineralogical banding were recorded. Accurate data for these granulites are much easier to obtain than for granitoid rocks because (1) the grains are more equidimensional and rarely, if ever, appear twice in the same sequence (see pls. 1 and 2), and (2) discriminating between subparallel contiguous grains is rarely a problem (as it is with, say, oligoclase).

Observations from sequences of length 35 or more comprise our basic data for examining the hypothesis that grain sequences form Markov chains, and when they exist, for identifying their properties. This hypothesis is evaluated by a procedure, described by Whitten and Dacey (1975), that uses the transition-probability matrices P_r to identify the lowest-order Markov chain (provided one exists) consistent with the sequence of minerals. The strategy is first to evaluate the hypothesis of a first-order chain against the alternative of a zero-order chain. If this hypothesis is rejected in favor of the alternative, the evidence suggests that the mineral sequences are independent and do not constitute a Markov chain (except as a degenerate form). If the alternative is rejected, then the hypothesis of a second-order chain is evaluated against the alternative hypothesis of a first-order chain. Successively, the hypothesis of an $(r+1)$-st order chain is tested against the alternative of an r-th order Markov chain, until the hypothesis is rejected for some value of r, or until there are insufficient data to continue the tests. Rejection of the $(r+1)$-st order chain indicates that the data support the hypothesis that the mineral sequences are adequately represented by a chain of r-th order. A *chi*-square test is used as an objective criterion for evaluating each hypothesis (Whitten and Dacey, 1975).

Chi-square values (table 1), calculated with a computer program adapted from Krumbein (1967), indicate that all five slides in set B may be represented by first-order Markov chains, although for slide 9 the evidence is ambiguous. The evidence is not consistent for the four slides of set A, because slide 1 and, possibly, slide 3 may be represented by first-order Markov chains and the other slides by second-order Markov chains.

As noted by Whitten and Dacey (1975), an inherent assumption of this series of tests is that the sequences derived from a thin section are homogeneous in the sense that all the grain transitions are described by a common transition-probability matrix. The validity of this assumption is checked for grain sequences that may be represented as first-order Markov chains by use of the *chi*-square statistic identified in appendix 1 to Whitten and Dacey (1975). The calculated values in table 2 are all less

TABLE 1

Calculated and tabulated *chi*-square values for tests for order of Markov chain

Hypothesis: The observed sequences form an $(r+1)$-st order chain
Alternative hypothesis: The observed sequences form an r-th order chain

Set	A				B					Tabulated values		
	Calculated values											
Slide	1*	2	3	4	5	6	7	8	9	Degrees of freedom	95% level	99% level
Number of Transitions	276	410	383	538	442	444	477	561	765			
Order r of chain												
0	31.4	51.4	29.2	45.6	50.2	17.1	36.5	28.4	48.7	4	9.5	13.3
1	19.5	35.6	21.6	41.5	17.6	14.3	18.4	19.8	23.1	12	21.0	26.2
2	29.7	45.5	43.3	47.6	—	—	—	—	49.2	36	51.0	58.6

* Transition sequences of length 30 or more were used for this slide only, because the lower limit of 35 eliminated nearly all transitions.

TABLE 2
Calculated and tabulated *chi*-square values for tests of homogeneity of sequences within slides

Slide	Calculated values	Degrees of freedom	Tabulated values 95% level	Tabulated values 99% level
1	44.4	42	57.96	66.36
2*	38.9	42	57.96	66.36
3	52.4	54	71.82	81.00
4*	46.9	48	59.84	73.44
5	26.6	48	59.84	73.44
6	40.3	36	50.76	58.68
7	36.9	48	59.84	73.44
8	51.8	42	57.96	66.36
9	60.8	54	71.82	81.00

* Slides having sequences that do not form first-order Markov chains.

than the corresponding tabulated χ^2 values, and this indicates that the sequences of one-step transitions comprising each of the seven slides can be considered homogeneous. Since the results in table 1 suggest that slides 2 and 4 form second-order Markov chains, the appropriate test of homogeneity for these slides uses second-order transition matrices; such tests were not conducted.

This set of tests provides persuasive, though certainly not conclusive, evidence that the sequences of mineral phases in all the thin sections are Markov chains. The chains are not identical, but are first-order Markov chains for slides 1, 3, and 5 to 9, and are second-order Markov chains for slides 2 and 4. This conclusion is not consistent with the finding of Kretz (1969) that grain types are randomly distributed through the rock but does support the claim of Flinn (1969) of a nonrandom distribution. It also is not consistent with the theory and empirical analyses of Vistelius for granitic rocks. His results indicated that sequences of mineral grains in granitic rocks form Markov chains, and, though the order and other features of these chains may vary from rock to rock, the sequences observed in an individual rock sample form a single type of Markov chain.

ADDITIONAL ANALYSIS OF MARKOV CHAINS

The estimated transition probabilities for the sequences of mineral phases are given by $P = P_1$ for first-order chains and by P_2 for second-order chains. However, the one-step transition matrices P provide useful information even for second-order chains, and table 3 gives P and Q for each of our nine slides.

Each $q(j)$ is an estimate of the frequency of occurrence of mineral phase j and, thereby, is an estimate of the probability that each grain is mineral j. In Markov chains, the occurrence of a mineral is conditioned by one or more preceding grains so that composition of $p(i, j)$ and $q(j)$ indicates if the occurrence of phase i increases, decreases, or does not alter the estimate of the probability that the next grain is j. Table 4 indicates for each slide if $p(i, j)$ is greater than, less than, or equal to $q(j)$, for all i, j pairs. This evidence strongly supports the conclusion that occurrence of a mineral type decreases the probability that the next grain in a sequence is of the same type and increases the probability that it is either of the other two types. This conclusion conflicts with Kretz's finding that mineral grains have a random distribution and indicates a structure in which, relative to a random distribution, adjacent grains are more likely to be of different, rather than of similar, composition.

A Markov chain is reversible if, when viewed in the reverse direction, the sequence is also a Markov chain. This is a desirable property of mineral sequences, for it implies that the existence of a chain is not a consequence of the direction in which the traverses are traced. It is known

TABLE 3

Estimated probabilities P and Q for the nine slides

Slide 1 ($N = 276$)				Slide 2 ($N = 410$)				Slide 3 ($N = 383$)			
	P		Q		P		Q		P		Q
0.05	0.55	0.41	0.08	0.08	0.42	0.50	0.16	0.16	0.30	0.55	0.11
0.09	0.41	0.50	0.54	0.12	0.35	0.52	0.45	0.08	0.42	0.50	0.48
0.08	0.74	0.18	0.37	0.23	0.58	0.18	0.39	0.13	0.62	0.26	0.41
Slide 4 ($N = 538$)				Slide 5 ($N = 442$)				Slide 6 ($N = 444$)			
	P		Q		P		Q		P		Q
0.14	0.47	0.39	0.22	0.16	0.51	0.33	0.26	0.22	0.47	0.30	0.25
0.22	0.32	0.45	0.43	0.34	0.25	0.41	0.42	0.24	0.40	0.36	0.46
0.28	0.55	0.17	0.34	0.25	0.58	0.17	0.31	0.29	0.55	0.16	0.29
Slide 7 ($N = 477$)				Slide 8 ($N = 561$)				Slide 9 ($N = 765$)			
	P		Q		P		Q		P		Q
0.17	0.47	0.36	0.24	0.17	0.52	0.31	0.29	0.18	0.51	0.31	0.29
0.24	0.36	0.41	0.45	0.31	0.40	0.29	0.46	0.30	0.42	0.28	0.47
0.29	0.57	0.14	0.31	0.37	0.49	0.14	0.26	0.38	0.53	0.09	0.24

Note: Mineral types (states) 1, 2, and 3 for each slide are, respectively, amphibole, scapolite, and pyroxene. N = number of transitions.

TABLE 4

Comparisons of $p(i, j)$ and $q(j)$

	Slides								
Differences	1	2	3	4	5	6	7	8	9
$p(1, 1) - q(1)$	—	—	+	—	—	—	—	—	—
$p(2, 2) - q(2)$	—	—	—	—	—	—	—	—	—
$p(3, 3) - q(3)$	—	—	—	—	—	—	—	—	—
$p(1, 2) - q(2)$	+	—	—	+	+	+	+	+	+
$p(2, 1) - q(1)$	+	—	—	0	+	—	0	+	+
$p(1, 3) - q(3)$	+	+	+	+	+	+	+	+	+
$p(3, 1) - q(1)$	0	+	+	+	—	+	+	+	+
$p(2, 3) - q(3)$	+	+	+	+	+	+	+	+	+
$\mathrm{p}(3, 2) - q(2)$	+	+	+	+	+	+	+	+	+

Notes:

+ indicates that $p(i, j) > q(j)$.

— indicates that $p(i, j) < q(j)$.

0 indicates that $p(i, j) = q(j)$ to two decimal places.

(Kemeny and Snell, 1960, p. 105) that a first-order chain is reversible if for all i, j pairs, $i \neq j$,

$$p(i, j) = q(j)p(j, i)/q(i). \tag{1}$$

The implementation of this test presumes that the transition probabilities are known precisely. However, it is reasonable to treat the transition probabilities of p_r as sample estimates obtained from a particular set of traverses on a particular small piece of a larger rock specimen. For sample estimates, the identity of equation (1) is replaced by $p(i, j)$ belonging to an interval $(q(j)p(j, i)/q(i) - l_1, q(j)p(j, i)/q(j) + l_2)$, where l_1 and l_2 are limits that reflect variability attributable to sampling variation. We know of no study that obtains these limits or suitable approximations. As a consequence, our test for reversibility relied on subjective comparison of $p(i, j)$ and $q(j)p(j, i)/q(i)$ for all pairs of minerals in those slides approximated by first-order chains. Typically, the differences are of the magnitude 0.02 when $p(i, j)$ is of magnitude 0.4, and the maximum difference is 0.07. Table 5 shows the comparison of both sides of equation (1) for the seven slides having first-order Markov chains; the differences are not considered significant, and we conclude tentatively that all these chains are reversible. The two second-order chains (slides 2 and 4) were not tested directly for reversibility, but there is no reason to anticipate that they would not pass our informal test.

All these chains are ergodic in that P_1 (for first-order chains) or P_2 (for second-order chains) has no zero entries. Since P_1 for each slide has no zero entries, each chain is also regular in the sense that there are no periodic cycles of mineral phases along the traverses.

The preceding tests underlie our conclusion that the sequences of mineral phases on each thin section of the analyzed Grenville calc-silicate

TABLE 5

Results of reversibility tests on each slide

Set		A		B				
Slide		1	3	5	6	7	8	9
Minerals i	j							
amphibole	scapolite	0.55* (0.61)	0.30 (0.35)	0.51 (0.55)	0.47 (0.44)	0.47 (0.45)	0.52 (0.49)	0.51 (0.49)
amphibole	pyroxene	0.41 (0.37)	0.55 (0.48)	0.33 (0.30)	0.30 (0.34)	0.36 (0.37)	0.31 (0.33)	0.31 (0.31)
scapolite	amphibole	0.50 (0.51)	0.50 (0.53)	0.41 (0.43)	0.36 (0.35)	0.41 (0.39)	0.29 (0.28)	0.28 (0.27)
scapolite	pyroxene	0.09 (0.08)	0.08 (0.07)	0.34 (0.32)	0.24 (0.26)	0.24 (0.25)	0.31 (0.33)	0.30 (0.31)
pyroxene	amphibole	0.08 (0.09)	0.13 (0.15)	0.25 (0.28)	0.29 (0.26)	0.29 (0.28)	0.37 (0.35)	0.38 (0.37)
pyroxene	scapolite	0.74 (0.73)	0.62 (0.59)	0.58 (0.56)	0.55 (0.57)	0.57 (0.60)	0.49 (0.51)	0.53 (0.55)

* For each i, j the first entry is $p(i, j)$ and the second (in parentheses) is $q(j)p(j,i)/q(i)$.

granulite are adequately approximated by Markov chains that are of first- or second-order and that are homogeneous, ergodic, regular, and reversible. It is significant that these are the conditions that Vistelius and co-workers, as reported by Whitten and Dacey (1975), attributed to sequences of mineral phases in ideal granitic rocks. However, the conformity between properties of this granulite and Vistelius' findings is not complete. His theory specified, and his empirical data supported, that all chains observed for a rock sample are homogeneous and, thereby, of the same order. In contrast, the chains observed for this granulite are of two different orders and, thereby, are not homogeneous. However, it is shown next that the five slides comprising set B are homogeneous.

The homogeneity of slides in set B is shown in two ways. First, the sequences for each pair of slides were combined into a single transition-probability matrix P, which was used to test for homogeneity of the component sequences. Second, a single transition matrix P was estimated from the sequences for all five slides, and it was used to test for homogeneity of sequences in set B. Table 6 shows the results of these tests, which strongly indicate that the sequences in set B are homogeneous and are described by a single first-order Markov chain. The transition probabilities of this chain, table 7, are estimated from all sequences of length 35 or more from all five slides comprising set B. For an informal test of

TABLE 6

Homogeneity tests for slides comprising set B

Slides	Calculated *chi*-square value	Degrees of freedom	Tabulated *chi*-square value at 0.95 level
5 & 6	86.4	90	113.4
5 & 7	72.7	102	125.5
5 & 8	93.8	96	120.0
5 & 9	116.9	108	132.8
6 & 7	84.9	90	113.4
6 & 8	99.4	84	106.3
6 & 9	115.2	96	120.0
7 & 8	94.3	96	120.0
7 & 9	111.1	108	132.8
8 & 9	110.2	102	125.9
Set B	259.2	252	289.8

Notes

Degrees of freedom $= m\ (m - 1)\ (s - 1)$, where m is number of mineral types (here, 3), and s is the number of individual sequences of $\geqslant 35$ transitions in the two compared slides.

The test statistic is

$$X^2 = \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{h=1}^{s} n_i^{(h)}\, [p^{(h)}(i,j) - p(i,j)]^2 \cdot [\mathrm{p(i,j)}]^{-1} ,$$

where tally matrix $T^{(h)}$ is based on transitions in the h-th sequence only, $p^{(h)}(i,j)$ is an entry in the $P^{(h)}$ derived from $T^{(h)}$, and

$$n_i^{(h)} = \sum_{j=1}^{m} p^{(h)}(i,j)$$

reversibility, these probabilities are used in table 8 to compare both sides of equation (1). Similar tests were not conducted for the slides comprising set A because they have different orders of Markov chains.

The results in tables 1, 2, 6, and 8 constitute the evidence that the grain sequences of set B comprise a first-order Markov chain with the transition matrix given in table 7. However, this evidence does not include a direct test, similar to those summarized in table 1, of the order of Markov chain. Results of such a test (table 9) cause rejection of the hypothesis of a first-order Markov chain and support the alternative of a second-order chain. If this test is admitted as evidence, it must be concluded that the sequences in set B form a second-order Markov chain. Because it is difficult to reconcile this conclusion with all other evidence about set B, it is necessary to rationalize the inconsistency or to reject the validity of the test reported in table 9. There are substantial reasons for the latter alternative.

When sequences from homogeneous serial thin sections are combined, intuitively, it may seem that the standard test (as in table 9) is

TABLE 7

Probabilities estimated from sequences of all slides in set B*

	Matrix P Amphibole	Scapolite	Pyroxene	Vector Q
Amphibole	0.18	0.50	0.32	0.27
Scapolite	0.29	0.37	0.34	0.45
Pyroxene	0.32	0.54	0.14	0.28

*Total number of transitions = 2689.

TABLE 8

Data for assessing reversibility of Markov chain for sequences in set B

i	j	$p(i,j)$	$q(j)p(j,i)/q(i)$
Amphibole	Scapolite	0.50	0.48
Amphibole	Pyroxene	0.32	0.33
Scapolite	Amphibole	0.29	0.30
Scapolite	Pyroxene	0.34	0.34
Pyroxene	Amphibole	0.32	0.31
Pyroxene	Scapolite	0.54	0.55

TABLE 9

Calculated and tabulated *chi*-square values for tests of order of Markov chain for sequences in set B

Hypothesis: The observed sequences form an $(r+1)$-st order chain
Alternative hypothesis: The observed sequences form an r-th order chain

Order r of chain	Calculated *chi*-square values	Degrees of freedom	Tabulated *chi*-square values 95% level	99% level
0	151.9	4	9.5	13.3
1	46.1	12	21.0	26.2
2	38.9	36	51.0	58.6

appropriate for ascertaining the order of a Markov chain. This has been the accepted procedure in the work of Vistelius and coworkers. However, such combined sequences provide estimates of a three-dimensional (rather than a linear) array of grains, and the application and interpretation of tests requires special care. The available tests for order of Markov chain require sequences that are independent and identically distributed. The tests for homogeneity (tables 2 and 6) provide convincing evidence that the sequences are identically distributed. However, a statistical test for independence of the sequences is not available, and there is no direct empirical evidence to indicate that grains on parallel, closely spaced slides are independent; as a result, indirect evidence must be used. Because the sequences from each slide in set B form a Markov chain, it is not unlikely that the serial thin sections actually cut a pervasive (penetrative) structure and that, as a result, the sequences in each slide are not independent of those in the other slides. If this is true, the tests in table 9 are inappropriate; hence, we tentatively conclude that the mineral sequences from the five slides in set B are generated by a common first-order (not a second-order) Markov chain.

The arguments used to support this conclusion may lack internal consistency. We decided it is appropriate to test for order of chain for sequences on traverses distributed in two-dimensional space (parallel traverses on a thin section) but inappropriate to test sequences on traverses distributed in three-dimensional space (parallel thin sections comprising set B). This reflects our willingness to assume that a two-dimensional array of traverses on a single slide has a dependent structure sufficiently weak that no serious error results from use of a test requiring independent sequences, but that the dependent structure of a three-dimensional array is too strong to justify use of the same test. In fact, macroscopic reexamination of our thin sections shows that the impersistent mineralogical banding is more apparent in slides 2 and 4 (set A) than in any of the other slides. For each of these slides this fact may be correlated with (A) a significant lack of independence of the traverses and (B) the rejection of the first-order Markov chain hypothesis (table 1). This question is especially critical in the analysis of metamorphic rocks because they are almost always compositionally banded. Properly, the relevant decisions should be guided by theoretical and empirical knowledge, but currently this does not exist. In the course of future work, we hope to test the effects of varying degrees of dependence between traverses.

It seems probable that the analysis of arrays of traverses presents problems answerable only in terms of statistical models that pertain to three-dimensional grain distributions. A model of three-dimensional structure could be analyzed for properties of grain sequences on a single plane (thin section) or on an array of planes (serial sections). However, a Markov-chain model for a linear traverse cannot resolve questions involving two and three dimensions. This limitation is similar to that applying to a one-dimensional physico-chemical model developed by Vistelius and coworkers for the genesis of grains in an ideal granite (Whitten and

Dacey, 1975). We contend that models for both the physical and the statistical properties of grains in rocks must incorporate a space that is three dimensional. A model of potential utility is that of the Markov random field, which is a multidimensional extension of the Markov chain; a nonelementary introduction to this was provided by Spitzer (1971).

THE INFLUENCE OF SEQUENCE LENGTH AND INCLUSION OF SPHENE

The preceding analysis has been based on sequences of length 35 or more, though Whitten and Dacey (1975) followed the advice of Vistelius and coworkers and recommended use of all sequences of length 10 or more. Also, the analysis has been based on only amphibole, scapolite, and pyroxene, although Kretz (1969) analyzed a similar rock on the basis of the three "states" scapolite, pyroxene, and all other minerals. To illustrate the effect of using these different definitions, the probabilities for slides 2 and 6, estimated from all sequences of length 10 or more for amphibole, scapolite, and pyroxene (method I), and when amphibole or sphene are used instead of amphibole (method II) are cited in table 10.

Comparison of values for method I with the corresponding values in table 3 indicates that inclusion of sequences of intermediate lengths 10 to 34 has little effect on the P matrices and Q vectors. Similarly, table 10 shows that inclusion of sphene with amphibole has only a minor effect on the probabilities. The *chi*-square values for the test of order of Markov chain for the sequences defined by methods I and II (table 11) corroborate the conclusions based on the longer sequences. Additionally, tests for order of Markov chain for all nine slides (although only those for slides 2 and 6 are reproduced in table 11) confirm the similarity of the matrices and vectors based on the two sequence lengths. These results encouraged us to rely on sequences with 35 or more transitions for our analyses. From the petrogenetic view point, it is interesting that the spatial distribution of the major minerals in both the short and the long sequences is apparently similar.

CONCLUSIONS AND SIGNIFICANCE

Understanding and modelling the kinetics of nucleation and crystallization of igneous and metamorphic rock assemblages is of considerable importance. However, the basic data are lacking and difficult to obtain (compare Rast, 1965), and observations of direct relevance are scarce in the geological literature. In the meantime, numerous indirect approaches (including that described in this paper) are beginning to emerge. It is appropriate to refer briefly to recent work that impinges on the problem.

Swanson (1974) examined the effects of nucleation density and growth rate on crystal growth in synthetic granodiorite, and Gray (1974) evaluated the effect of rate of nucleation of plagioclase, clinopyroxene, and opaques on mineral-grain density per unit volume in some diabase dikes. Byerly and Vogel (1974) claimed (A) that grain-boundary-network changes during progressive regional metamorphism of impure marbles can be modelled in terms of growth of preexisting grains, changes in grain neighborhoods, and nucleation and growth of new grains or phases, and (B)

TABLE 10

Inclusion and exclusion of sphene for slides 2 and 6*

Method I

Slide 6 ($N = 931$):

	Matrix P: Amphibole	Matrix P: Scapolite	Matrix P: Pyroxene	Vector Q
Amphibole	0.09	0.43	0.48	0.15
Scapolite	0.12	0.36	0.52	0.46
Pyroxene	0.19	0.59	0.22	0.39

Slide 6 ($N = 923$):

	Matrix P: Amphibole	Matrix P: Scapolite	Matrix P: Pyroxene	Vector Q
Amphibole	0.21	0.49	0.30	0.29
Scapolite	0.30	0.37	0.33	0.45
Pyroxene	0.35	0.55	0.10	0.26

Method II

Slide 2 ($N = 1130$):

	Matrix P: Amphibole or sphene	Matrix P: Scapolite	Matrix P: Pyroxene	Vector Q
Amphibole or sphene	0.08	0.47	0.45	0.17
Scapolite	0.15	0.35	0.51	0.45
Pyroxene	0.22	0.56	0.22	0.39

Slide 6 ($N = 945$):

	Matrix P: Amphibole or sphene	Matrix P: Scapolite	Matrix P: Pyroxene	Vector Q
Amphibole or sphene	0.23	0.47	0.30	0.30
Scapolite	0.31	0.36	0.33	0.44
Pyroxene	0.36	0.54	0.10	0.26

* These P matrices and Q vectors are based on all sequences of 10 or more transitions; N is the total number of transitions included.

TABLE 11

Chi-square values for tests of order of Markov chains for sequences summarized in table 9

Hypothesis: The observed sequences form an $(r+1)$ order chain
Alternative hypothesis: The observed sequences form an r-th order chain

	Calculated *chi*-square values Method I		Calculated *chi*-square values Method II		Degrees of freedom	Tabulated *chi*-square values 95% level	Tabulated *chi*-square values 99% level
Slide	2	6	2	6			
Order r of chain							
0	86.2	58.6	103.1	59.1	4	9.5	13.3
1	56.6	20.4	45.5	19.2	12	21.0	26.2
2	43.8	—	49.9	—	36	51.9	58.7

that data on such networks can be analyzed as input for stochastic models of grain-transition probabilities. Of particular importance was Kretz's (1973, 1974) detailed study of methods of extracting information on the kinetics of crystallization from actual rocks. Kretz (1973) showed that, in metasedimentary rocks of the Yellowknife Group, Canada, compositional profiles in garnets of different sizes permit evaluation of the rate of crystal growth and that the form of the crystal-size distribution yields an expression for the rate of nucleation. These expressions led to an equation for the garnet-producing reaction rate. Kretz (1973, p. 19) concluded that (A) garnet crystals were constantly being created during the period of garnet crystallization, and (B) the nuclei formed at preferred sites in the rock, but that potential nucleation sites were sufficiently abundant to give rise to ". . . an essentially random distribution of crystals".

In several other studies of garnet in metamorphic rocks, the random nucleation and spatial distribution of crystals has been cited as important. Jones and Galwey (1964, p. 87 and 92) concluded that random nucleation of garnet occurred in each band of the metasedimentary rocks at Ardara, Donegal, Eire, and that ". . . garnets were apparently randomly dispersed over the sections studied". Jones, Morgan, and Galwey (1972), in further considering the size distribution of garnets in sundry metamorphic rocks, based a new probability model on spatially random nucleation sites. Earlier Kretz (1966, p. 158) had made a very detailed study of grain-size for certain metamorphic minerals in relation to nucleation and growth; he concluded that garnet distribution (in a sample from the aureole of a granite) ". . . may with confidence be regarded as random. Hence, it is inferred to be random in three-dimensions as well". As mentioned earlier, Kretz (1969) also adduced detailed evidence to support the contention that the mineral phases in the calc-silicate granulite studied in the present paper are randomly distributed.

These concepts of randomly distributed grains in metamorphic rocks are primarily, though not entirely, based on garnet occurring as a minor rock constituent and on scapolite–pyroxene–amphibole–sphene assemblages. Flinn's (1969, p. 361) analyses were based on the major constituents of more quartzo-feldspathic rocks and indicated that ". . . the grains, instead of being distributed at random, are specially arranged so that grains of the same phase tend not to occur in contact with each other". He concluded that this fabric arises from grain-boundary migration leading to insertion of grains of one phase between pairs of like grains of other phases. Pending more thorough investigation, we think it necessary to allow that minor and major constituents may have dissimilar spatial distributions in analogous rocks.

When observed in traverses normal to the weak mineralogical banding, the sample studied by us shows a distinctive nonrandom grain distribution. The transition probabilities on the diagonal of our P matrices are smaller than the corresponding fixed-probability Q-vector values. This implies that contacts between grains of the same major mineral are always less abundant than would be expected if the grains were randomly distributed. This generalization applies to all nine slides when transition-sequence lengths of 35 or more or of 10 or more are used with amphibole alone or with amphibole combined with sphene. The sequences of grains resemble first-, and sometimes second-order Markov chains, although there is a possibility that some represent chains of even higher order.

The work of Rogers and Bogy (1958), Mahan and Rogers (1968), Kretz (1969), and Flinn (1969) reflected distinct differences between $p\ (i, j)$ and $p\ (j, i)$, $i \neq j$. Flinn (1969, p. 368) concluded that such differences ". . . are probably significant, in which case they could imply a polar pattern of distribution of grains . . ." within the rocks studied. Despite comparable differences between $p\ (i, j)$ and $p\ (j, i)$ in all the slides examined by us, we are satisfied that reversibility of the Markov chains of order-one has been established; in these cases, the sequences cannot be polar in the sense used by Flinn.

The unequivocal evidence for nonrandom distribution of grains in granitoids (Vistelius and coworkers; Moore, ms) and in the Grenville granulites (present paper) cannot necessarily be extrapolated to other igneous and metamorphic rocks. The need for additional empirical data on the spatial distribution of mineral phases in such rocks is acute. Models based on nucleation, crystallization, growth rates, grain-boundary migration, and kinetics will necessarily require significant adjustments according to whether the mineral grains are randomly or nonrandomly distributed.

Vistelius and coworkers concluded that the Markov property of the granites examined by them was a feature resulting from magmatic crystallization in a system analogous to that examined experimentally by Tuttle and Bowen (1958). Even if that petrogenetic interpretation were correct for granites, it is obvious that the present calc-silicate Grenville granulite is a metasedimentary rock and that, despite having similar Markovian properties, it owes its present mineralogy to high-grade neocrystallization in the solid state. A significant problem is posed by the need to explain the Markovian grain distribution that is shared by the present granulite and the granitic rocks studied previously.

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