Melt Network in a Partially Molten Rock

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MELT NETWORK IN A PARTIALLY MOLTEN ROCK

（部分溶融した岩石内での液相のネットワークについての研究）

Chapter 1

THE MULTIPHASE GRAIN CONTROL PERCOLATION

- Its Implication For a Partially Molten Rock -

Chapter 2

CONNECTIVITY OF MELT PHASE

IN A PARTIALLY MOLTEN MULTIPHASE CRYSTALLINE ROCK

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Chapter 1

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Abstract

A model of melt percolation named the multiphase grain control percolation (the MGCP) is proposed to estimate the bulk properties in a multiphase grain mixture where the distribution of melt phase at the grain boundary is controlled by the surrounding grain species or their combinations, such as in a partially molten rock. According to the connection of melt phase at the corner and edge element of grain boundary, the MGCP can be divided into three models, i.e. the corner percolation, the edge percolation and the corner-edge (CE) percolation. The CE percolation is a fundamental model of actual melt network in which the corner and edge element with melt phase chain each other. In order to estimate connectivity of melt phase in a binary grain system, however, the corner and edge percolation, which are applicable for the connection of the corner and edge elements with melt phase, respectively, are found to be able to substitute for the CE percolation. Connectivity of melt phase changes as a function of modal composition of grains in a multiphase grain system. Assuming the combination of grains around the corner and edge element with melt phase in a binary grain system, we obtain critical grain fraction where connectivity of melt phase changes drastically. It is found that the critical grain fraction estimated from the MGCP does not coincide with that does from the ordinary percolation in which the distribution of melt phase is assumed to be random. In addition to connectivity of melt phase, it is also needed to introduce the grain-

controlled melt distribution for estimating the bulk properties, such as electrical conductivity, in a partially molten rock. As a geophysical application of the MGCP, we make the connectivity diagram (modal composition diagram of connectivity of melt phase) of a partially molten peridotite by using stability criteria of melt phase obtained from partial melting experiment. From this diagram, we predict that melt network is fully connecting if volume fraction of olivine exceeds 0.64 (64%) for a natural peridotite composed of olivine, orthopyroxene and clinopyroxene and 0.38 (38%) for a synthetic peridotite composed of olivine and orthopyroxene, respectively.

Introduction

Percolation of melt phase in a partially molten rock is one of the most important physical process in the earth's upper mantle, especially beneath the volcanic areas. It controls not only magma migration rate [McKenzie, 1984 ; Scott and Stevenson, 1984] but also bulk properties of partially molten layer, such as electrical conductivity [e.g. Shankland and Waff, 1977], seismic wave velocities [e.g. O'Connel and Budiansky, 1977] and their attenuation [e.g. Mavko, 1980]. It is well known that, even if only small amount of melt phase exists, macroscopic response of melt and solid mixture is much different from that of single (solid) phase when network of melt phase connects extensively [Ziman, 1979]. Therefore, in order to make precise interpretation of geophysical observations about partially molten layer, we must relate connectivity of melt phase to physical condition and modal composition in it.

Generally, connectivity of melt phase in a partially molten rock depends on both the volumetric fraction and the distribution of melt phase. Under the textural equilibrium, the distribution of melt phase at the grain boundary is controlled by melt-solid and solid-solid interfacial energies [Bulau et al., 1979; Waff and Bulau, 1979]. For a monomineralic rock that consists of the same shape and size of grains, connectivity can be obtained from the volume fraction of melt phase and the interfacial energies between melts and solids because melt phase is uniformly distri-

buted at every grain boundary [Beere, 1975 ; Park and Yoon, 1985; von Bargen and Waff, 1986]. In the case of a poly-mineralic rock, however, it is insufficient to specify the volume fraction of melt phase and the interfacial energies among melt and solid phases for obtaining connectivity of melt phase. Connectivity of melt phase also depends on the distribution of various kind of grains because, at a grain boundary, combination of the interfacial energies which controls the distribution of melt phase changes according to the combination of grains around it.

In a limited range of degree of partial melting, connectivity of melt phase is controlled by the distribution of corner and edge elements of grain boundaries occupied by melt phase [Toramaru and Fujii, 1986]. For this case, taking advantage of percolation theory [Shante and Kirkpatrick, 1971; Stauffer, 1979, 1981], connectivity of melt phase may be obtained statistically. However, the distribution of the element occupied by melt phase in a partially molten rock would not be a priori random as normally assumed in the ordinary percolation, but is likely to be correlated with each other through randomly distributed species of solid phases. Theoretical and experimental approaches including interfacial energies indicate that the stable existence of melt phase on the grain boundary is controlled by surrounding mineral species and/or their combinations. In other words, the distribution of the melt elements is determined by the distribution of the mineral grains through relative difference in the interfacial energies : i.e. the melt elements

have some nearest neighbor dependence (short-range ordering).

In this paper, we propose a model of melt percolation in a multiphase grain mixture where the existence of melt phase on the grain boundary is controlled by the randomly distributed grain species. Connectivity of melt phase is estimated by using this model which is named the multiphase grain control percolation (hereafter abbreviated as the MGCP). In the model calculation by the MGCP, we try to get a critical grain fraction (modal composition) for the mixture of polymineralic grains where connectivity of melt phase changes drastically by assuming various conditions for the existence of melt phase at grain boundaries. First of all, a simple model of the MGCP is introduced. We demonstrate the difference of connectivity between the MGCP and the ordinary percolation. As a geophysical application of the MGCP, we will present connectivity diagram (modal composition diagram for connectivity of melt phase) for a partially molten peridotite based on a result of three dimensional numerical simulation.

Model and definition

We approximate all grains as simple convex polyhedrons (on the two dimension, they are polygons) which are entirely the same size and shape and enable to fill the space : i.e. we treat network of grain boundaries around hexagons, squares and triangles in the two dimensional model and tetrakaidecahedrons and simple cubics in the three dimensional model. Although the diamond structure is a popular network geometry, it will not be discussed because polyhedral grains can not be defined in this network. It is also assumed that there are two well mixed (i.e. randomly distributed) grains, grain A and B, with volumetric fraction of ϕ and $(1-\phi)$, respectively.

Melt phase is only possible to stably exist on the edge and corner elements of grain boundary. Although face is one of the elements of the grain boundary, stable existence of melt phase is not possible there [Waff and Bulau, 1979; Cooper and Kohlstedt, 1982]. We call an edge and a corner element occupied by melt phase as an occupied edge and an occupied corner, respectively. This is analogous to an occupied bond and an occupied site in the ordinary percolation. In a partially molten rock, an edge or a corner element becomes an occupied element only when the configuration of grain species around it is specified by some rule. This rule can be deduced from thermodynamical consideration including physical properties of solids and melts, such as interfacial energies. However, our purpose is not to debate the deduction of the rule further in detail but to clarify the effect

of grain-controlled melt distribution onto the macroscopic response of the partially molten rock. (Deduction of the rule from the termodynamical consideration is described by Nakano and Fujii [1988].) For the rule to judge the configuration of grains around the occupied corner and edge, the following rule can be the simplest without loosing any important application :

If a corner or edge element is surrounded by at least $\underline{M}$ of grain A among the adjacent $\underline{N}$ grains, it is occupied.

The rule for each $\underline{M}$ is regarded as condition $\underline{M}$ for the occupied corner or edge. The number $\underline{M}$ can vary from $\underline{0}$ to $\underline{N}$. The number $\underline{N}$ varies with types of network of grain boundaries, e.g. $\underline{N} = \underline{2}$ for the edge around the two dimensional grain and $\underline{N} = \underline{4}$ for the corner of tetrakaidecahedron. Note that condition $\underline{1}$ is equivalent to that all corner or edge elements around grain A are occupied. Concentration of occupied elements, $\underline{p}$ (numbers of occupied elements per numbers of total elements), is related to volumetric fraction of grain A, which is given as following.

$$\underline{p} = \sum_{\underline{k}=\underline{M}}^{\underline{N}} \left(\frac{\underline{N}}{\underline{k}} \right) \underline{\phi}^{\underline{k}} \, \underline{(1-\phi)}^{\underline{N}-\underline{k}}. \qquad [1]$$

Three types of percolation through the cluster of occupied elements are introduced :

The corner percolation : When all edge elements are occupied, two occupied corner elements connect each other if they are nearest neighbor.

The edge percolation : When all corner elements are occupied, two occupied edge elements connect each other if they are nearest neighbor.

The corner-edge (CE) percolation : When not all of edge and corner elements are occupied, two occupied edges at nearest neighbor position connect each other if a corner element between them is occupied, and vice versa.

For the model of the network of melt phase in a partially molten rock, it is possible to use them as the approximation for the limited range of degree of partial melt, e.g. it is appropriate to apply the edge percolation when degree of partial melt is very small and to apply the corner percolation when the melt phase on the corner element is large enoughly to directly connect with neighbouring corner elements [Jurewicz and Watson, 1985] or the Ostwald ripening is occurred. The CE percolation might be the most important for the practical applications because network of melt phase consists of both the corner and edge elements alternatively. Unlike the assumption in the ordinary percolation, existence of melt phase on the edge and corner elements is not determined independently. The edge or corner percolation are found to be able to substitute for almost all CE percolation, where the configuration of grains around the occupied corner and edge is determined by the combination of condition M for each elements, as described in Appendix A in detail. Therefore, we will consider mainly the edge and corner percolation in the following section.

In our model, connectivity of occupied elements is defined as

Connectivity is a probability that some fraction of occupied elements belong to the infinite cluster of occupied elements.

From the analogy of the ordinary percolation, we expect that connectivity in the MGCP is a function of $\underline{\phi}$ and has only one critical grain fraction $\underline{\phi}^*$ where connectivity changes from 0 to 1 drastically. So, connectivity in the MGCP could be characterized by $\underline{\phi}^*$, i.e. connectivity is expected to be characterized by a critical grain fraction as

if $\underline{\phi} < \underline{\phi}^*$, the network of occupied elements is non-connective,

and

if $\underline{\phi} > \underline{\phi}^*$, the network of occupied elements is connective.

Grain-site translation

In the MGCP, the connection of the occupied elements whose distribution is controlled by the randomly distributed grain A becomes a subject of interest, while the connection of randomly distributed occupied elements does in the ordinary percolation. Because of this similarity about the randomly distributed grain A in the MGCP with the randomly distributed occupied element in the ordinary percolation, we expect that there can be some correspondences between them. The edge and corner element in the MGCP obviously correspond to the bond and site element in the ordinary percolation, respectively. So that, one might expect that the critical edge and corner concentration in the MGCP will be the same value for the critical bond and site concentration in the ordinary percolation, respectively. However, the expectation is generally incorrect and, moreover, there is a rigorous relationship between the edge percolation of condition 1 and the ordinary site percolation as shown in the following example.

In case of square grains, square lattice obviously corresponds to the grain boundary. On this lattice, critical bond concentration of the ordinary bond percolation (which is likely to correspond to the edge percolation) is exactly obtained as 1/2 [Sykes and Essam, 1964]. For the edge percolation of condition 1, an occupied edge is surrounded by at least one grain A which is indicated by closed circles in Fig. 1 (a). Considering a cluster of occupied edges as shown by thick lines in Fig. 1 (b), it can be regarded as a cluster of grains A (shaded squares

) because all edges around grain A are occupied. Regarding grain A as occupied site (which is called the grain-site translation, hereafter), connection of the occupied site is the same as that in the ordinary site percolation on the matching lattice [Sykes and Essam, 1964] of square lattice (Fig. 1 (c)). Therefore, the edge percolation of condition 1 around square grains should be equivalent to the ordinary site percolation on a lattice with eight coordination number (Fig. 1 (d)). Since critical site concentration on this lattice is 0.407 (which is obtained from the matching property [Sykes and Essam, 1964] applied on the result of numerical simulation [Stauffer, 1979, 1981]), so that ϕ^* for the edge percolation of condition 1 around square grains should be 0.407. Note that critical edge concentration, p^*, calculated from equation [1] with $N = 2$ and $M = 1$ is 0.648, which does not coincide with the critical bond concentration of 0.500 for the ordinary bond percolation on the square lattice.

Critical grain fraction for the edge percolation of condition 1 around 2 dimensional grains (i.e. hexagon and triangle) can be obtained according to the same procedure described above and listed in Table 1. An exact critical grain fraction, 0.500, is obtained by using the grain-site translation for the edge percolation with condition 1 around hexagonal grains. Because connection of occupied site is the same as that of the ordinary site percolation on the triangular lattice (Fig. 1 (e)) and critical site concentration on the lattice, 0.500, is exactly obtained in the ordinary percolation [Stauffer, 1979, 1981].

Although the grain-site translation is possible for the three dimensional edge percolation and the two and three dimensional corner percolation of condition 1, it needs, however, to specify rather complex lattice with large coordination number to perform the site percolation in the ordinary percolation scheme.

In the case of the edge and corner percolation for condition M (M > 1), the grain-site translation does not become simple to estimate connectivity of occupied elements. For example, consider the edge percolation of condition 2, in which an occupied edge is always surrounded by two grain A. Namely, occupied edge is covered with the shell of grain A. When the network of the occupied edge is fully connected, the shell should be fully connecting. At the bottle neck between two clusters of occupied edges, connection of the shell is clearly different from that of occupied site in the ordinary site percolation as shown in Fig. 2. In the case of the ordinary site percolation (Fig. 2 (a)), an occupied site at the bottle neck between two clusters, C_1 and C_2, connects at least two adjacent occupied sites. However, in the case of the edge percolation of condition 2 after applying the grain-site translation (Fig. 2 (b)), an occupied site (i.e. the shell of occupied edge) at the bottle neck between two clusters, C_3 and C_4, connects at least three adjacent occupied sites.

Therefore, it is not easy to get p^* by critical site and bond concentration for the ordinary percolation. So, numerical calculation is needed to get p^* for the MGCP.

Numerical simulation

To determine a critical grain fraction for various types of grain shape, the numerical calculation was performed by using the Monte Carlo method. As an example, the procedure is described below for the corner percolation of condition 2 around hexagonal grains.

First, hexagonal grains A and B with volumetric fraction ϕ and $(1-\phi)$ are distributed randomly, and the Monte Calro trials are made for at least 10^5 of total grains for all trials. At each trial, occupied corners are marked according to the rule of condition 2. As a result of these procedures, concentration of occupied corner, p, in average, takes the value calculated from equation [1] with N = 3 and M = 2. Finally, the sizes of every cluster of occupied corners are counted by using the cluster multiple labeling technique [Hoshen and Kopleman, 1976]. We always regard the largest cluster as the infinite cluster of occupied corners. By this approximation, connectivity, C, is calculated as [Stauffer, 1979, 1981],

$$C = \max(Nc) / No, \qquad [2]$$

where Nc and No are numbers of occupied corners in a cluster and total numbers of occupied corners, respectively. To judge the critical grain fraction clearly, we also calculate the mean size of finite occupied corner cluster, MSC, which diverges at critical point as does in the case of ordinary (site) percolation and is obtained from :

$$\underline{MSC} = (\Sigma \underline{Nc}^2 - \underline{max(Nc)}^2) / (\underline{No} - \underline{max(Nc)}), \qquad [3]$$

where summation takes for all clusters.

One example for the case of $\underline{M} = \underline{2}$ for the hexagonal grains ($\underline{N} = \underline{3}$) is shown in Fig. 3. Total number of grains and corners are 5×10^5 and 1.5×10^6, respectively. Maximum value of MSC is 5.7×10^4. It is clear that both C and MSC change sharply within the narrow range of grain fraction. The value centered in this range can be regarded as the critical grain fraction, which can be determined within the range of about 0.01 for all simulations. Critical grain fraction obtained from numerical simulation coincides with those obtained from the grain-site translation as described in the previous section. Results of critical grain fractions and critical edge and corner concentration for all variation of condition M are summarized in Table 1.

Two characteristics are found in Table 1. First, critical edge and corner concentration for the MGCP are always different from critical site and bond concentration for the ordinary percolation when the same network of grain boundary is applied. It seems, at this moment, to be no systematic trend of the difference of critical values between the MGCP and the ordinary percolation. Secondly, the value of critical edge and corner concentration decreases with increasing the value of M of condition M. Therefore, in any grain mixture, network of melt phase becomes easy to connect extensively when condition M with larger M is applied.

Connectivity diagram

Connectivity diagram is a mineral composition diagram for connectivity of melt phase in a partially molten rock [Toramaru and Fujii, 1986]. After translating the stability criteria of melt phase obtained from the partial melting experiment into the appropriate rule for the MGCP, connectivity diagram can be constructed.

Since melt phase in a partially molten rock under the textural equilibrium is only possible to exist at the corner elements surrounded by 4 grains and the edge elements surrounded by 3 grains [e.g. Bulau et al., 1979], most of mantle material can be approximated as equal sized tetrakaidecahedral grains.

For the synthetic peridotite composed of olivine (OL) and orthopyroxene (OPX), Fujii et al. [1986] reported that melt phase stably existed at all corner elements and the edge elements of grain boundary except at those edge elements surrounded by two or three OPX grains in the water-free specimen. From the view point of the MGCP, it is appropriate to use the edge percolation of condition 2 ($N = 3$) to make connectivity diagram if we regard OL and OPX as grain A and B, respectively. From Table 1, critical grain fraction of OL for this condition is 0.38. Therefore, we can predict that, in this system, melt network is extensively connecting if volume fraction of OL exceeds 0.38.

For the natural peridotite mainly composed of OL, OPX and clinopyroxene (CPX) crystals, Toramaru and Fujii [1986] concluded that melt phase were morphologically stable only on the

edge element surrounded by OL-OL-OL and on the corner element surrounded by OL-OL-OL-OL and OL-OL-OL-OPX (Fig. 4). According to the discussion in Appendix B, we can obtain connectivity diagram for this peridotite by using critical grain fraction for the edge percolation of condition 3 (N = 3) in binary grain mixture, i.e. the above conclusion for melt phase stability implies the OL tube connection. Regarding OL and two pyroxenes as grain A and B, respectively, critical grain fraction of OL is 0.63 (Table 1). Namely, melt phase in this partially molten natural peridotite becomes extensively connecting, if volume fraction of OL exceeds 0.63 which is independent on the relative ratio of CPX to OPX (a line with symbol A in Fig. 5). The result by Toramaru and Fujii [1986], who used the ordinary percolation, are also shown by a curve TF for comparison.

In these two examples, connectivity of melt phase in the partially molten peridotite is a function of the volume fraction of OL alone. This result is, however, exceptional case from the specific condition used for existence of melt phase at the corner and edge elements. In general, connectivity of melt phase becomes dependent on the volume fraction of pyroxenes. For example, if melt phase is possible to exist at the corner elements surrounded by OL-OL-OL-OL and OL-OL-OL-OPX and the edge elements surrounded by OL-OL-OL and OL-OL-OPX in a OL-OPX-CPX system, connectivity diagram can be obtained from numerical simulation of the CE percolation for three different solid phase mixture and the results are also shown by a curve with symbol B in Fig. 5. From Fig. 5, it is clear that critical grain fraction of this

system depends not only volume fraction of OL but also that of OPX.

Discussions and conclusions

The MGCP can be classified as one of the correlated percolation. However, it differs from the ordinary correlated percolation in respect that correlation among occupied elements is caused by the types of grains and their combination around the occupied elements. Therefore, the rule which controls the configuration of various phases of grains is the most important factor for the MGCP. The rule we used implies that grain A has more attractive properties of melt phase than that of grain B and the melt attraction is the additive one. This rule is widely applicable in nature, such as connectivity diagrams for the natural and synthetic peridotite. In general, the rule which determines the configuration of grains around the occupied elements is very sensitive for the physical condition and chemical composition of a partially molten rock. To estimate connectivity of melt phase in partially molten layer in earth's upper mantle, it needs to relate condition M for the edge and corner element with stability criteria of melt phase on grain boundaries by using solid-solid and solid-melt interfacial energies [Toramaru and Fujii, 1986].

Although there are some ambiguities what rule should be applied to each observations, it is likely to be correct that the distribution of melt phase in a partially molten rock is not random but depends on the distribution of various kind of grains in it. Network configuration for such a correlated melt distribution is clearly different from one estimated by the ordinary percolation. The difference of the configuration of melt network

between the MGCP and the ordinary percolation should affect the estimation not only for connectivity but also of another macroscopic response of the partially molten system.

Electrical conductivity is one example. Archie's law is well known empirical law in geophysical observations and suggests that the electrical conductivity, EC, and the volume fraction of melt phase, v, hold the nonlinear relationships as

$$EC \propto v^m \qquad [4]$$

where the exponent m takes the value more than 1 [Archie, 1942]. Although there are many theoretical studies about Archie's law [e.g. Kirkpatrick, 1973; Webman et al., 1975; Sen et al., 1981; Yonezawa and Cohen, 1983], it can also be demonstrated the relationship of EC and v by using the MGCP. Since conductance of solid phase is negligibly small in comparison with that of melt phase, it is possible to regard solid phase as an insulator. For simplicity, we assume that all corner element is occupied and the occupied edge and non-occupied edge are the conductor and insulator, respectively, so that the network of melt phase consists of the conductance path.

If the occupied edge is randomly distributed, EC and the edge concentration, p ($\propto$ v), hold linear relationships as predicted by effective medium approximation [Kirkpatrick, 1973 ; Shankland and Waff, 1974]. In addition, if the conductance of occupied edges are assumed to be uniform, it is expected that the nonlinearlity between EC and p in Archie's law is explained by the correlated melt distribution. Although there are some models

of the ordinary correlated percolation which can explain it, it should be noted that the power law relation between EC and p is also appeared in the MGCP, in which the distribution of correlated occupied edge depends on the randomly distributed grains, For example, exponent m is obtained as 1.4 from the numerical calculation of EC for the two dimensional square binary grain system where the occupied edge is distributed by using the rule of condition 2 (Fig. 6). Since critical concentration of occupied edge for this MGCP (0.49) and occupied bond for the ordinary bond percolation (0.5) around square grains are almost the same, the simulation seems to suggest that the occupied edge cluster of infinite size in the MGCP containes more dead ends relative to that in the ordinary percolation.

Although a question whether the exponent, m = 1.4, holds the same value on the three dimensional model of the MGCP would remain unanswered, it is clear that the correlated melt distribution caused by the distribution of grains plays an significant role in the Archie's law.

In our model of the MGCP, the variation of the grain size was not taken into consideration. Generally, the corner and edge percolation is enable to be regarded as the ordinary site percolation by using the grain-site translation. Percolation theory suggests that connectivity of the occupied sites in the ordinary site percolation is determined by a few parameters alone (e.g. coordination number of the lattice and dimensionality of the system) and is not affected by geometrical irregularity [Stauffer, 1979, 1981] . Therefore, little effect of grain size

distribution might be expected.

As demonstrated in the previous section and in the Fig. 5, it will be straightfoward procedure to extend the MGCP from binary grain system to polymineralic grain system composed of more than three kind of grains. Although, for many cases, the MGCP through polycrystalline solids is enable to reduce to that through binary grain system as discussed in Appendix B, it needs further investigations such as the correlation with polychromatic percolation [Zellen, 1977].

Appendix A : Reduction from the CE percolation to the edge or corner percolation.

The actual network model consists of the corner and edge elements chained each other, so that the fundamental approach will be to consider the CE percolation in every case. For many cases, however, it needs not to consider the CE percolation for the estimation of connectivity of occupied elements. Except for a few cases, the CE percolation in the binary grain system, where the distributions of the occupied edge and corner are separately determined by condition M, is equivalent to the edge or corner percolation.

For example, consider the CE percolation in hexagonal binary grain mixture where melt network is constructed by the occupied corner elements satisfied with condition 2 and the occupied edge elements satisfied with condition 1 : i.e.

An occupied corner element is surrounded by at least two grain A among three grains,

and

An occupied edge element is surrounded by at least one grain A among two grains.

Consider two adjacent occupied corners (Fig. A1), these corners C_1 and C_2 in Fig. A1 are both surrounded by two or three grains A. As shown in Fig. A1, it is clear that at least one of grains located at X and Y is grain A. Therefore, the edge ele-

ment among these occupied corners is always surrounded by at least one grain A. In other words, an edge element among two occupied corners is automatically an occupied edge. In this consequence, connectivity of occupied elements is controlled by the distribution of occupied corners alone, even though network of melt phase in this system is composed of both occupied corners and occupied edges.

For all combinations of condition M for corner and edge elements in hexagonal and tetrakaidecahedral binary grain system, it is possible to reduce the CE percolation to the edge or corner percolation as a result of similar considerations described above.

Although it is also possible to reduce from the CE percolation to the edge or corner percolation for almost all combination of condition M for each element, there are a few exceptions in two dimensional square and triangular and three dimensional cubic binary grain system. For such exceptions, it needs to estimate connectivity of occupied edges and corners by judging to label the cluster of both elements at the same time. Reduction from the CE percolation to the edge or corner percolation for all system are summarized in Table 2. In the case that the reduction is not possible, we performed numerical simulation to get critical grain fraction, ϕ^*, which are shown by numeric instead of symbols in Table 2.

Appendix B : Model for connectivity diagram of the natural peridotite

Toramaru and Fujii [1986] obtained the expressions of stability criteria for existence of melt phase on the elements of grain boundary in a partially molten rock composed of at most three different phases of minerals as a function of possible interfacial energies. Applying this criteria to the result of the partial melting experiment of the natural peridotite composed of OL, OPX and CPX crystals, they predict that melt phase are morphologically stable only on the edge elements surrounded by OL-OL-OL and the corner elements surrounded by OL-OL-OL-OL and OL-OL-OL-OPX.

Compared to the corner and the edge percolation in the binary grain mixture, two new aspects should generally be introduced in the MGCP to estimate connectivity for this peridotite : (1) three kind of grains must be introduced in the model of the MGCP, and (2) since the condition for the existence of melt phase on the edge and the corner element are given separately, the estimation of connectivity in this peridotite needs the CE percolation. There are, however, some conditions for which it can be reduced to the edge percolation in binary grain mixture as follows.

For example, consider a unit composed of the edge-corner-edge elements shown in Fig. A2 in which P, Q, R and S are edges and O represents a corner. If any two edges of this unit are occupied by melt phase, they should be both surrounded by OL-OL-OL. Since grain shape is tetrakaidecahedron, the corner element, O, between

these edge elements is always surrounded by OL-OL-OL-OL. In other words, the corner element between any two occupied edges is automatically occupied by melt phase. Therefore, network of melt phase in the partially molten peridotite is equivalent to the network of the occupied edges and we can estimate connectivity by applying the edge percolation. Although melt phase is possible to exist on the corner elements surrounded by OL-OL-OL-OPX, these elements should locate at the perimeter of the network of melt phase. Since the distribution of occupied edges in this peridotite is controlled by the distribution of the OL grains alone, it is not necessary to distinguish two pyroxenes but sufficient to introduce binary grains, OL and other minerals (i.e. pyroxenes, PX).

Although Toramaru and Fujii [1986] also discussed the effect of the different mean grain size among OL, OPX and CPX onto connectivity, we can neglect this effect by following reason. Except for the corner elements at the perimeter, network of melt phase in the peridotite is always covered with OL grains for the conditions deduced from the experimental results discussed above. In other words, network of melt phase is in the tube made only by OL. In order to connect the melt network extensively, it is necessary to connect this OL tube extensively. Since the formation of OL tube is not affected by the difference of the mean grain size between OL and PX, we can neglect the effect of the difference of the mean grain size between OL and two pyroxenes onto connectivity of melt phase in the peridotite.

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Figure captions

Fig. 1 Correspondence between the edge percolation of condition 1 around the two dimensional grains and the ordinary site percolation. (a) Configuration of the square grain A (closed circle) and B (open circle) around an occupied (thick line) and non-occupied edge (double thin lines). (b) A cluster of occupied edge (thick lines). The edges around grain A (shaded squares) are always occupied in the case of condition 1. (c) Connection of the occupied site after the grain-site translation. (d) The matching lattice of the square lattice, which indicates eight coordination number. (e) Connection of occupied site after the grain-site translation for the two dimensional hexagonal (left), square (middle) and triangular (right) grains. An occupied site (solid circle) can connect the adjacent sites (open circle) through the break lines.

Fig. 2 Schematic diagram indicating the difference of connection of two occupied site clusters between (a) the ordinary site percolation and (b) the edge percolation after applying the grain-site translation. Break lines denote the occupied edges.

Fig. 3 Example of result of the Monte Carlo simulation to obtain critical grain fraction ϕ^* for the corner percolation of condition 2 around the two dimensional hexagonal grains. By this simulation, ϕ^* and critical corner concentration, p^*, can be determined as 0.55 and 0.56, respectively. (a) Mean size of finite occupied corner cluster, MSC (equation [3]), vs. occu-

pied corner concentration, p. MSC diverges when network of occupied corners connects extensively. The mean values and variances of MSC for every 0.01 division of p are represented by the cross bars. (b) Fraction of grain A, ϕ, vs. p. ϕ and p relate each other by equation [1] with $N = 3$ and $M = 2$. (c) Connectivity of occupied corners, C (equation [2]), vs. p. C changes from 0 to 1 if network of occupied corners becomes fully connecting.

Fig. 4 Three types of "occupied" corner-edge-corner elements in a natural peridotite composed of OL, OPX and CPX grains, in which an occupied edge must be surrounded by three OL grains. All grains are approximated by the equal size tetrakaidecahedrons. (a) The corner elements at both ends are not occupied because of CPX grains. (b) One corner element is not occupied because of CPX grain. The other is occupied because it is surrounded by OL-OL-OL-OL or OL-OL-OL-OPX grains. (c) The corner elements at both ends are occupied because they are both surrounded by OL-OL-OL-OL or OL-OL-OL-OPX grains. (Modified after Toramaru and Fujii [1986]).

Fig. 5 Connectivity diagram for a peridotite composed of OL, OPX and CPX crystals. Melt network is fully connecting in the area shown by hatched side. Boundary A and TF, which are obtained from the model of the MGCP and the ordinary percolation [Toramaru and Fujii, 1986], respectively, are predicted for the natural peridotite in which melt phase can exist at the corner element surrounded by OL-OL-OL-OL or OL-OL-OL-OPX and the edge element surrounded by OL-OL-OL. Boundary B is the case that melt

phase can exist at the corner element surrounded by OL-OL-OL-OL or OL-OL-OL-OPX and the edge element surrounded by OL-OL-OL or OL-OL-OPX. Volume fraction of OL at P, Q, S, T and R are 0.63, 0.63, 0.72, 0.82 and 0.37, respectively.

Fig. 6 Result of the numerical calculation of the macroscopic electrical conductivity, EC, of the two dimensional conductor network around the square grains. Two kind of conductors, H and L whose ratio of conductance is 10^6 : 1, are distributed with the number fraction of p and (1-p), respectively. Total number of them is 10^4. Top : distribution of conductor H is the same as that of occupied edge in the edge percolation of condition 2, Bottom : conductor H is distributed randomly.

Fig. A1 A unit of corner (C_1) - edge (E_0) - corner (C_{γ_2}) elements around the two dimensional hexagonal grains. If both C_1 and C_2 are surrounded by at least two grain A, one of two grains located at X and Y is a grain A. Therefore, E_0 is always beside at least one grain A.

Fig. A2 The grain boundary surrounded by four tetrakaidecahedral grains. In the case that edge element P is surrounded by OL-OL-OL grains, corner element O is always surrounded by OL-OL-OL-OL grains if one of edge elements among Q, R and S is surrounded by OL-OL-OL grains.

Table 1. Critical values for the MGCP

Critical grain fraction, ϕ^*

Corner percolation

Grain	Condition number, M							
	1	2	3	4	5	6	7	8
HX	0.29	0.55	0.80					
SQ	0.20	0.43	0.62	0.84				
TR	0.12	0.27	0.42	0.58	0.74	0.89		
TD	0.10	0.23	0.40	0.63				
SC	0.03	0.11	0.20	0.30	0.41	0.53	0.66	0.80

Edge percolation

Grain	Condition number, M			
	1	2	3	4
HX	0.500*	0.80		
SQ	0.407	0.70		
TR	0.30	0.63		
TD	0.18	0.38	0.63	
SC	0.10	0.24	0.42	0.64

Critical corner/edge concentration, p^*

Corner percolation

Grain		Condition number, M							
	OS	1	2	3	4	5	6	7	8
HX	0.698	0.64	0.56	0.51					
SQ	0.593	0.59	0.58	0.51	0.50				
TR	0.500*	0.54	0.51	0.50	0.50	0.50	0.50		
TD	0.45	0.35	0.23	0.18	0.15				
SC	0.311	0.25	0.21	0.20	0.18	0.18	0.18	0.18	0.18

Edge percolation

Grain		Condition number, M			
	OB	1	2	3	4
HX	0.653*	0.750*	0.64		
SQ	0.500*	0.648	0.49		
TR	0.347*	0.51	0.40		
TD	0.41	0.45	0.32	0.25	
SC	0.250	0.35	0.25	0.21	0.18

Symbols

* : exact solution
HX : 2-D hexagon
SQ : 2-D square
TR : 2-D triangle
TD : 3-D tetrakaidecahedron
SC : 3-D simple cubic
OS : critical site concentration of ordinary percolation
(values obtained from Stauffer [1981])
OB : critical bond concentration of ordinary percolation
(values obtained from Stauffer [1981])

Table 2. Reduction from the CE percolation to the edge or corner percolation

---

2-D hexagon

		corner			
M	0	1	2	3	
0	*	C1	C2	C3	
edge 1	E1	E1	C2	C3	
2	E2	E2	E2	C3/E2	

2-D square

		corner				
M	0	1	2	3	4	
0	*	C1	C2	C3	C4	
edge 1	E1	E1	0.41	C3	C4	
2	E2	E2	E2	E2	C4	

2-D triangle

		corner					
M	0	1	2	3	4	5	6
0	*	C1	C2	C3	C4	C5	C6
edge 1	E1	E1	E1	0.43	0.58	C5	C6
2	E2	E2	E2	E2	E2	0.75	C6

3-D tetrakaidecahedron

		corner				
M	0	1	2	3	4	
0	*	C1	C2	C3	C4	
edge 1	E1	E1	C2	C3	C4	
2	E2	E2	E2	C3	C4	
3	E3	E3	E3	E3	C4/E3	

3-D simple cubic

		corner							
M	0	1	2	3	4	5	6	7	8
0	*	C1	C2	C3	C4	C5	C6	C7	C8
1	E1	E1	E1	0.20	0.30	C5	C6	C7	C8
edge 2	E2	E2	E2	E2	0.31	0.41	C6	C7	C8
3	E3	E3	E3	E3	E3	0.45	0.54	C7	C8
4	E4	E4	E4	E4	E4	E4	E4	0.69	C8

Symbols

M : condition number (M = 0, 1, ...)
* : always connecting
CM : enable to reduce to the corner percolation of condition M
EM : enable to reduce to the edge percolation of condition M
CM/EM : enable to reduce to the corner or edge percolation (in this case, critical grain fraction for both percolation takes the same value as shown in Table 1)
numeral : critical grain fraction, ϕ^*, for the CE percolation

Note

Row of M = 0 is the corner percolation, and defined in the text.
Column of M = 0 is the edge percolation, and defined in the text.

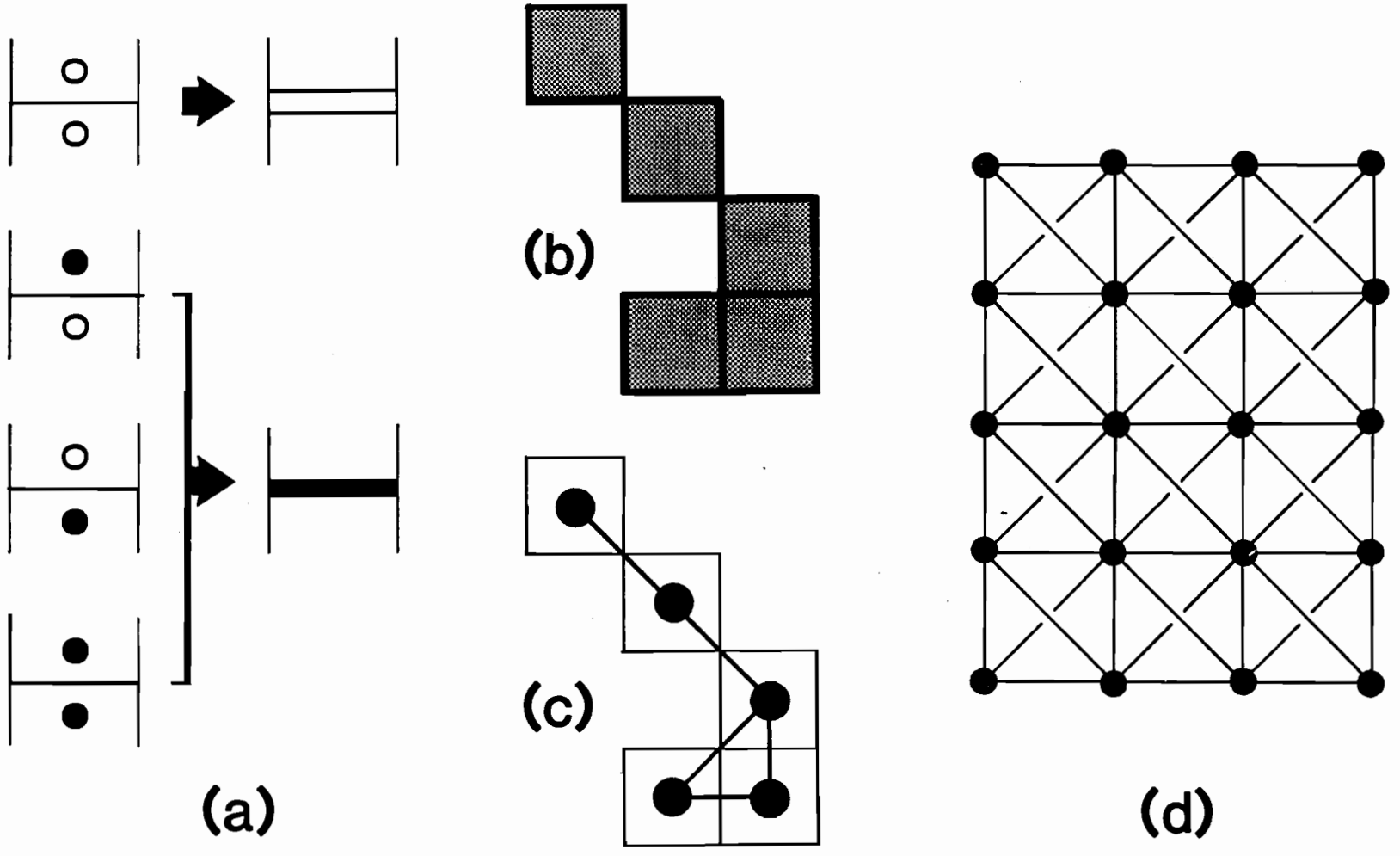


Fig. 1

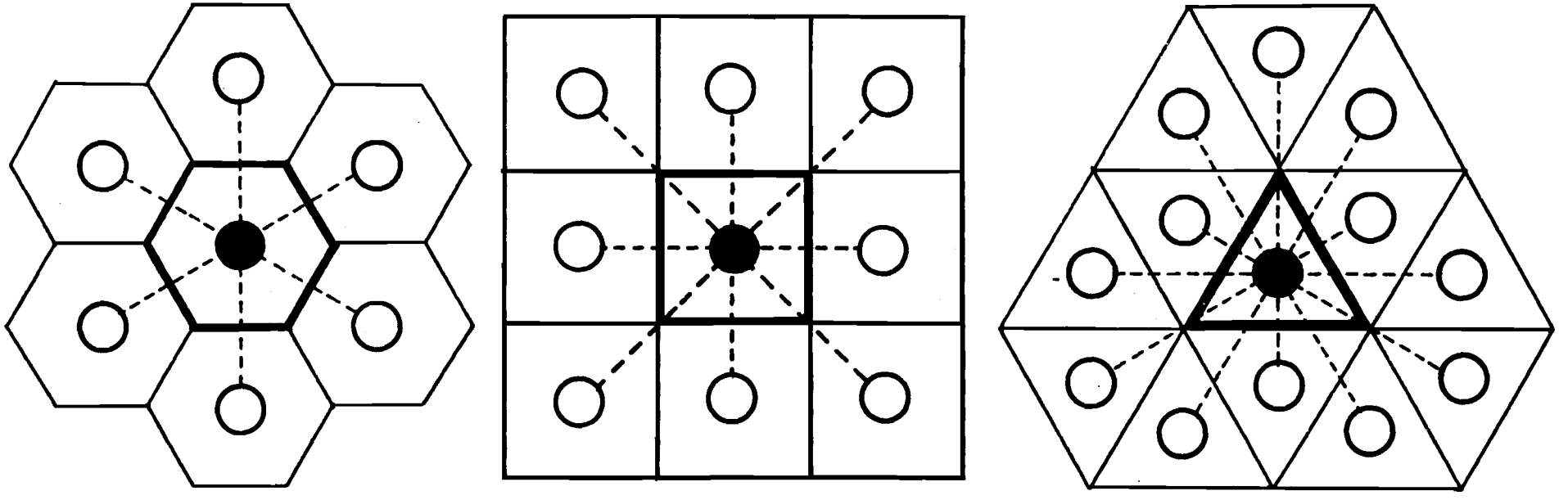


Fig. 1(e)

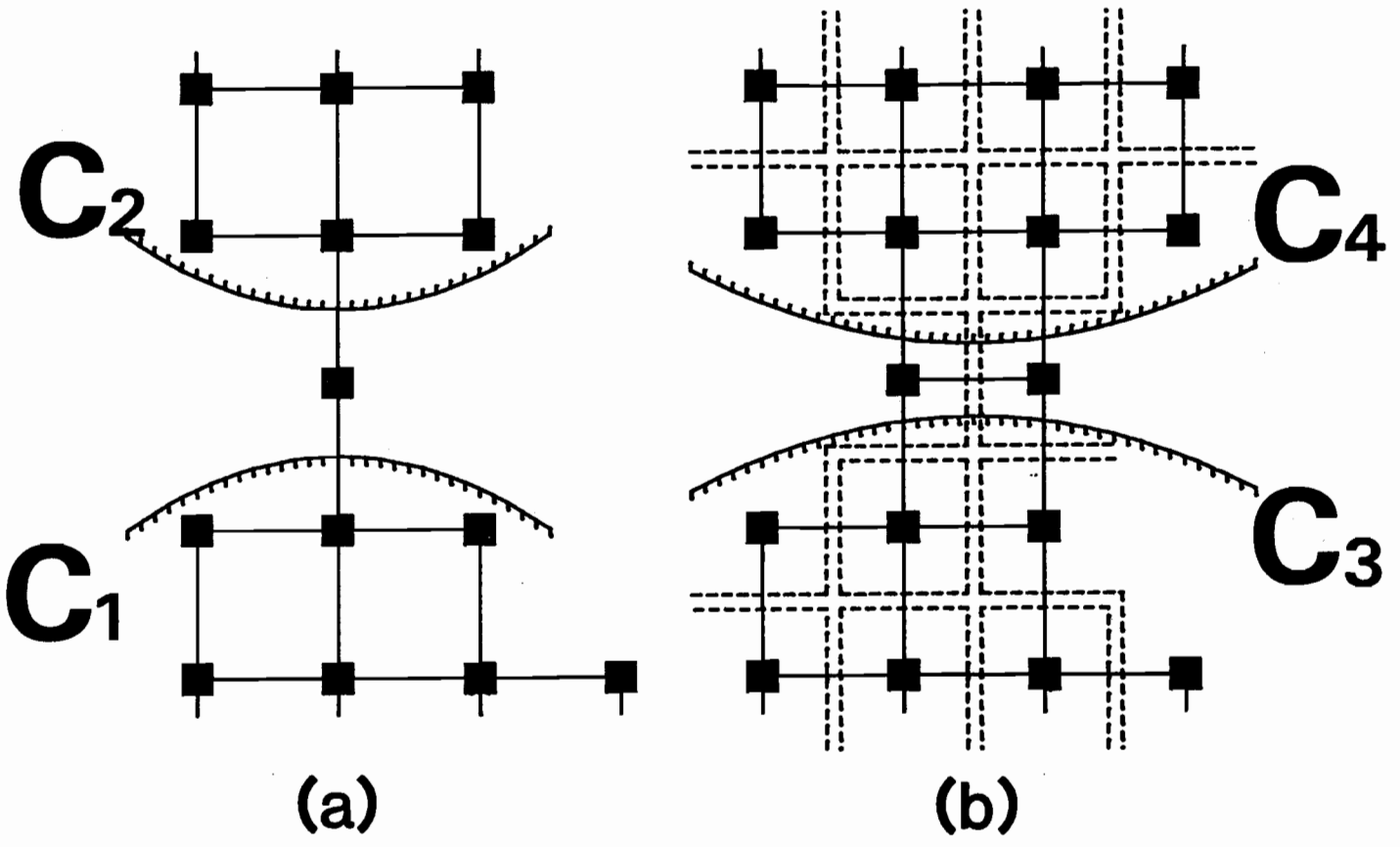


Fig. 2

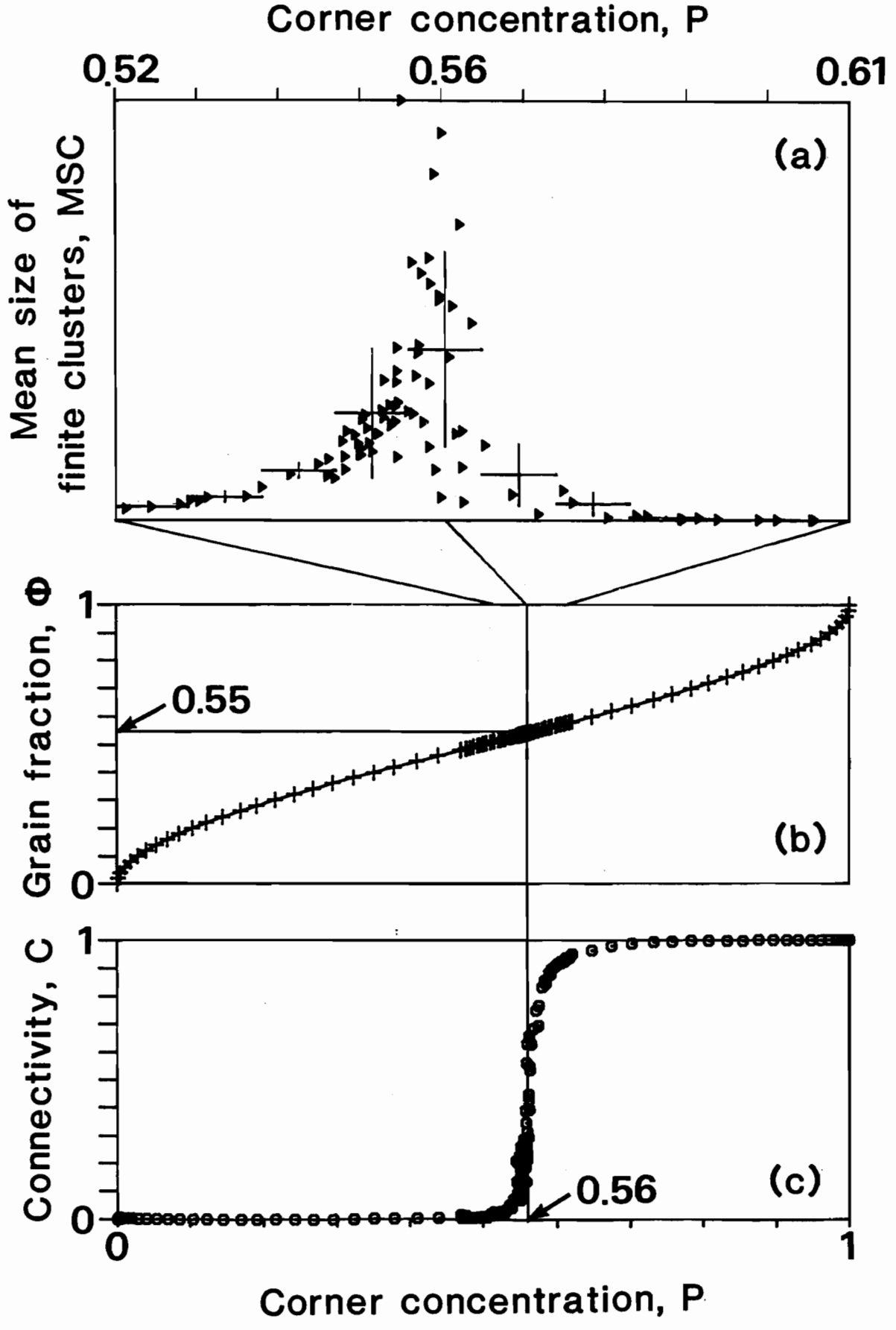
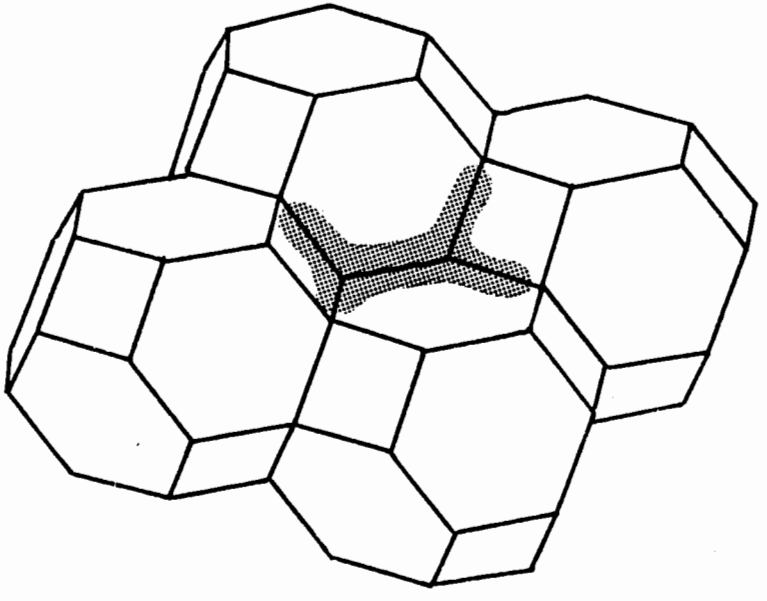

Corner concentration, P
0.52
0.56
0.61
(a)
Mean size of finite clusters, MSC
Grain fraction, Φ
1
0.55
0
(b)
Connectivity, C
1
0
0.56
(c)
0
1
Corner concentration, P

Fig. 3



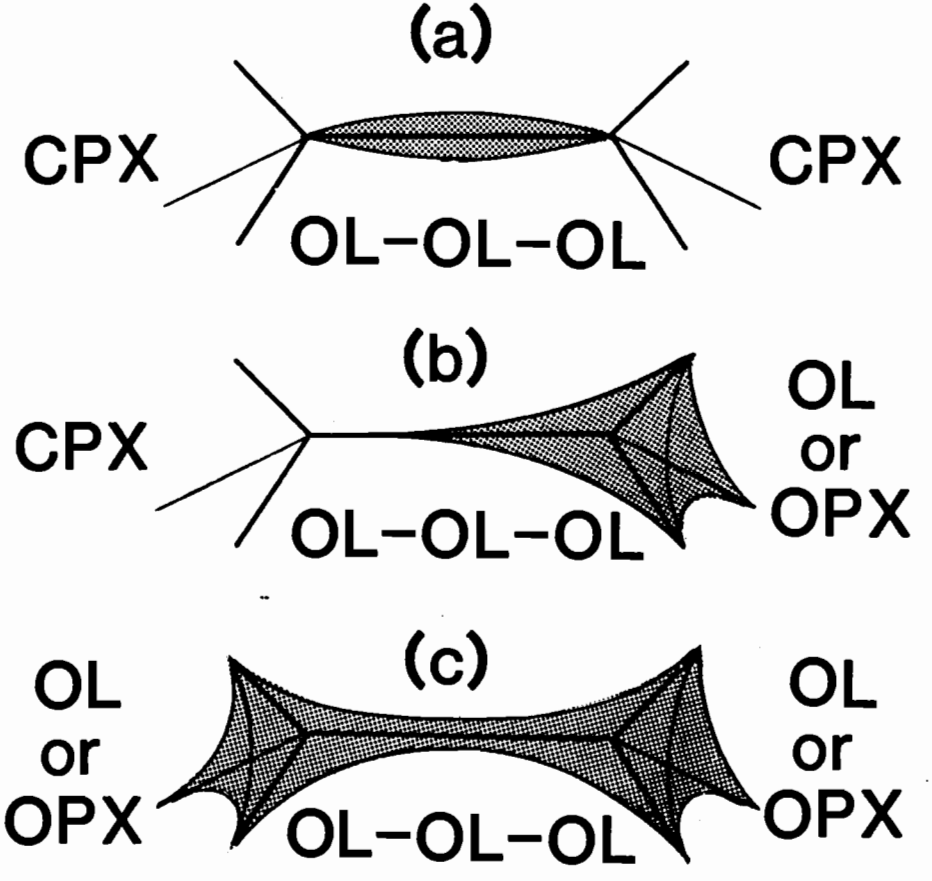

(a)
CPX
CPX
OL–OL–OL
(b)
CPX
OL
or
OPX
OL–OL–OL
(c)
OL
or
OPX
OL
or
OPX
OL–OL–OL

Fig. 4

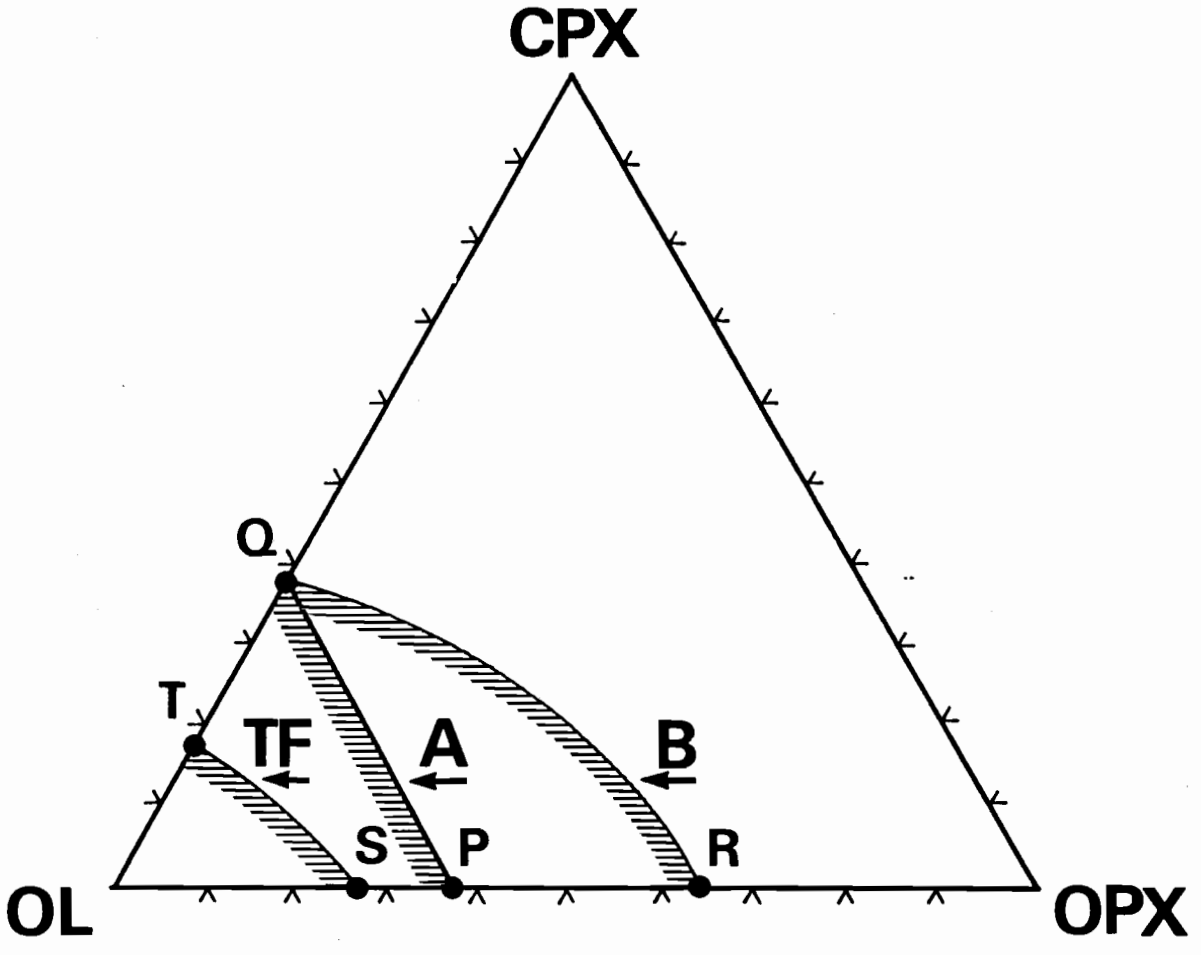


Fig. 5

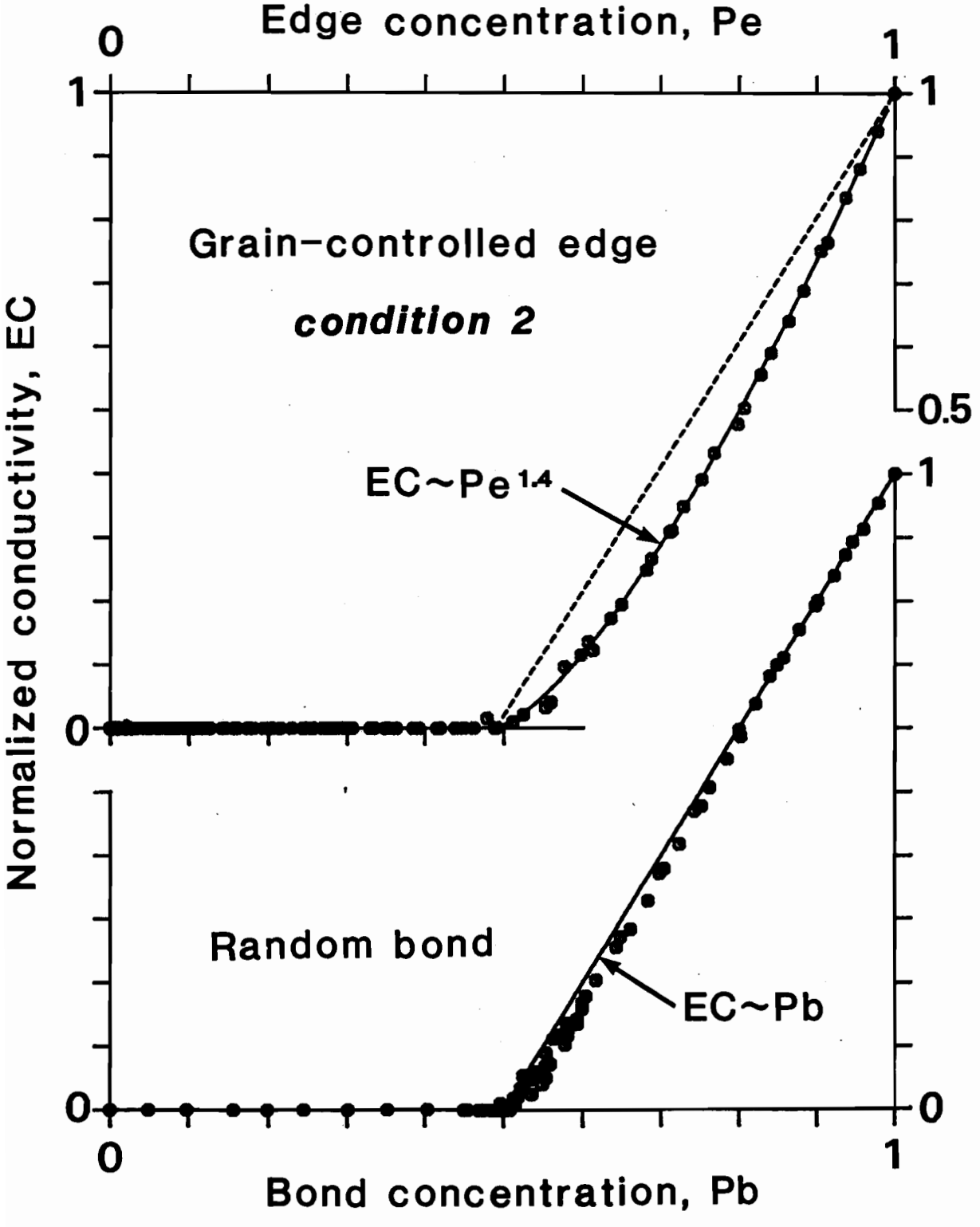

Edge concentration, Pe
0
1
1
1
Grain-controlled edge
condition 2
0.5
EC~Pe^1.4
Normalized conductivity, EC
1
0
Random bond
EC~Pb
0
0
1
Bond concentration, Pb

Fig. 6

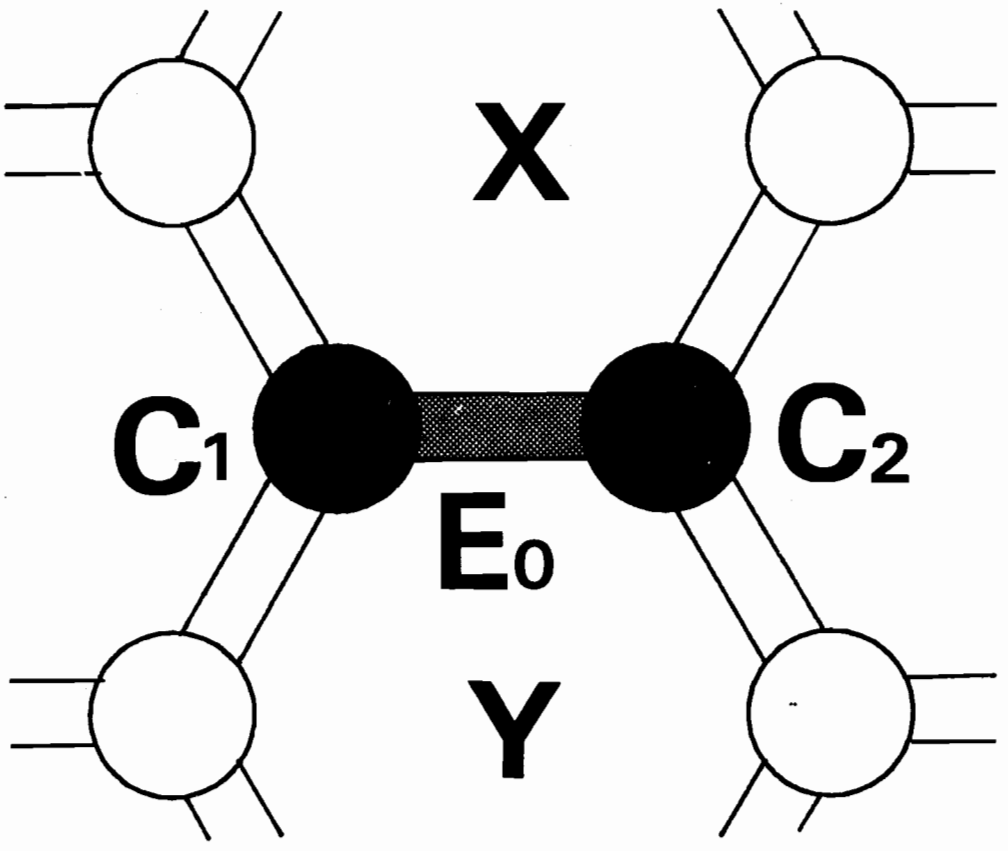


Fig. A1

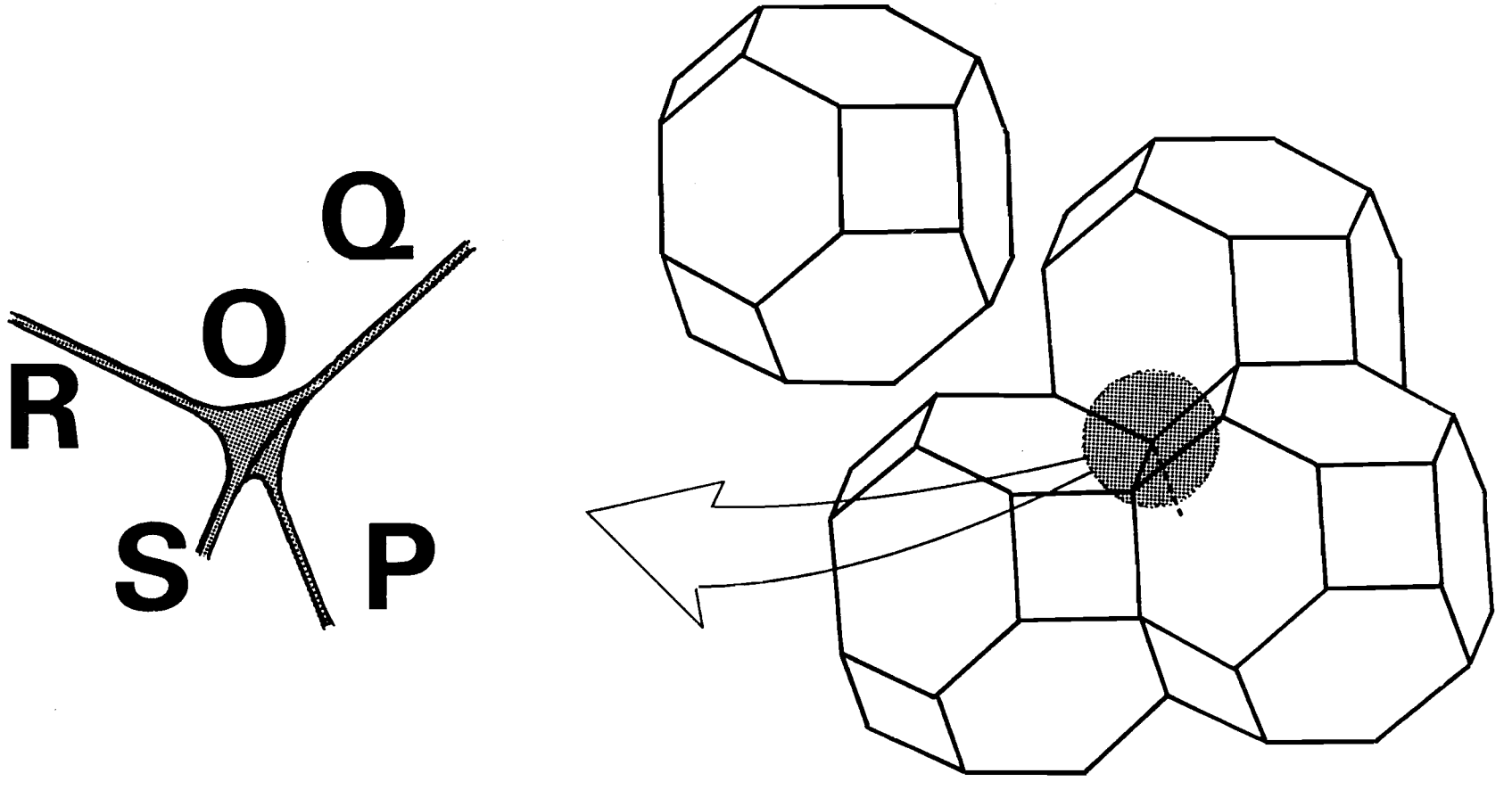


Fig. A2

Chapter 2

CONNECTIVITY OF MELT PHASE IN A PARTIALLY MOLTEN MULTIPHASE CRYSTALLINE ROCK

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Abstract

Connectivity of melt phase in a partially molten multiphase crystalline rock is considered. Under the textural equilibrium where interfacial energies among melt and solid phases control the morphology and redistribution of melt phase, permitted range of interfacial energies to exist melt phase on the corner region of multiphase grains is determined according to the combination of grain species around the corner. Microscopic connectivity between two adjacent corners could also be calculated as a function of interfacial energies. The result shows that melt phase can exist more stably and with larger volume at the corner surrounded by larger number of grains with smaller interfacial energies. By using the model of the multiphase grain control percolation (the MGCP), critical volume fraction of solid phase and melt phase where connectivity of melt phase changes drastically are obtained.

Introduction

Connectivity of melt phase in a partially molten rock is one of the most fundamental factors to control the magma transport process under the volcanic area [Frank, 1968; Turcotte, 1982; McKenzie, 1984; Scott and Stevenson, 1984; Stevenson, 1986]. Various geophysical observations such as electrical conductivity [Shankland and Waff, 1977], seismic wave propagation and attenuation [Mavko, 1980 ; Shankland et al., 1981] in the partially molten layer in earth's upper mantle are also depend on it.

From geometrical consideration, it is known that melt network can be extensively connecting if volume fraction of melt phase exceeds 0.15 [Ziman, 1979]. However, this value is an upper limit when distribution of melt phase at the grain boundary is a priori random. In partially molten layer, melt and solid phases are undergone the textural equilibrium where interfacial energies among melt and solids control the morphology and redistribution of the melt phase on the grain boundary [Bulau et al., 1979, Waff and Bulau, 1979]. Under this condition, it is enable to connect melt phase extensively even when volume fraction of melt phase is very small compared to the upper limit and the critical melt fraction can be determined theoretically [Beere, 1975; Wray, 1976; von Bargen and Waff, 1986].

As demonstrated by experimental studies [Toramaru and Fujii,

1986; Fujii et al., 1986], connectivity of melt phase in a partially molten polymineralic rock is also affected by volume fraction of minerals. Due to the variety of interfacial energies among melt and polymineralic solid phases, distribution of melt phase on the grain boundary is determined by the surrounding grain species or their combinations. For example, in a partially molten peridotite, melt phase can exist around olivine crystals and it looks like that pyroxines prevent the connection of network of melt phase [Toramaru and Fujii, 1986]. Therefore, the multiphase grain control percolation (the MGCP) [Nakano and Fujii, 1987; Chapter 1 of this paper] is a fundamental factor to estimate the connectivity of melt phase in a partially molten rock.

Although both volume fraction of melt phase and volume fraction of minerals in a partially molten polymineralic rock are important factors to determine the connectivity of melt phase, it is poorly understood about the relation between connectivity and mineral composition of the rock. In this paper, we study connectivity of melt phase as a function of both volume fraction of polymineralic solid phases and melt phase. First, thermodynamical consideration including interfacial energies will be made to determine the condition to exist melt phase on the multiphase grain boundary. This is an extension of the study for the single solid with melt system. By assuming that the system is the two dimensional and solid phases are binary hexagonal grains,

relationship between existence of melt phase on a corner and its surrounding grain species are obtained as a function of interfacial energies. And, by taking advantage of the model of the MGCP proposed by Nakano and Fujii [1987; Chapter 1 of this paper] , connectivity of melt phase will be estimated as a function of both volume fraction of solid phases and melt phase.

Thermodynamical consideration

In a partially molten system under the textural equilibrium, chemical potentials for i-th component in solid phase, M^i_S, and melt phase, M^i_M, take the same value and relate with interfacial energy, T_{SM}, between melt and solid as follows [Bulau et al., 1979] :

$$M^i_S = M^i_M = M^i_O - 2\, V^i_S\, T_{SM}\, C_{SM} \qquad [\ 1\ ]$$
$$C_{SM} = (1/2)\ (\ 1\ /\ R_{SM} + 1\ /\ R_{SM}'\ )$$

where M^i_O is chemical potential for i-th component when boundary surface is flat. V^i_S is a factor with unit of volume and equal to $((\partial M^i_M\ /\ \partial P_M)^{-1} - (\partial M^i_S\ /\ \partial P_S)^{-1})^{-1}$, where P_M and P_S are surface pressure in melt and solid phase, respectively [Landau and Lifshitz, 1970]. C_{SM} represents the mean curvature of the boundary surface between two phases. R_{SM} and R_{SM}' are principal radii of curvature and positive when they have centers inside melt phase. Since all terms in equation [1] is a constant in single solid with melt system, it becomes a constant mean curvature condition of two phase boundary [von Bargen and Waff, 1986] :

$$C_{SM} = \text{constant}. \qquad [\ 2\ ]$$

In the case of multiphase solid A, B, ... with melt system under the textural equilibrium, equation [1] becomes

$$V_A^i \, T_{AM} \, C_{AM} = V_B^i \, T_{BM} \, C_{BM} = \ldots = \text{constant}, \qquad [\ 3\ ]$$

where subscripts A, B, ... represent solid phase A, B, ..., respectively. If we assume that V_S^i takes the same value for all solid and melt phases (or $-V_S^i \times T_{SM}$ (S = A, B, ...) is regarded as newly defined interfacial energy between solid and melt phase), equation [3] can be reduced as follows :

$$T_{AM} \, C_{AM} = T_{BM} \, C_{BM} = \ldots = \text{constant}. \qquad [\ 4\ ]$$

Hereafter, binary solids, A and B, with melt system is considered and equation [4] is used for the basic equation to determine the equilibrium interface between melt and solid phases.

Since all interfacial energies is positive, equation [4] states that sign of curvature of all melt and solid interfaces is the same. If not all of the sign is the same, melt phase surrounded by the surface with positive curvature is morphologically unstable [Toramaru and Fujii, 1986]. Generally, volume of melt phase surrounded by the positive curvature surface is larger than that by negative curvature surface [Wray, 1975; von Bargen and Waff, 1986]. So, we assume that all interfaces between melt and solid has negative curvature to study the connectivity of melt phase in a partially molten rock with very small melt fraction.

To solve equation [4] explicitly, boundary conditions around the boundary surface are needed. If we assume that all interfacial energies among solid and melt phases is isotropic,

force balance at dihedral edge shown as Fig. 1 can be used for those conditions : i.e. from force balance at point P in Fig. 1, dihedral angles, Θ_{AB}^{MA} and Θ_{AB}^{MB}, can be calculated as

$$\Theta_{AB}^{MA} = \arccos((T_{AM}^2 + T_{AB}^2 - T_{BM}^2)/(2 T_{AM} T_{AB}))$$
$$\Theta_{AB}^{MB} = \arccos((T_{BM}^2 + T_{AB}^2 - T_{AM}^2)/(2 T_{BM} T_{AB})), \qquad [5]$$

where T_{AB} is the interfacial energy between two solids A and B. Note that this definition of dihedral angle is usually not used in single solid with melt system but defined as [Jurewicz and Watson, 1984]

$$\Theta = 2 \arccos(T_{SS} / (2 T_{SM})). \qquad [6]$$

However, this definition is insufficient to study the melt morphology in a partially molten multiphase solid with melt system as described in following section.

Solid phases is assumed to be the polyhedral grains. When melt fraction is very small and interfacial energies take appropriate values, melt phase exists only at the corner region of the grains as shown in Fig. 2 (a) [Bulau et al., 1979]. In this case, boundary surface of melt and solids is a part of sphere whose radius, $R_S = -1/C_{SM}$, is determined by equation [4]. However, this solution is only possible when melt phases at the corner are isolated. If melt phases at the corner region of grains are microscopically connecting shown as Fig. 2 (b), it becomes too complex to solve equation [4] because additional

boundary conditions are needed to connect melt phase smoothly [von Bargen and Waff, 1986]. In this paper, our analysis will be restricted to the critical state when melt phase at the two adjacent corners just connect with each other, so that it is enough to analyse the case when melt phase is isolately distributed at corner region of polyhedral grains.

In binary solid with melt system, there is a possibility that the existence of melt phase at each corner is determined by its surrounding grain species because solution of equation [4] with boundary condition [5] is permitted only in a limited range of interfacial energies T_{AA}, T_{BB}, T_{AB}, T_{AM} and T_{BM}. For simplicity, we assume that interfacial energies among solid phases, T_{AA}, T_{BB} and T_{AB}, take the same value : i.e.

$$T_{AA} = T_{BB} = T_{AB} = T_S. \qquad [7]$$

Geometrical consequence of this assumption is that all faces of polyhedral grains should be intersected with equal angle. In this paper, relative interfacial energies T_A and T_B between melt and solids defined as follows are used instead of T_{AM} and T_{BM}.

$$T_A = T_{AM} / T_S$$
$$T_B = T_{BM} / T_S. \qquad [8]$$

In the case of single solid with melt system, critical volume fraction of melt phase at the critical state can be estimated from equations [2] and [6] [Wray, 1975; von Bargen and Waff,

1986]. Fig. 3 (a) and (b) show the critical volume fraction of melt phase as a function of dihedral angle in two dimensional and three dimensional system. Critical volume fraction of melt phase in the three dimensional system is enable to become effectively zero when dihedral angle is less than 60° (this dihedral angle is the one defined by equation [6]). And from Fig. 3 (a) and (b), we notice that critical volume fraction of melt phase varies mildly as a function of dihedral angle. So, we firstly consider about the critical volume fraction of solid phases by obtaining the condition to exist the solution of equation [4] with boundary condition [5]. And, after the analysis, we try to get the critical melt fraction by solving the equation exactly.

Two dimensional binary hexagonal grain system

Hereafter, we call solid phases as grains. In the case that system is the two dimensional and all grains is equal size hexagon, interfaces between melt and solids are part of circles as shown in Fig. 4. In this binary grain with melt system, there are four types of corners where melt phase is enable to exist (Table 1) : e.g. corner 0 means that the corner is surrounded only by grains B, corner 1 is surrounded by one grain A and two grains B and so on.

For each types of corners, range of T_A and T_B to exist melt phase are mapped on the different area of T_A-T_B plane and obtained as follows. First, dihedral angle appeared in the corner must be enable to define : i.e.

$$\cos \theta < 1. \qquad [9]$$

Secondly, edge length, L, of melt phase, which is a distance from corner of grains (point 0 in Fig. 4) to intersection point of two interfaces between melt and grain, must be positive : i.e.

$$L > 0. \qquad [10]$$

For each type of corner in the two dimensional binary hexagonal grains with melt system, edge length expressed by dihedral angles is represented as follows.

Corner 0 (B-B-B corner) :

$$L_{BB}^{MB} = R_B \left((1/3^{1/2}) \cos \Theta_{BB}^{MB} - \sin \Theta_{BB}^{MB}\right) \qquad [11]$$

Corner 1 (A-B-B corner) :

$$\begin{aligned} L_{AB}^{MB} &= R_A \left((1/3^{1/2}) \cos \Theta_{AB}^{MA} - \sin \Theta_{AB}^{MA}\right) \\ &= R_B \left((2/3^{1/2}) \cos \Theta_{BB}^{MB} - \right. \\ &\qquad \left. (1/3^{1/2}) \cos \Theta_{AB}^{MB} - \sin \Theta_{AB}^{MB}\right) \end{aligned} \qquad [12]$$

$$\begin{aligned} L_{BB}^{MA} = R_B \left((2/3^{1/2}) \cos \Theta_{AB}^{MB} - \right. \\ \left. (1/3^{1/2}) \cos \Theta_{BB}^{MB} - \sin \Theta_{BB}^{MB}\right) \end{aligned} \qquad [13]$$

Corner 2 (A-A-B corner) :

$$\begin{aligned} L_{AB}^{MA} &= R_B \left((1/3^{1/2}) \cos \Theta_{AB}^{MB} - \sin \Theta_{AB}^{MB}\right) \\ &= R_A \left((2/3^{1/2}) \cos \Theta_{AA}^{MA} - \right. \\ &\qquad \left. (1/3^{1/2}) \cos \Theta_{AB}^{MA} - \sin \Theta_{AB}^{MA}\right) \end{aligned} \qquad [14]$$

$$\begin{aligned} L_{AA}^{MB} = R_A \left((2/3^{1/2}) \cos \Theta_{AB}^{MA} - \right. \\ \left. (1/3^{1/2}) \cos \Theta_{AA}^{MA} - \sin \Theta_{AA}^{MA}\right) \end{aligned} \qquad [15]$$

Corner 3 (A-A-A corner) :

$$L_{AA}^{MA} = R_A \left((1/3^{1/2}) \cos \Theta_{AA}^{MA} - \sin \Theta_{AA}^{MA}\right) \qquad [16]$$

In these equation, R_A and R_B are radius of circles which bound the grain A and B and melt phase, respectively and take the values determined by equation [4] :

$$\begin{aligned} R_A &= -1/(2\ C_{AM}) = T_A\ R \\ R_B &= -1/(2\ C_{BM}) = T_B\ R \end{aligned} \qquad [17]$$

where R is a constant.

For corner 0 and 3 (equation [11] and [16]), conditions described in equations [9] and [10] are satisfied if

$$1/2 < T_B < 1/3^{1/2} \qquad [18]$$

and

$$1/2 < T_A < 1/3^{1/2}, \qquad [19]$$

respectively. Left hand sides of the inequalities in [18] and [19] represent the conditions described by equation [9]. And right hand sides denote the conditions for negative curvature of interfaces between melt and solids (i.e. positive value of edge length of melt phase , L, in equation [10]). For corner 2 and 3, range of T_A and T_B can not be simply expressed like [18] and [19]. By the numerical calculation about the conditions described by equations [9] and [10] for equations [12] and [13], we get Fig. 5 which shows the range of T_A and T_B where melt phase can exist on corner 2. As comparing equations [14] and [15] to equations [12] and [13], it is clear that the range of T_A and T_B for corner 3 becomes the one which T_A and T_B is exchanged on Fig. 5. By superimposing these ranges, we can get the relationships between relative interfacial energies, T_A and T_B, and the corner type where melt phase can exist (Fig. 6).

It is enough to consider only the case of $T_A > T_B$ on T_A-T_B map

shown in Fig. 6. If melt phases surrounded by interfaces with positive curvature and negative curvature coexist in a system, melt phase surrounded by interface with positive curvature is morphologically unstable [Toramaru and Fujii, 1986]. Therefore, melt phase can exist only in the one of four areas numbered from 1 to 4 on the T_A-T_B map. In area 1, it is enable to stably exist melt phase on corner 0 alone. In area 2, melt phase can coexist stably on corner 0 and 1. And in area 3 and 4, it is enable to coexist melt phase on corner 0, 1 and 2 and 0, 1, 2 and 3, respectively. From this classification, we know that melt phase always exists on corner 0 when melt phase can be located at the corner surrounded by grain A. In other words, melt phase covered with grain B alone is the most stable.

Volume (or area in present analysis) of melt phase on each types of corner can be obtained in the case that interfacial energies lie in the range to exist melt phase on the corner. It can be expressed by the dihedral angles (equations [5] and [8]) and the edge lengths of melt phase (equations [11] - [16]) as follows.

Corner 0 (B-B-B corner) :

$$S_0 = 3 R_B^2 ((L_{BB}^{MB} / R_B) \cos \Theta_{BB}^{MB} + \Theta_{BB}^{MB} - \pi/6) \qquad [20]$$

Corner 1 (A-B-B corner) :

$$S_1 = R_B^2 ((L_{BB}^{MA} / R_B) \cos \Theta_{BB}^{MB} + \Theta_{BB}^{MB} +$$

$$(L_{AB}^{MB} / R_B) \cos \theta_{AB}^{MB} + \theta_{AB}^{MB} - \pi/3) + \quad [21]$$
$$R_A^2 ((L_{AB}^{MB} / R_A) \cos \theta_{AB}^{MA} + \theta_{AB}^{MA} - \pi/6)$$

Corner 2 (A-A-B corner) :

$$S_2 = R_A^2 ((L_{AA}^{MB} / R_A) \cos \theta_{AA}^{MA} + \theta_{AA}^{MA} +$$
$$(L_{AB}^{MA} / R_A) \cos \theta_{AB}^{MA} + \theta_{AB}^{MA} - \pi/3) + \quad [22]$$
$$R_B^2 ((L_{AB}^{MA} / R_B) \cos \theta_{AB}^{MB} + \theta_{AB}^{MB} - \pi/6)$$

Corner 3 (A-A-A corner) :

$$S_3 = 3 R_A^2 ((L_{AA}^{MA} / R_A) \cos \theta_{AA}^{MA} + \theta_{AA}^{MA} - \S/6). \quad [23]$$

Since R_A and R_B contain an arbitary constant, R, as shown in equation [17], these equations can give us the informations only about the relative values of the volume of melt phase on each types of corner. By calculating the relative values, the order of volume of melt phase on each types of corner can be obtained as follows :

$$S_0 > S_1 > S_2 > S_3. \quad [24]$$

Therefore, melt phase at the corner surrounded only by grain B is the most largest.

To connect melt phase on two adjacent corners (Fig. 7), sum of two edge length of melt phase, L_{CEC}, obtained from equation [11] - [16] should be greater than edge length of the grain, L_E :

$$L_E < L_{CEC}. \quad [25]$$

We call two adjacent corner as a CEC unit. In the two dimensional binary hexagonal grain with melt system, there are nine types of CEC unit shown in Table 2. Each unit is constructed by combination of various types of corners and, therefore, conditions to connect melt phase as described by equation [20] are different among them. If we assume that edge length, L, of a CEC unit is zero when melt phase can not exist on one of two corners, we can regards the relative value of L_{CEC} for each CEC unit as microscopic connectivity : i.e. CEC unit with the largest L_{CEC} is the most connective. Name of CEC unit (0 - 8) shown in Table 2 is determined by this connective order : i.e.

$$L_{CEC0} > L_{CEC1} > \ldots > L_{CEC8}. \qquad [26]$$

Therefore, if CEC unit 8 is microscopically connecting, all CEC units are microscopically connecting. In other words, melt phase covered with grain B alone is the most connective, because CEC unit 0 is constructed by two corner 0 which are surrounded only by the grain B.

The multiphase grain control percolation

As demonstrated in the previous section, existence of melt phase on the corner in the binary grain with melt system under the textual equilibrium is determined by the surrounding grain species through relative interfacial energies, TA and TB. To connect such a localized melt phase extensively over the system, three elementary conditions must be satisfied : (1) Melt phases exist both on the two adjacent corners and (2) they are microscopically connecting. (3) These two conditions are realized extensively over the system. Condition (1) and (2) are related with interfacial energies shown in previous section. The model of the multiphase grain control percolation (the MGCP) proposed by Nakano and Fujii [1987; Chapter 1 of this paper] is a simple model to consider the condition (3).

Outline of the model of the MGCP is as follows. For simplicity, we consider the corner percolation which treats the melt network constructed by the melt phase on the corner. According to the naming of the MGCP, a corner where melt phase can exist is called as an occupied corner. Basic assumption of the MGCP is that distribution of occupied corners is determined by some rule specified by the surrounding grain species or their combinations. If the rule is specified and grains are assumed to be well-mixed, relation between the number density (or volume fraction if all grain is assumed to be equal size) of grain A (or B) and

number density of occupied corner can be obtained statistically. Connectivity of melt phase is defined as a probability that some fraction of the occupied corners belong to the infinite cluster of occupied corners. From numerical simulation or, in some cases, analytic procedures supported by percolation theory [Stauffer, 1981], we can obtain critical grain fraction of grain A (or B) where connectivity of melt phase changes drastically.

First, we try to estimate the connectivity of melt phase in the two dimensional binary hexagonal grain with melt system without considering the condition (2) : i.e. we regard that melt phase is always microscopically connecting when two adjacent corners are occupied. Area 1 - 4 of interfacial energies shown in Fig. 6 can be translated into the rule which determines the types of corners where melt phase can exist. This rule is almost the same one used by Nakano and Fujii [1987; Chapter 1 of this paper] :

> If a corner is surrounded by at least M (i.e. 0 - 3) of grains B among the adjacent 3 grains, it is occupied.

From Table 1 about the corner percolation presented by Nakano and Fujii [1987; Chapter 1 of this paper], we can obtain the critical grain fraction of grain B for area 1 - 4 on TA-TB map in Fig. 6 (Table 3 (a)). This result shows that, at any conditions in consideration (i.e. system is undergone the textural equilibrium and melt fraction is very small), it is always

enable to connect melt phase extensively when the volume fraction of grains with smaller interfacial energy (i.e. grain B) exceeds 0.8 (80 %).

If we take the condition (3) into consideration, CEC unit is a element which constructs the melt network. Classification of CEC unit obtained in previous section can be regarded as the rule of the MGCP. If we slightly modify the corner-edge (CE) percolation [Nakano and Fujii, 1987; Chapter 1 of this paper], it is easy to obtain the connectivity of melt phase as a function of types of CEC unit which is microscopically connecting. In Table 2 (b), critical grain fraction of grain B is shown as a function of the types of CEC units. Obviously, this result becomes the more specified version of the case of the corner percolation described above.

When volume fraction of grain B exceeds 0.8 in the binary hexagonal grain system, critical volume fraction of melt phase can be easily calculated as follows. In this condition, connective melt network is possible to covered mainly with grain B. As described in equation [26], the most connective CEC unit is the one covered with grain B, so that it is enough to consider the critical state that edge length of melt phase on corner O is equal to a half of edge length of the hexagonal grains :

$$L_{BB}^{MB} = 1/2\ L_E. \qquad [27]$$

Combining it with equations [11] and [17], an arbitary con-

stant R is expressed as a function of L_E and relative interfacial energies. And by using equations [11] - [16] and [20] - [23], volume fraction of melt phase on each types of corners can be expressed as a function of L_E and dihedral angles. Since number densities of each types of corners are determined by the volume fraction of grains as shown in Table 1, critical volume fraction of melt phase, F, becomes as follows :

$$F = (8\ 3^{1/2} / L_E^2)\ (\ \phi_B^3\ S_0 + 3\ \phi_A\ \phi_B^2\ S_1 + 3\ \phi_A^2\ \phi_B\ S_2 + \phi_A^3\ S_3\ ), \qquad [28]$$

where ϕA and ϕB are volume fraction of grain A and B, respectively. Note that volume of melt phase is zero on the corner which is not satisfied with the condition of relative interfacial energies as shown in Fig. 6. Examples of critical volume fraction of melt phase as a function of relative interfacial energies are shown in Fig. 8.

Discussion

In previous section, we restrict ourselves to consider the connectivity of melt phase in the two dimensional system. In the three dimensional system, it is expected that correspondence between the types of corners and classification of the area of interfacial energies on T_A-T_B map is similar with that in two dimensional system. Since melt phase always exists on the corners surrounded only by the grain B when the two dimensional binary hexagonal system is under the condition in consideration, therefore, in the three dimensional system, it should be also realized that existence of melt phase is easy on the corner surrounded only by the grain B. This condition means that melt network is connective if grain B around the melt phase is extensively connecting. In other words, connective melt network in a partially molten system can be covered only with grains with smallest relative interfacial energy.

This situation can be observed in some partial melting experiments of the peridotite [Toramaru and Fujii, 1986; Fujii et al., 1986]. In a partially molten peridotite composed of olivine and pyroxene, relative interfacial energies of olivine is generally small compared to that of pyroxene [Toramaru and Fujii, 1986]. Therefore, it can be predicted that melt network in partially molten peridotite is almost covered with olivine tube. The MGCP can be applicable to estimate the volume fraction

of olivine for such connective melt network. By using the value calculated by Nakano and Fujii [1987; Chapter 1 of this paper], critical volume fraction for binary tetrakaidecahedral grains which is usually adopted in the three dimensional model is 0.63. So, we can predicted that melt network can be connective in a partially molten peridotite under the textural equilibrium if volume fraction of olivine exceeds 0.63 (63 %).

In the three dimensional case critical volume fraction of melt phase is calculable when melt phase can exist only on the corners surrounded by grain B. In this case, number density of the corner with melt phase, p, is calculated as

$$p = \phi^N \qquad [29]$$

where ϕ is volume fraction of grain B and N is numbers of grains around the corner. This relation is hold at critical state and, therefore, critical volume fraction of melt phase in binary solid with melt system takes the value multiplied the critical volume fraction of melt phase in single solid by p. Since critical volume fraction of grain B is 0.63 in the three dimensional tetrakaidecahedral grain system (N = 4), critical volume fractions of melt phase takes the value as shown in Fig. 2 (b) multiplied by 0.157.

In this paper, variations among solid-solid interfacial energies are neglected. Validity of this assumption is not obvious because there are a little experimental measurement of inter-

facial energies. In a partially molten synthetic peridotite composed of olivine and orthpyroxene, Fujii et. al. [1986] reported that interfacial energies among solid phases took almost the same value. To judge the validity of this assumption, it is expected that many measurements of dihedral angles defined by equation [5] (Fig. 1) instead of equation [6] are performed in the future.

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Figure captions

Fig. 1 Definition of dihedral angles, Θ_{AB}^{MA} and Θ_{AB}^{MB}. At a intersection point, P, of three interfaces among solids and melt phases, three forces T_{AM}, T_{BM} and T_{AB} denoted as thick arrows are balanced.

Fig. 2 Sketches of melt shape in a partially molten system. (a) Melt phase exists at the corner of grain in isolation. (B) Melt phases at adjacent two corners are macroscopically connecting.

Fig. 3 Critical volume fraction of melt phase, F, and mean curvature of solid - melt interface, C, expressed by dihedral angle, theta (defined by equation [6] in text). These diagram are drawn for the system composed of single solid with melt phase. Solid phase is assumed to be (a) the two dimensional hexagonal grains and (b) the three dimensional beta-tetrakaidecahedron [Wray, 1975], respectively. Value of F_C and F_O are 0.00622 (0.622 %) and 0.03562 (3.562 %), respectively.

Fig. 4 Schematic picture showing melt shape at a corner of the two dimensional hexagonal grain. R_A, R_B and R_C are radius of circles bounded melt phase on solid phases A, B and C, respectively. T_A, T_B and T_C are relative interfacial energies between melt phase and solid phase A, B and C, respectively (defined by equation [8] in text). L_{AB}^{MC}, L_{AC}^{MB} and L_{BC}^{MA} are distances from corner of hexagon, O, to intersection point of three interfaces

among melt phase and two solid phases, A and B, A and C and B and C, respectively. In text, these distances are called as edge length of the melt phase.

Fig. 5 Permitted range of relative interfacial energies, T_A and T_B, to exist melt phase on corner type 2 in the two dimensional binary hexagonal grain with melt system under the textural equilibrium.

Fig. 6 Classification of the region on the map of relative interfacial energies, T_A and T_B. According to the conditions to exist melt phase on the four types of corners in binary hexagonal grain with melt system under the textural equilibrium, four area labeled by 1 - 4 can be identified in the case of $T_A > T_B$. In area 1, it is possible to exist melt phase on corner type 0 alone. In area 2, melt phase can exist on both corner type 0 and 1. In area 3 and 4, melt phase is possible to exist on corner type 0, 1 and 2 and 0, 1, 2 and 3, respectively.

Fig. 7 Schematic figure showing the edge length of melt phase, L_1 and L_2, and edge length of the the hexagonal grain, L_E. Microscopic connectivity of the CEC unit, L_{CEC}, described in text is $L_1 + L_2$. Shaded area is melt phase.

Fig. 8 Critical volume fraction of melt phase to connect melt network extensively over the system expressed as a function of relative interfacial energies, T_A and T_B, in the two dimensional

hexagonal binary grain with melt system under the textural equilibrium. Thick lines denote the boundaries of permitted range to exist melt phase at various types of corner as shown in Fig. 6. Numerics represent the values of critical melt fraction. Volume fractions of the grain B (i.e. solid phase with smaller relative interfacial energy) are (a) 0.8 and (b) 0.9, respectively.

Table 1 Name of corner

Corner name	Configuration	Probability*
0	B >- B (B)	ϕ_B^3
1	B >- A (B)	$3\,\phi_A\,\phi_B^2$
2	A >- A (B)	$3\,\phi_A^2\phi_B$
3	A >- A (A)	ϕ_A^3

---

* ϕ_A and ϕ_B are number density of grain A and B, respectively.

Table 2 (a) Name of CEC unit

CEC 0	CEC 1	CEC 2
B B >-< B B	B B >-< A B B A >-< B B	B A >-< A B
CEC 3	**CEC 4**	**CEC 5**
A B >-< B B B B >-< B A	A A >-< B B B A >-< B A A B >-< A B B B >-< A A	A A >-< A B B A >-< A A
CEC 6	**CEC 7**	**CEC 8**
A B >-< B A	A A >-< B A A B >-< A A	A A >-< A A

Table 2 (b) Specification of CEC unit

CEC Name	Edge length	Probability*	Corner Name
0	$2\ L_{BB}^{MB}$	ϕ_B^4	0,0
1	$L_{BB}^{MA} + L_{BB}^{MB}$	$2\ \phi_A\ \phi_B^3$	0,1
2	$2\ L_{BB}^{MA}$	$\phi_A^2\ \phi_B^2$	1,1
3	$2\ L_{AB}^{MB}$	$2\ \phi_A\ \phi_B^3$	1,1
4	$L_{AB}^{MA} + L_{AB}^{MB}$	$4\ \phi_A^2\ \phi_B^2$	1,2
5	$2\ L_{AB}^{MA}$	$2\ \phi_A^3\ \phi_B$	2,2
6	$2\ L_{AA}^{MB}$	$\phi_A^2\ \phi_B^2$	2,2
7	$L_{AA}^{MA} + L_{AA}^{MB}$	$2\ \phi_A^3\ \phi_B$	2,3
8	$2\ L_{AA}^{MA}$	ϕ_A^4	3,3

* ϕ_A and ϕ_B are number density of grain A and B, respectively.

Table 3 Critical fraction of grain B in binary hexagonal grain system

Corner percolation

Corner names	area	critical fraction
0	1	0.80
0 - 1	2	0.55
0 - 2	3	0.29
0 - 3	4	0.00**

CEC percolation

CEC unit names	critical fraction
0	0.80
0 - 1	0.80
0 - 2	0.80
0 - 3	0.55
0 - 4	0.50
0 - 5	0.50
0 - 6	0.29
0 - 7	0.20
0 - 8	0.00**

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* area on the map of interfacial energies, TA and TB numbered in Fig. 6.

** always connecting.

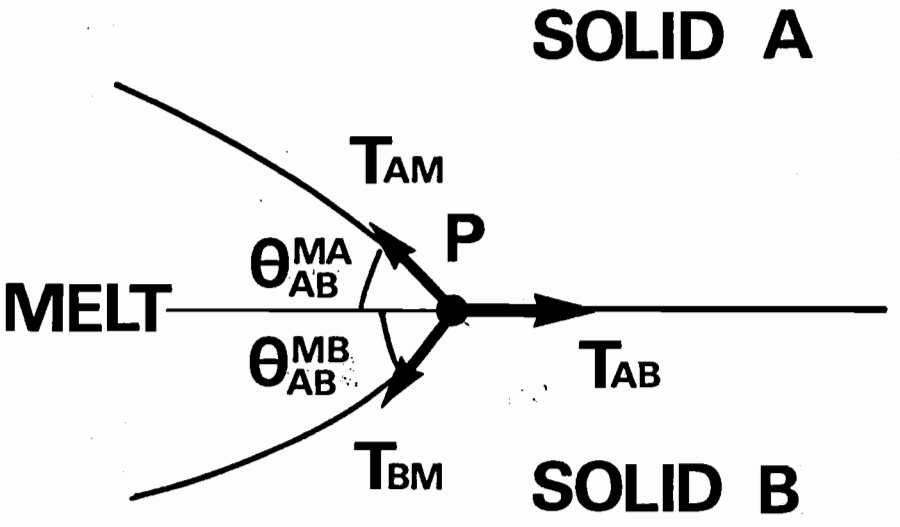


Fig. 1

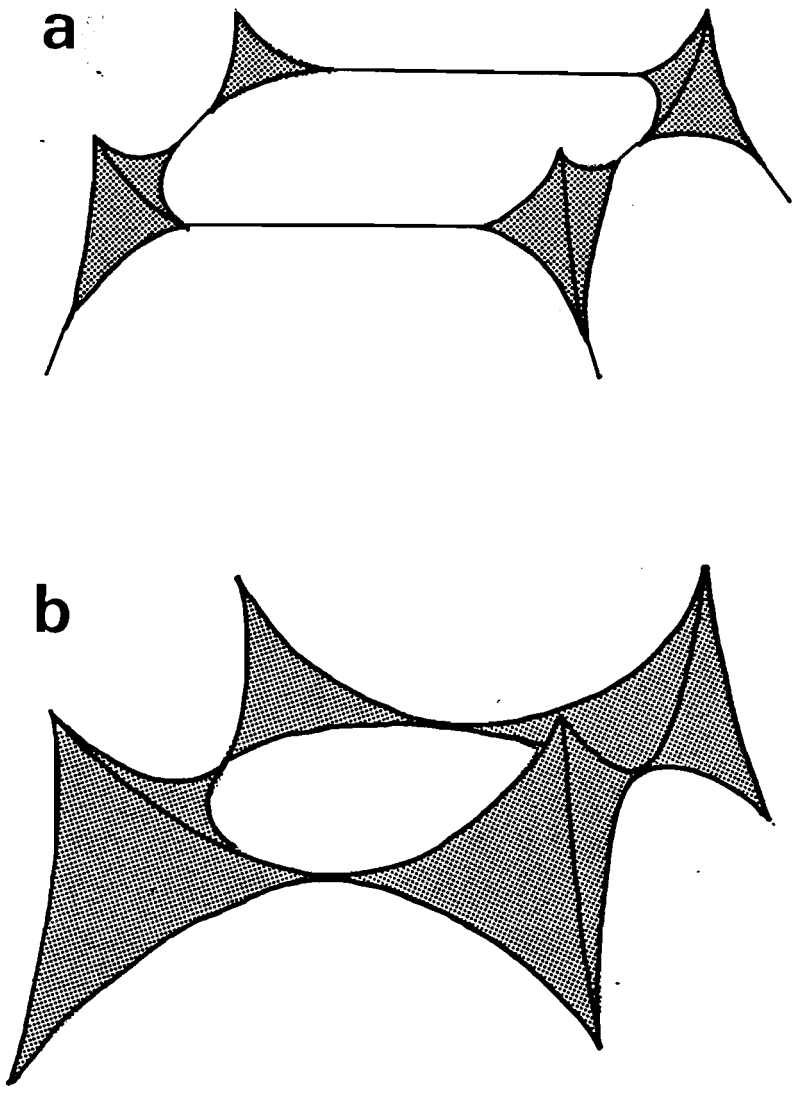


Fig.2

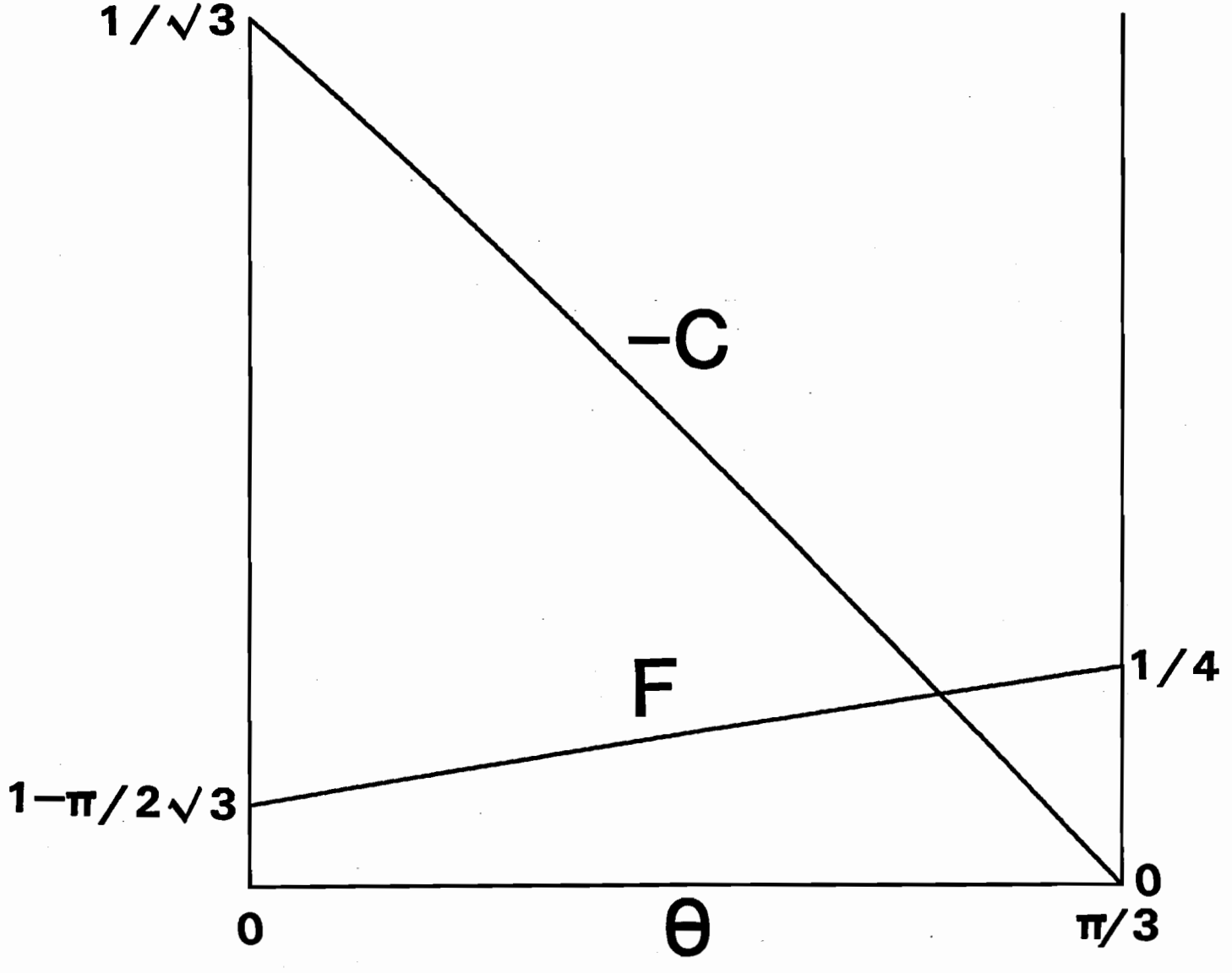
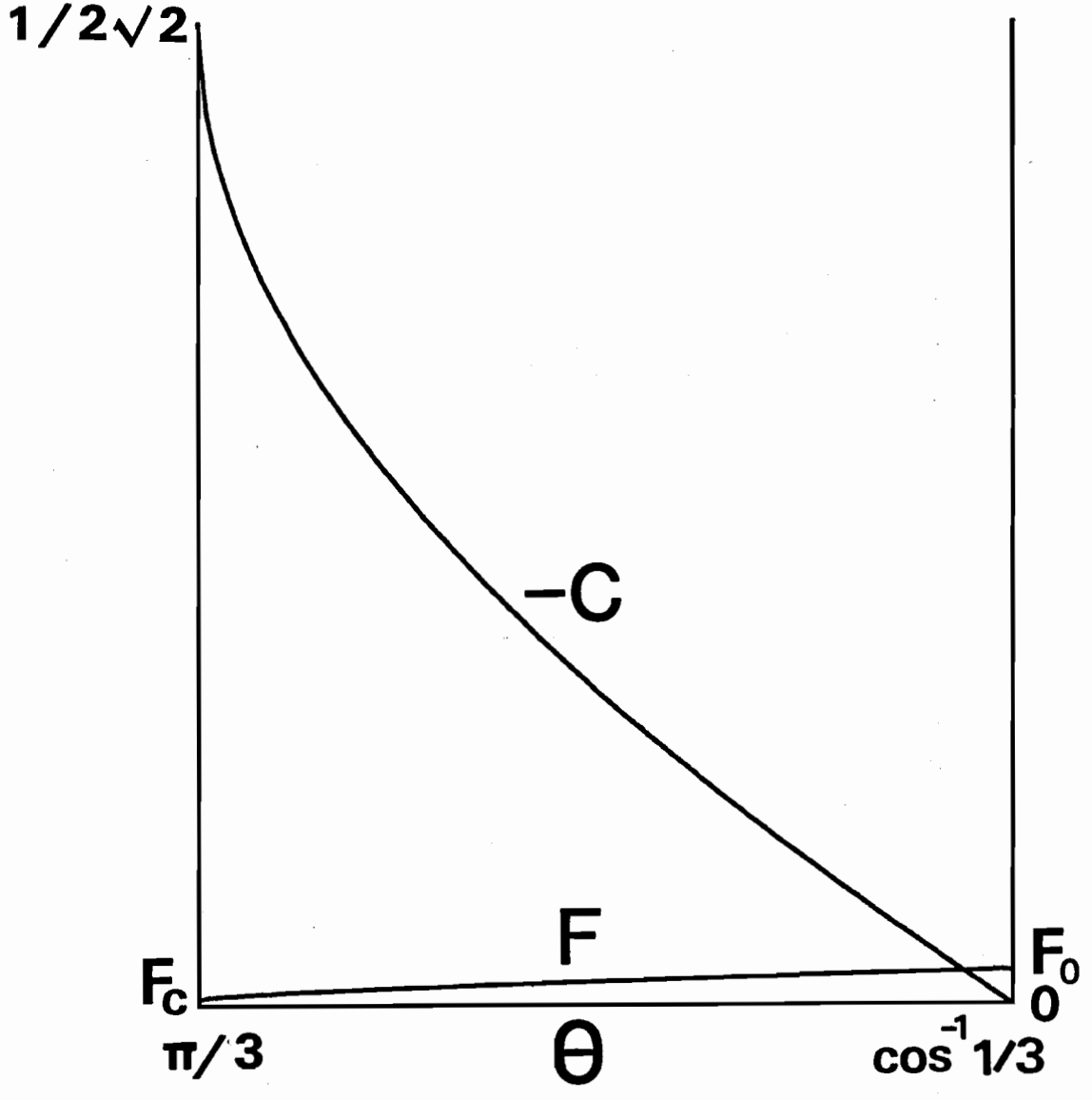


Fig.3(a)



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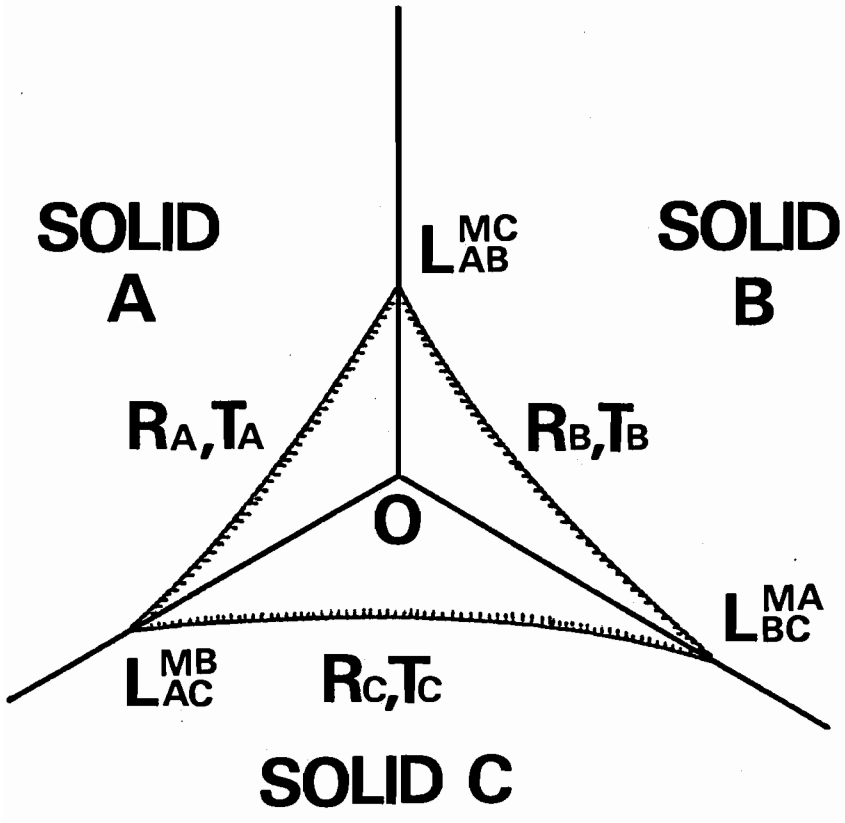

Fig.4

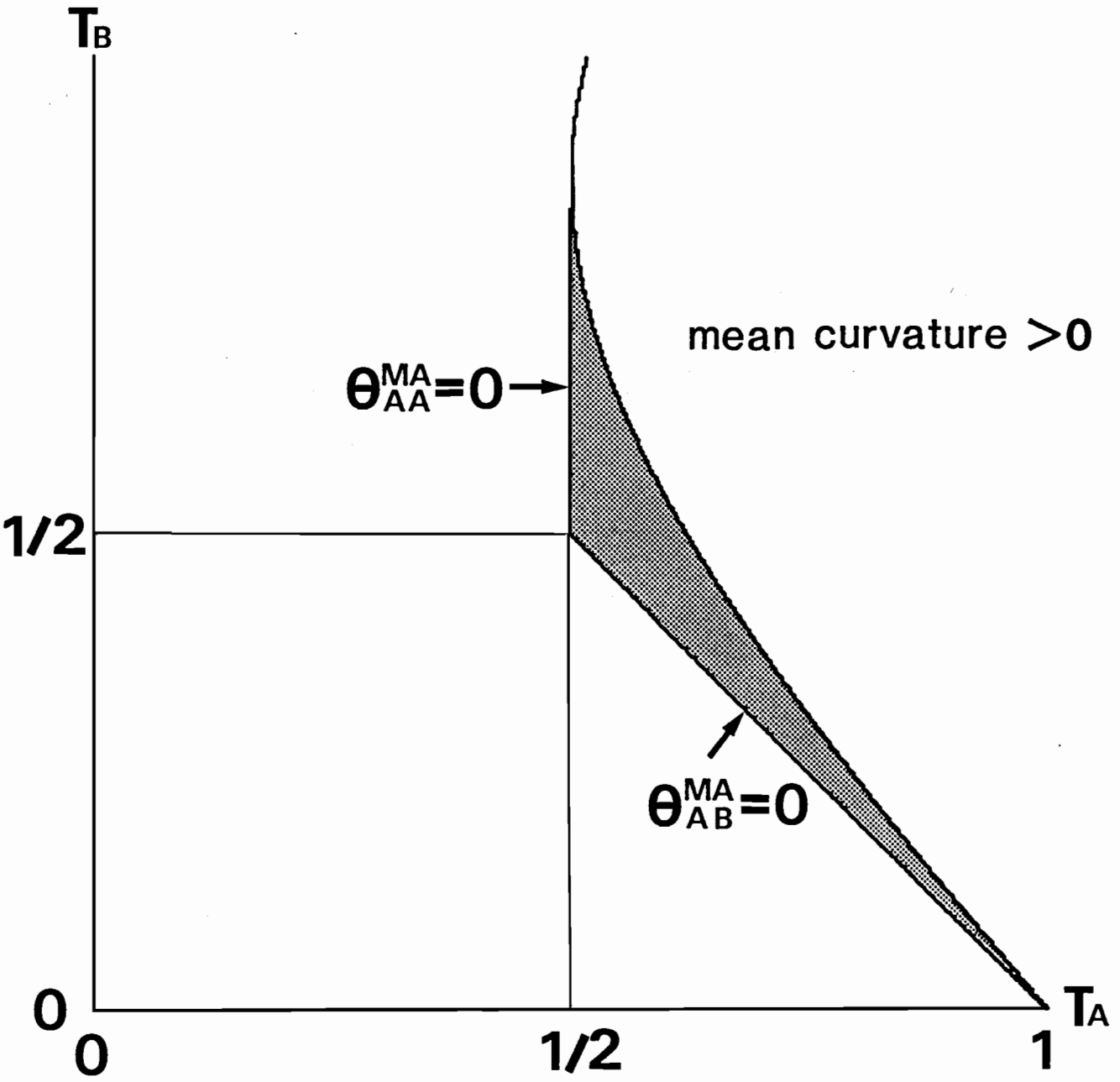

Fig.5

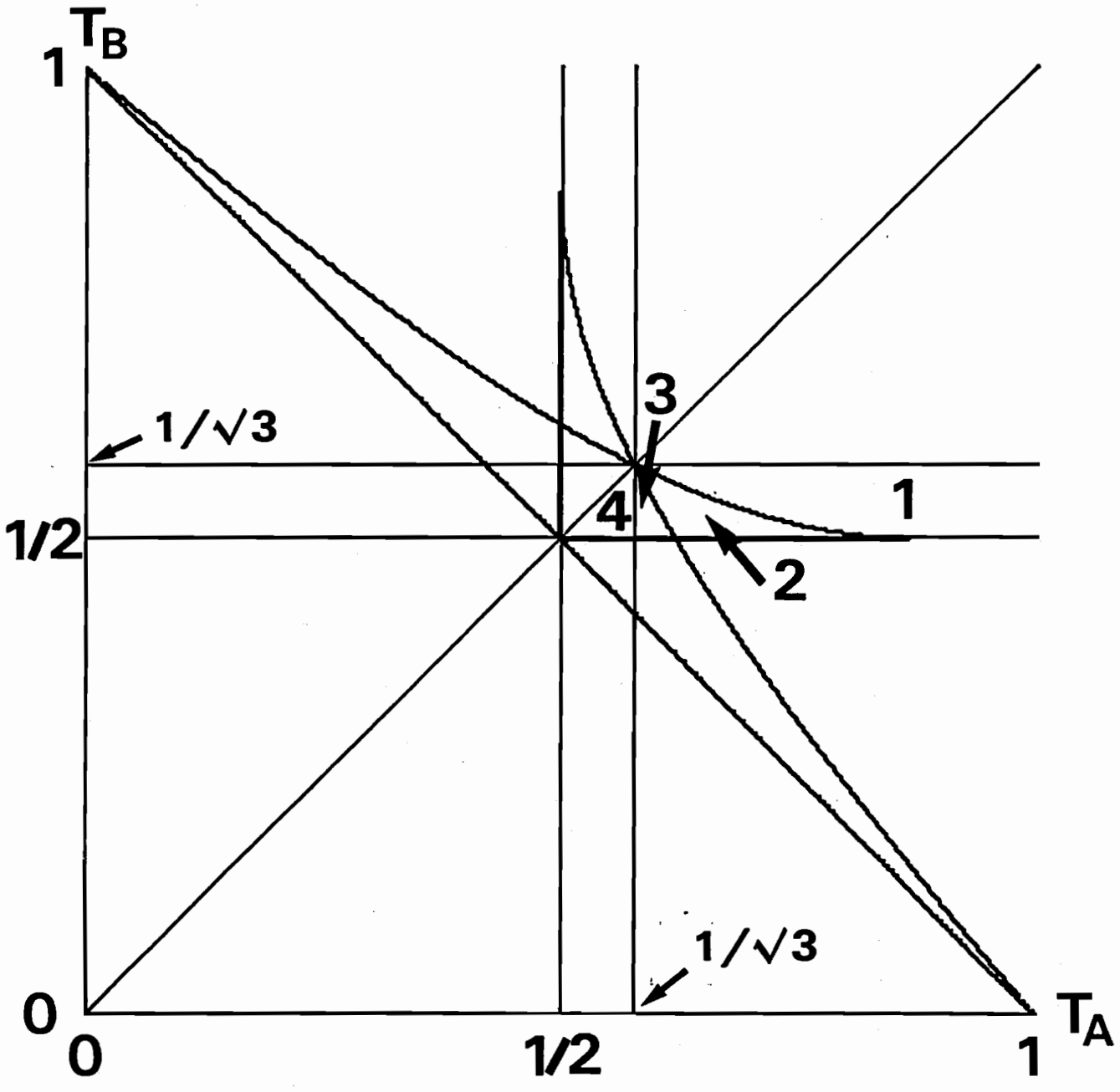

Fig.6

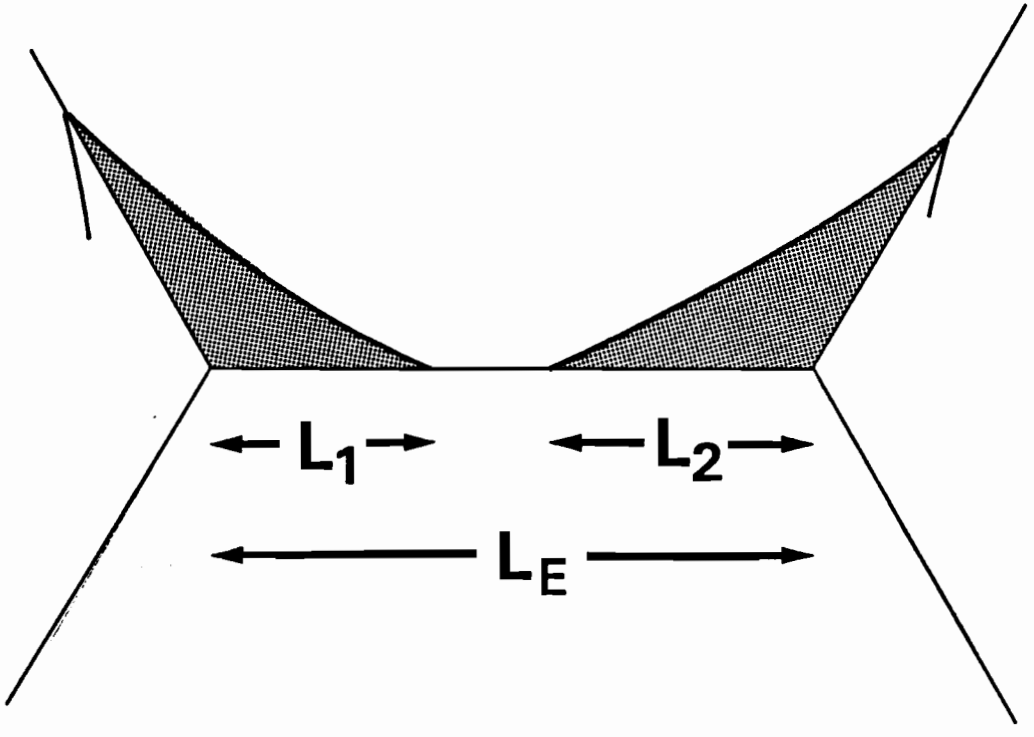

Fig.7

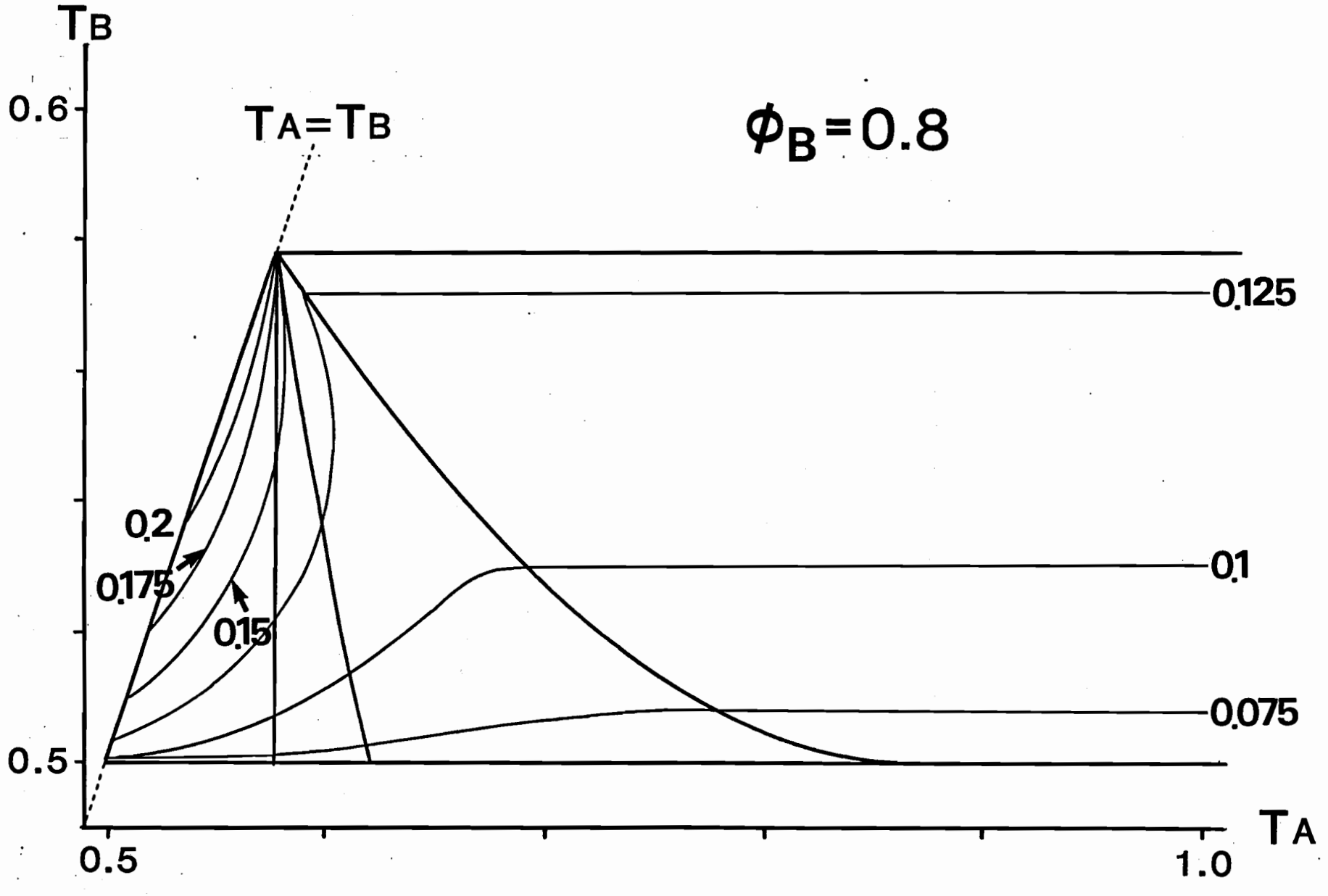

Fig.8(a)

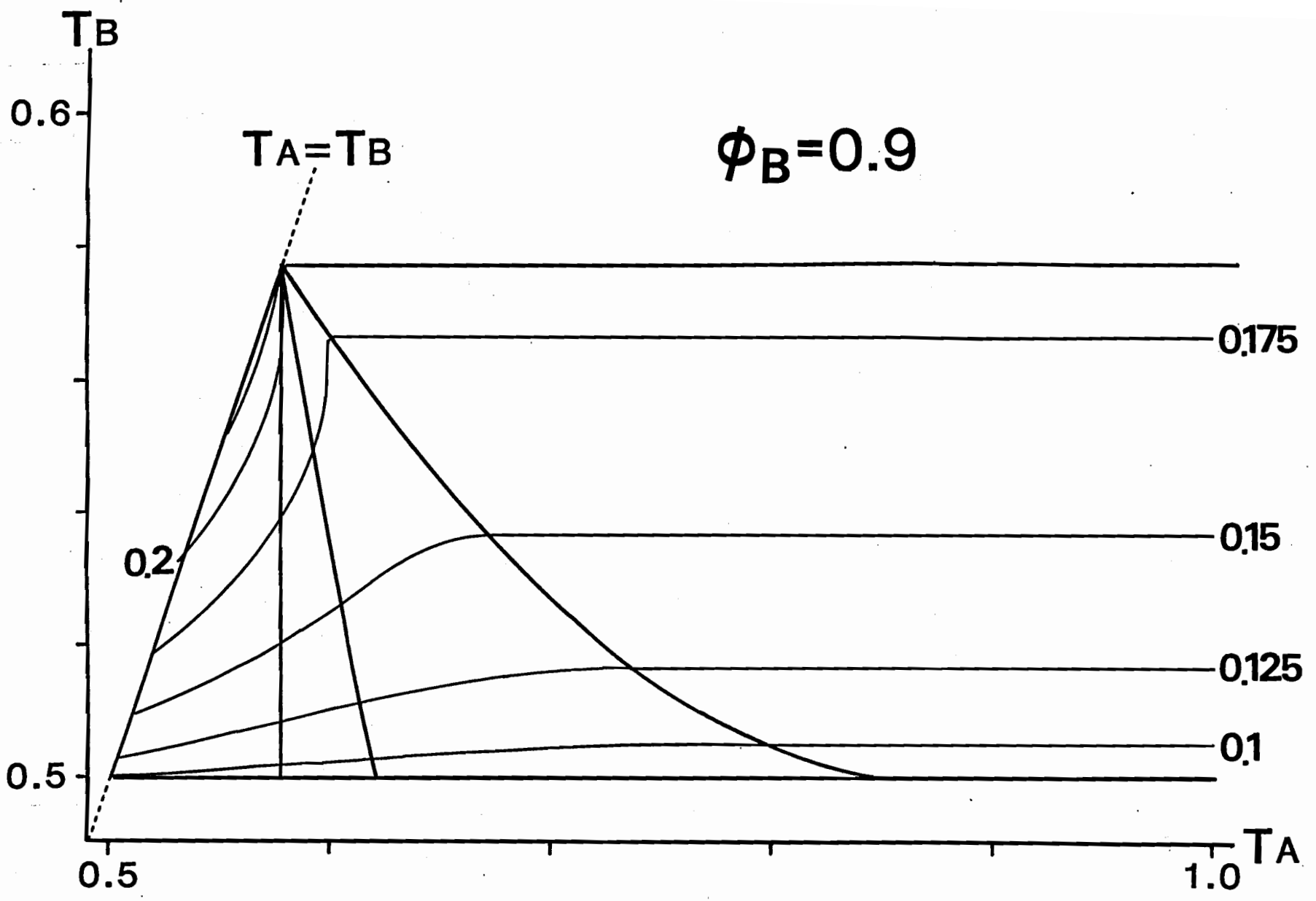

Fig.8(b)