

Research
Report

Design of Grain Oriented Microstructure by the Monte Carlo Simulation of Sintering and Isotropic Grain Growth

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等方的粒成長下での焼結・粒成長のモンテカルロシミュレーション による粒子配向組織設計

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Abstract

Fabrication of dense and highly textured ceramics is significantly important for the improvement of their anisotropic properties by the templated grain growth (TGG) method. Monte Carlo simulation based on the Potts model was carried out through computation for the design of TGG processing, in which anisometric template particles are mixed with fine matrix particles and organic binder and aligned by tape casting before heat treatment. Thus, four initial parameters affecting the microstructure after sintering with isotropic grain growth were investigated; 1) mixing ratio of template/matrix particles, 2) size and 3) aspect ratio of the template particles, and 4) initial porosity (caused

by the removal of binder). The fraction of oriented grains in the simulated microstructure was found to increase with increasing template/matrix mixing ratio and aspect ratio of template, and with decreasing template size and initial porosity. The residual porosity was shown to decrease with decreasing template/matrix mixing ratio and template size, and with decreasing initial porosity. The study suggests that computational design would give a guiding principle in terms of the initial preparation conditions for the ceramics having both a large fraction of oriented grains and low residual porosity.

Keywords

Computer simulation, Textured ceramics, Microstructural design, Templated grain growth, Isotropic grain growth

要 旨

テンプレート粒成長法 (TGG法) で作製する機能性セラミックスの異方的な物理特性を向上させるためには、高密度、高配向度のセラミックスの作製が重要である。そうした機能性セラミックスの設計を目的として、Pottsモデルに基づくモンテカルロシミュレーションを行った。ここで、TGG法は、異形状のテンプレート粒子と微細なマトリックス粒子およびバインダーの混合工程と、熱処理の前工程として行うテープ成形によるテンプレート粒子の配向工程と、からなる。そこで、作製するセラミックスの微細構造に影響する4つの因子について検討した。つまり、テンプレ

ート粒子の(1)配合割合、(2)粒径、(3)アスペクト比と、(4)初期気孔率 (バインダーの脱脂に起因) である。計算微組織中の配向粒子の割合は、テンプレート粒子の配合割合およびアスペクト比が増大するほど増加し、また、テンプレート粒子の粒径と初期気孔率が減少するほど増加した。さらに、残余気孔率は、テンプレート粒子の割合と粒径および初期気孔率が減少するほど減少した。このように、本研究は、シミュレーションによる設計によって、配向粒子の割合が高く、かつ、残余気孔率が低いセラミックスを合成するための初期条件の選定に重要な指針が得られることを示唆した。

キーワード

計算機シミュレーション, 配向セラミックス, セラミックス微細組織設計,
テンプレート粒成長法, 等方粒成長

1. Introduction

Texture engineering is an effective approach to enhancing the mechanical properties (*e.g.*, fracture toughness and bending strength) or physical properties (*e.g.*, piezoelectric, pyroelectric, magnetic and thermoelectric properties) of ceramics composed of crystals with anisotropy in these properties. Among the several proposed texturing methods, tape casting was applied to fabricate the piezoelectric PbNb_2O_6 ,¹⁾ Bi_2WO_6 ²⁾ and $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ ^{3, 4)} ceramics with preferred orientation. The strategy of this method evolved into the templated grain growth (TGG) method. The TGG method was developed to fabricate highly textured ceramics: *e.g.*, Si_3N_4 ,⁵⁾ Al_2O_3 ,⁶⁻⁸⁾ $\text{Al}_2\text{O}_3 \cdot 3\text{SiO}_2$ (Mullite),⁹⁾ BaTiO_3 ,¹⁰⁾ $\text{CaBi}_4\text{Ti}_4\text{O}_{15}$,¹¹⁾ $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})_3\text{-PbTiO}_3$,^{12, 13)} $(\text{ZnO})_5\text{In}_2\text{O}_3$,¹⁴⁾ $(\text{Ca}_{2.70}\text{Na}_{0.15}\text{Bi}_{0.15})\text{Co}_4\text{O}_9$ ¹⁵⁾ and Na_xCoO_8 .¹⁶⁻¹⁷⁾ In this method, a small amount of template particles with an anisotropic (*e.g.*, platelike or needlelike) shape are used as the seed materials for the grain growth. The template particles are aligned with a specific orientation by tape casting and then upon heat treatment they grow at the expense of matrix particles (*i.e.*, fine and equiaxed particles). Thus, the development of the texture gives a unique microstructure with enhanced mechanical or physical properties.

For the increase in these properties, both a high density (low residual porosity) and a high degree of orientation (large fraction of oriented grains) are significantly important. The TGG method is typically composed of the following processing stages: 1) mixing template particles, matrix particles and organic binder, 2) tape casting and stacking to form a green compact, 3) dewaxing the binder from the compact and 4) sintering the dewaxed body to make a dense ceramic. Thus, various initial (*i.e.*, presintering) conditions and process parameters affect the microstructure of a TGG-processed ceramic; that is, a) volume ratio of template to matrix particles, b) template size and ratio of template to matrix particles, c) aspect ratio of template particles, d) initial porosity (caused by dewaxing), e) sintering temperature, f) sintering time and g) amount of liquid phase (in the case of liquid-phase sintering). In addition to the given

parameters, growth mechanisms (*i.e.*, isotropic or anisotropic growth, vapor-, liquid- or solid-phase sintering, diffusion-controlled or reaction-limited sintering) must also be important factors.

Many studies have been dedicated to the experimental investigation on the effect of these parameters; some of the typical examples are the effect of the volume ratio of the template to the matrix particles,⁷⁻⁸⁾ sintering temperature and time,⁷⁻⁸⁾ and the amount of liquid⁷⁾ in grain-oriented Al_2O_3 ceramics fabricated by the TGG method with a liquid phase. However, it is difficult and time-consuming to experimentally optimize the initial and process parameters because these parameters are closely related to one another. Moreover, conventional sintering theory cannot deal with such complicated systems.

Alternatively, it is considered that a simulation of the grain growth using the Monte Carlo (MC) method is a useful approach to the understanding of the grain growth behavior and microstructural development in the systems that are difficult to treat a conventional sintering theory and an experimental approach. Firstly, Anderson et al. proposed the simulation model (*i.e.*, the Potts model) of grain growth based on the MC technique.¹⁸⁾ Then, Matsubara, Brook and co-workers proposed a grain growth and sintering model for the systems containing second-phase particles (dispersed particles) and a liquid phase.¹⁹⁻²²⁾ Indeed, these studies showed that the MC simulations expressed good agreement with the experimental results of grain growth and sintering behavior.¹⁹⁻²²⁾ Therefore, the MC simulation is expected to be a powerful tool for specifying optimal initial and sintering conditions in order to design complex microstructures.

In this study, the MC simulation was carried out in order to design TGG-processed ceramics having both a large amount of oriented grains and low residual porosity. Here, we examine the ceramics, which have an isotropic crystal structure (*e.g.*, regular perovskite-type materials) and grow isotropically without a liquid phase. Then, we focus on the initial process parameters, a) the mixing ratio of template to matrix particles, b) the size and c) the aspect ratio of template particles and d) initial

porosity, because these parameters would most typically affect the microstructures. The present work examines the effect of these four parameters and discusses the validity of the MC simulation for the design of highly textured functional ceramics.

2. Simulation

2.1 Calculation model

The simulation of grain growth was carried out on a 2-dimensional triangular lattice on the basis of the Potts model.¹⁸⁾ The lattice size for the calculation is 224 by 224 cells and periodic boundary conditions were imposed. In the lattice, 12 cells near the outermost edge were treated as external space that is the same as pores (see, **Fig. 1** (a)). In the rest of the cells (*i.e.*, the 200 by 200 cells in the gray-colored area illustrated in **Fig. 1**(a)), the cells were randomly set as solid or pore cells (see, **Fig. 1** (b)). All cells contact with 6 adjacent cells. For each cell, an orientation number (Q), which represent the direction of crystal orientation, was distributed at random. It is necessary to give a total Q of more than 50 in order to express the sintering behavior¹⁸⁾ and thus we gave Q numbers ranging 1 to 90 in this study. Template particles were composed of solid cells having the same Q number as shown in **Fig. 1** (b). Q numbers ranging from 1 to 90 were randomly distributed throughout the cells for matrix particles.

A cluster of cells consisting of those having the same Q number was regarded as a single-crystal particle. The Q numbers, 65-90, were set to represent the particles with the crystal axis uniaxially oriented. Thus, the Q numbers of 65-90 were assigned to the cells for template particles and some of the cells for matrix particles that fortuitously had the same orientation as the template particles.

Table 1 summarizes the initial conditions of the MC simulation of the TGG process. The initial size of the matrix particles was that of a 1 by 1 cell. Four initial parameters were examined; 1) the mixing ratio of template to matrix particles (runs #1, 2-1, 2-2 and 2-3), 2) the particle size of template particles (runs #1, 3-1 and 3-2), 3) the aspect ratio of template particles (runs #1, 4-1 and 4-2), and 4) initial porosity (runs #1, 5-1 and 5-2) (see, **Table 1**). Here, run #1 is treated as the standard.

We set the excess free energy at the boundary between two adjacent cells (interface energy γ) in the following manner. For a solid-solid interface, when the two adjacent cells had the same orientation number (*i.e.*, $Q_i = Q_j$ for cells i and j), the interface energy was set at zero ($\gamma = 0$). In the case of $Q_i \neq Q_j$, the interface energy was set at γ_{GB} ($\gamma = \gamma_{GB}$, the grain boundary energy). For the interface between a solid cell and a pore cell, we set γ at $\gamma = \gamma_{SV}$, *i.e.*, the

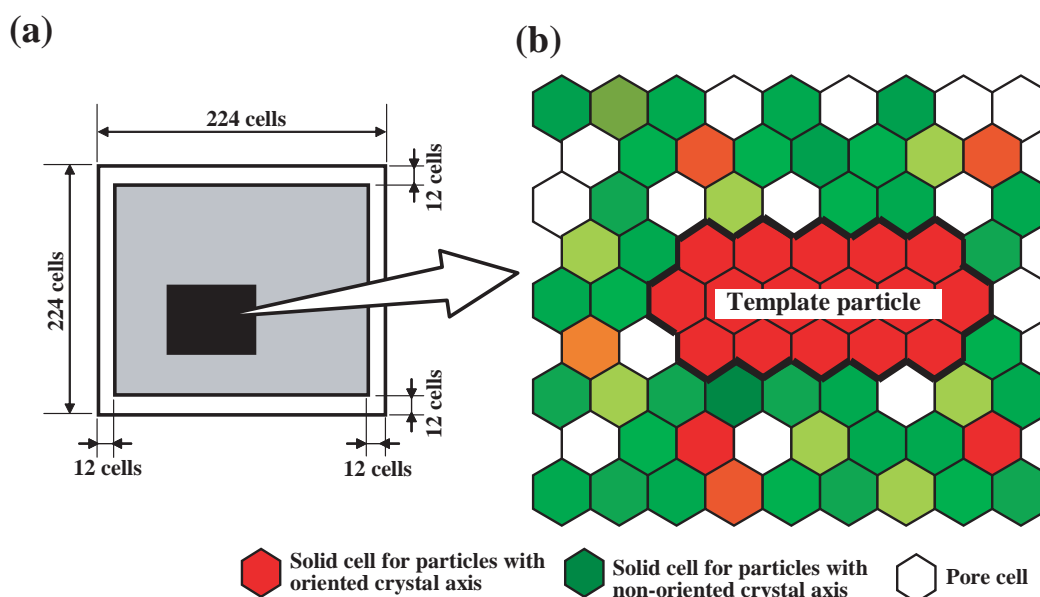


Fig. 1 Schematic diagram of (a) the calculation lattice and (b) the particles models of template particles, matrix particles and pores for the templated grain growth method.

surface energy of the solid particles. In this work, we set the values of γ_{GB} and γ_{SV} at 1 and 1.4, respectively. These values are comparable to the values of oxide materials such as Al_2O_3 .^{23, 24)} When the two adjacent cells are both pores, we set the value of γ at 0.

2. 2 Algorithm in the simulation

At first, a cell was selected at random from the lattice. When the selected cell was a solid, a change in the Q number of the solid to the Q number of one of the adjacent cells was attempted. If the attempted total energy change (ΔE) equaled zero or less, the Q number was changed, otherwise it was not changed. On the other hand, when the selected cell was a pore and its neighboring cell was a solid, one of the following two attempts was performed (the sink mode and the high-diffusion mode). In the sink mode, the pore cell moves at a random walk through the solid particles (composed of solid cells) starting from the position of the adjacent solid cell (*i.e.*, volume diffusion). When the pore reaches the grain boundaries, the cell, which initially was a pore, was changed to a solid. Simultaneously, the cell at the surface of the solid particles was changed to a pore. This attempt contributes to the densification of ceramic materials. In the high-diffusion mode, the pore cell moves through the grain boundaries or along the solid surface (*i.e.*, grain boundary or surface diffusion). This attempt contributes to the

growth of pores but contributes little to the densification of a ceramic body. In these modes, the attempts were made for the case in which ΔE equals zero or less.

The frequency factor was given as a value between 0 and 1 for the grain growth (F_{gg}), pore diffusion in the sink mode (F_{sink}) and that in the high-diffusion mode (F_{hd}). Here, we set the values of F_{sink} and F_{hd} at $F_{sink} + F_{hd}$ is less than 1. The values of F_{gg} , F_{sink} and F_{hd} represent the relative values of the diffusion coefficients of (1) grain boundary diffusion that restricts a grain growth, (2) volume diffusion of pores and (3) grain boundary and surface diffusion of pores. In this study, we set these values as $F_{gg} = 0.5$, $F_{sink} = 0.1$ and $F_{hd} = 0.5$.²⁵⁾

The time scale was measured in terms of Monte Carlo steps (MCS).¹⁸⁾ One MCS is defined as N attempts (selection of a cell from the lattice) irrespective of success or failure, where N is the total number of cells.

2. 3 Methods for evaluation of the fraction of oriented grains

Figure 2 shows the typical example of initial configuration and microstructural development in the present computational study. We set known amounts of template and matrix particles, and pores in the initial configuration (see, Fig. 2 and Table 1). These particles and pores were randomly distributed in the calculation lattice. In addition, all the

Table 1 Initial conditions of the Monte Carlo simulation for the TGG Process.

Run	Fraction of matrix particles (%) ¹⁾	Template particles			Porosity (%) ¹⁾	Template/matrix mixing ratio ³⁾ (%)
		Size ²⁾	Fraction (%) ¹⁾	Aspect ratio		
1	63.9	5 × 25	16.3	5	19.8	20.3
2-1	80.0	-	0.0	5	20.0	0.0
2-2	75.9	5 × 25	4.1	5	20.0	5.1
2-3	71.8	5 × 25	8.1	5	20.1	9.3
3-1	64.1	3 × 15	16.2	5	19.7	20.2
3-2	64.1	4 × 20	16.2	5	19.7	20.2
4-1	63.9	8 × 16	16.3	2	19.8	20.4
4-2	63.9	3 × 42	16.4	14	19.7	20.4
5-1	71.5	5 × 25	18.1	5	10.4	20.3
5-2	55.5	5 × 25	14.4	5	30.1	20.3

1) Area fraction 2) Size of matrix particles was 1 by 1 cell as a comparison

3) Area of template particles / (area of template and matrix particles) × 100 %

template particles were located without tilt. After being sintered for a given time (t MCS), the total area of all oriented grains were calculated. Here, we define the fraction of oriented grains as the area ratio of all oriented grains to all grains as expressed in Eq. (1),

$$\text{Fraction of oriented grains} = (T + M_{\text{orient}}) / (T + M_{\text{orient}} + M_{\text{random}}) \times 100 [\%] \dots (1)$$

where T , M_{orient} and M_{random} are the areas of template particles, matrix grains oriented similarly to the templates and randomly oriented matrix grains, respectively (see, Fig. 2). Then, the porosity was calculated by Eq. (2),

$$\text{Porosity} = (\text{the total area of all pores}) / (\text{total area}) \times 100 [\%] \dots (2)$$

3. Results and discussion

3.1 Initial mixing ratio of template to matrix particles

Figure 3 shows the effect of the initial mixing ratio of template to matrix particles (template/matrix mixing ratio) on the development of the microstructure. With no template particles (run #2-1), the grains grew in a rather equiaxed shape with similar diameters. On the contrary, the bimodal microstructure of large anisometric grains and small round particles was exhibited for the system containing 5-20 % template particles (runs #2-2, 2-3 and #1). The former and the latter particles originated mainly from templates and matrix particles, respectively.

The template particles increased in size by incorporating adjacent matrix particles; this is because the large template particles tend to incorporate smaller particles (the template particles were larger than the matrix particles). Simultaneously, the rest of the matrix particles grew by coalescing with each other. The template particles grew preferably in the perpendicular direction rather than in the lateral direction and matrix particles grew into an equiaxed shape. This growth behavior is typical for the isotropic growth. Oriented grains originated mainly from the template particles as well as from part of the grown matrix particles, which had coincidentally the same crystal orientations as the templates.

These results on the grain growth and microstructure development suggest that the current simulation seems to be able to express the TGG process.

Figure 4 (a) shows the change in the fraction of oriented grains with time as a function of initial

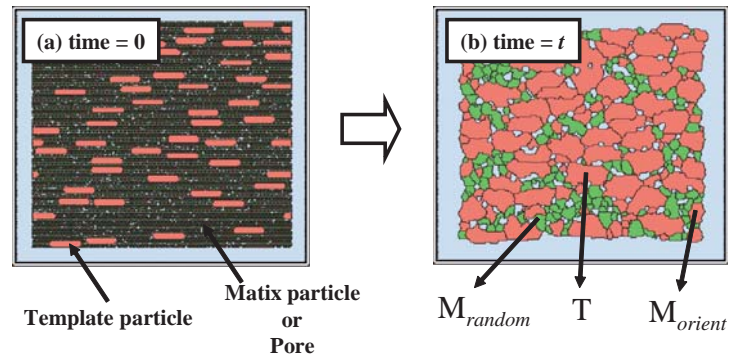


Fig. 2 Initial configuration and microstructure developed at a given time (t Monte Carlo steps); T : the grains developed from template particles (oriented-grains), M_{orient} : the oriented-grains grown from matrix particles, M_{random} : the non-oriented grains grown from matrix particles.

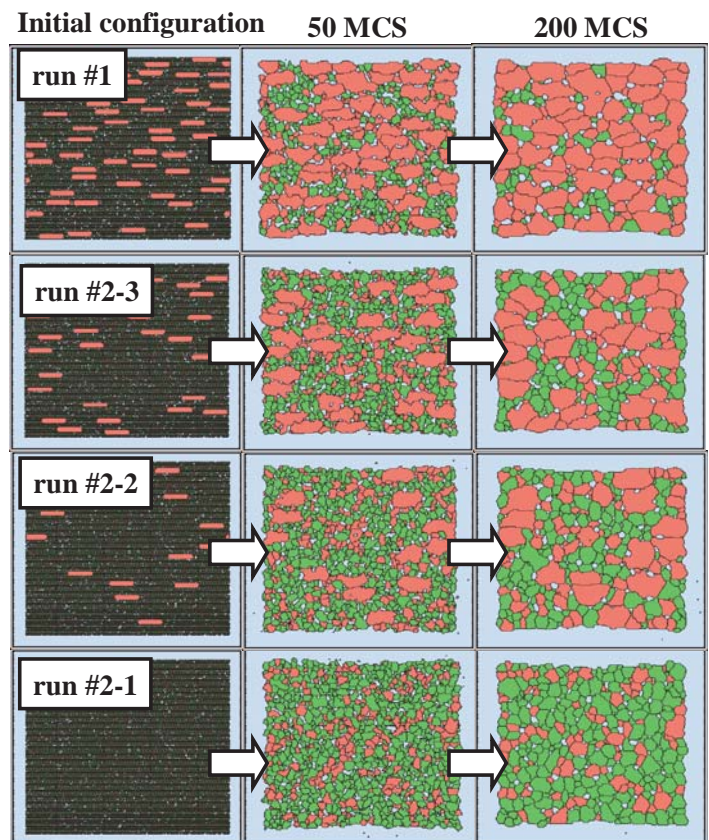


Fig. 3 Development of microstructure for the cases with different initial mixing ratios of template to matrix particles; run #1: template particle = 20.3 %, run #2-1: 0.0 %, run #2-2: 5.1 % and run #2-3: 9.3 %.

template/matrix mixing ratio. An increase in initial template/matrix mixing ratio resulted in an increased fraction of oriented grains. The number of matrix particles in contact with template particles increased with increasing initial template/matrix mixing ratio; a larger number of matrix particles were incorporated into the template particles and thus the fraction of oriented grains was increased. These simulation results are in accordance with the experimental results for TGG processing of Al_2O_3 ceramics with a liquid phase⁷⁾ although the system treated in the current computational study is different from that of the experiment (anisotropic growth with a liquid phase).

It should be noted that the fraction of oriented grains were ~30 % for the system with the template/matrix ratio of 0.0 % as a result of the originally assigned ratio of 26/90 for the number of oriented cells/total Q number. Thus, the dotted line in Fig. 4(a) must be considered as the fraction of oriented grains for the randomly oriented system under this simulation condition.

Figure 4 (b) shows the change in porosity with time as a function of initial template/matrix mixing ratio. An increase in initial template/matrix mixing ratio resulted in increased residual porosity. This result is consistent with the fact that the system including coarse particles is difficult to densify.

It was found that an increase in initial template/matrix mixing ratio gave an increased fraction of oriented grains and increased residual porosity as shown above. An increase in the fraction of oriented grains enhances the physical properties of functional ceramics while an increase in residual porosity can reduce these properties. Thus, it is important to specify the optimal template/matrix mixing ratio in order to attain the best properties.

3.2 Initial size of template particles

Figure 5 shows the effect of the initial template particle size on the development of the microstructure. The size of the resultant grains increased with increasing initial template size (see, run #1 in Fig. 3, runs #3-1 and 3-2 in Fig. 5). Because the initial template/matrix mixing ratio was a given constant in all the runs, an increase in template particle size resulted in a decreased initial number of template particles. Thus, an increase in initial template size resulted in an increase in the interval between template particles, thereby resulting in an increased resultant grain size due to the increase in space for template particles to grow at the expense of adjacent fine matrix particles. A similar experimental result was reported in the TGG processing of the anisotropic Al_2O_3 system with a liquid phase.⁷⁾

Figure 6 (a) shows the change in the fraction of

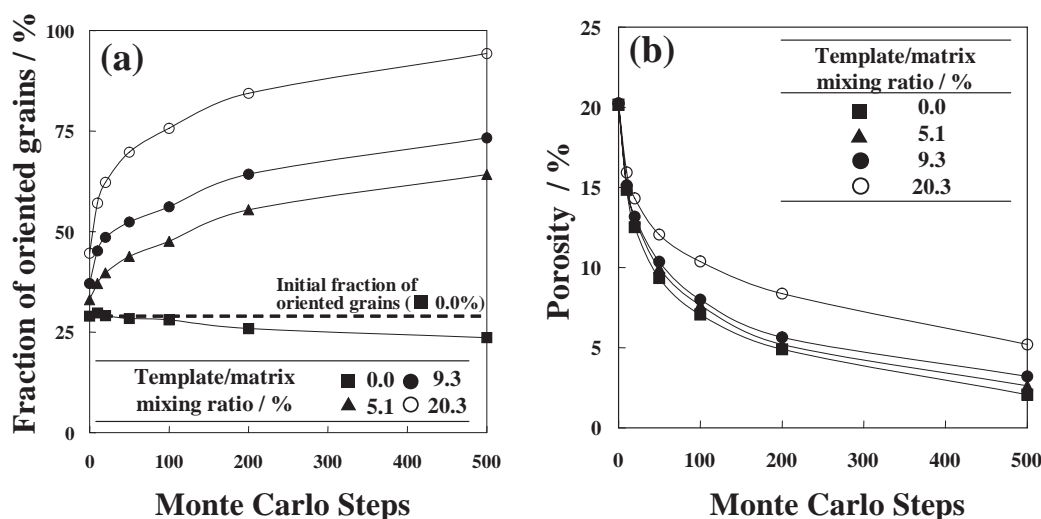


Fig. 4 (a) Change in the fraction of oriented grains with time as a function of initial mixing ratio of template to matrix particles; run #2-1(■): template particle = 0.0 %, run #2-2(▲): 5.1 %, run #2-3(●): 9.3 % and run #1(○): 20.3 %. (b) Change in porosity with time as a function of initial mixing ratio of template to matrix particles; run #2-1(■): template particle = 0.0 %, run #2-2(▲): 5.1 %, run #2-3(●): 9.3 % and run #1(○): 20.3 %.

oriented grains as a function of initial template particle size. The fraction was increased with decreasing initial template particle size. The possibility that template particles preferably entrap matrix particles depends on both the difference in size and that in area of the interface between the template and matrix particles. The size effect represents the extent to which larger particles tend to entrap smaller particles. The interface effect represents the frequency at which two adjacent

particles combine with each other. In the current simulation, the area of the interface had a predominant effect; that is, the increase in the initial number of template particles gave an increased area of template/matrix particle interface, thereby giving an increased fraction of matrix particles entrapped in the template particles (*i.e.*, the fraction of oriented grains was increased).

Figure 6 (b) shows the change in porosity with time as a function of initial template particle size. Decrease in the initial template particle size resulted in increased porosity. This result is consistent with the fact that the system including coarse particles is difficult to be densified in general.

3.3 Initial aspect ratio of the template particles

Figure 7 shows the effect of the initial aspect ratio of template particles on the development of the microstructure. The aspect ratio of grains developed during 200 MCS increased with increasing initial aspect ratio (see, run #1 in Fig. 3, runs #4-1 and 4-2 in Fig. 7). Because particles grew isotropically, the aspect ratio of grains decreased with time. However, the template particles with high initial aspect ratio (run 4-2) still had an anisotropic microstructure. The initial aspect ratio of the template particles was found to have a significant effect of enhancing anisotropic microstructural development even in the

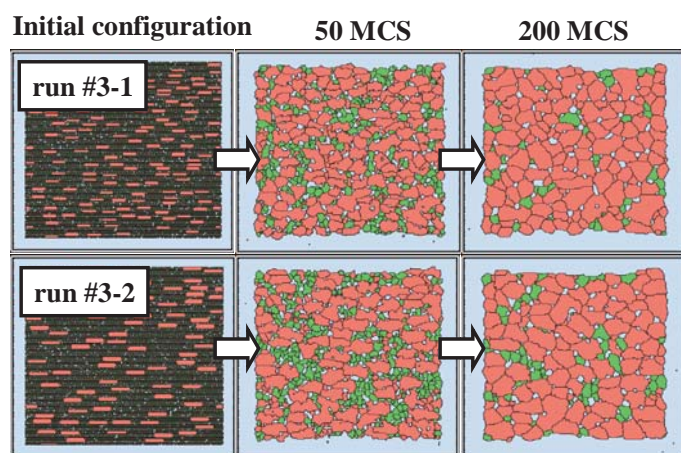


Fig. 5 Development of microstructure for cases with different initial template particle sizes; run #3-1: template particle size = 3×15 and run #3-2: 4×20 . (see, run #1 in Fig. 3 as a comparison: template particle size = 5×25).

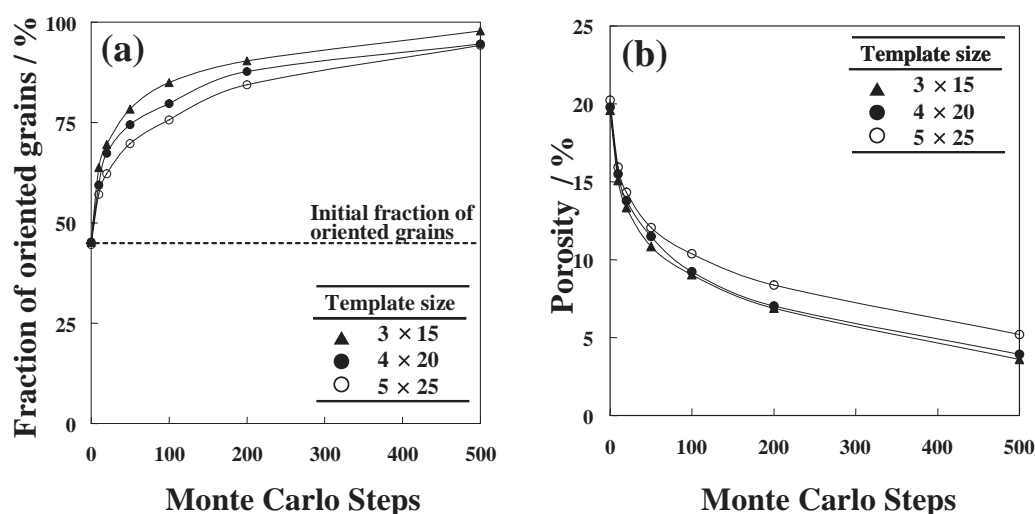


Fig. 6 (a) Change in the fraction of oriented grains with time as a function of initial template particle sizes; run #3-1(▲): template particle size = 3×15 , run #3-2(●): 4×20 and run #1(○): 5×25 .
(b) Change in porosity with time as a function of initial template particle sizes; run #3-1(▲): template particle size = 3×15 , run #3-2(●): 4×20 and run #1(○): 5×25 .

materials that grew isotropically.

Figure 8 (a) shows the change in the fraction of oriented grains as a function of the initial aspect ratio of the template particles. The fraction was increased with increasing initial aspect ratio. The increase in initial aspect ratio resulted in an increased area of template/matrix interface, thereby increasing the fraction of the matrix particles incorporated into the template particles. Although the effect of the initial aspect ratio was not examined experimentally, the simulation results would be

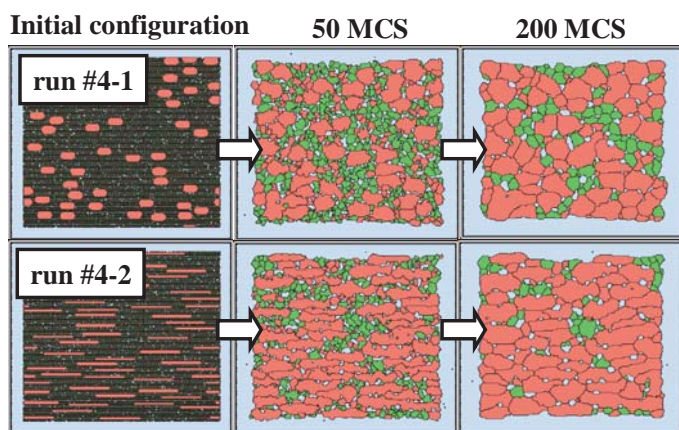


Fig. 7 Development of microstructure for the cases with different initial aspect ratios of template particles; run #4-1: aspect ratio = 2 and run #4-2: 14. (see, run #1 in Fig. 3 as a comparison: aspect ratio = 5).

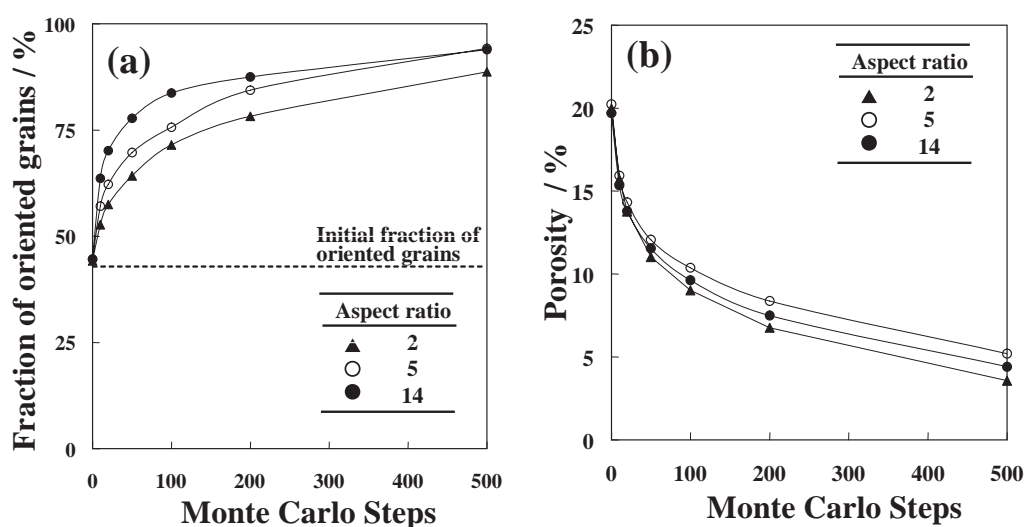


Fig. 8 (a) Change in the fraction of oriented grains with time as a function of initial aspect ratio of template particles; run #4-1(▲): aspect ratio = 2, and run #1(○): 5 and run #4-2(●): 14.
(b) Change in porosity with time as a function of initial aspect ratio of template particles; run #4-1(▲): aspect ratio = 2 and run #1(○): 5 and run #4-2(●): 14.

reasonable.

Figure 8 (b) shows the change in porosity with time as a function of the initial aspect ratio of the template particles. There is no consistent tendency in the relationship between the initial aspect ratio and the residual porosity. When template particles have the same aspect ratio, an increase in the area of the interface between the template and matrix particles results in decreased residual porosity. Additionally, there is another effect when template particles have different aspect ratios: that is, the different curvatures of the particles result in different surface tensions, thereby changing the reduction rate of residual porosity. Thus, a possible interpretation for the current simulation result is that residual porosity was determined by the complicated combination of the interface and curvature effects.

3.4 Initial porosity

Figure 9 shows the effect of initial porosity on the development of the microstructure. Particle size increased with decreasing initial porosity (see, run #1 in Fig. 3, runs #5-1 and 5-2 in Fig. 9). This is consistent with the fact that pores disturb grain growth in general.

Figure 10 (a) shows the fraction of oriented grains as a function of initial porosity. A large porosity, such as 30 %, inhibited an increase in the fraction of oriented grains. Because pores attached to template

particles suppress the growth of template particles, it is important to reduce porosity and increase the growth rate of template particles. Thus, liquid-phase sintering and reaction-bonded sintering would have the effect of enhancing the texture development.⁷⁻⁹⁾

Figure 10 (b) shows the change in porosity with time as a function of initial porosity. Residual porosity at a given time decreased with decreasing initial porosity. This is due to the same reason as

explained above. An increase in the number of interfaces (not only between template and matrix particles but also matrix and matrix particles) results in decreased porosity.

These initial porosity effects are in accordance with the results reported for the presintering conditions for $\text{Bi}_{0.5}(\text{Na}, \text{K})_{0.5}\text{TiO}_3$ ceramic preparation; that is, cold isostatic pressing of green specimen (giving decrease in the initial porosity) causes the resultant ceramics to have an increased degree of orientation (*i.e.*, the fraction of oriented grains) and increased density (*i.e.*, decreased residual porosity).²⁶⁾

As shown above, the MC simulation was carried out for the development of the microstructure in an isotropic growth system during the TGG process. The computational studies expressed reasonably the effect of some typical initial parameters on the microstructural development of TGG processed ceramics. For the enhancement of the physical properties of functional ceramics, it is essentially necessary to fabricate ceramics having both a higher fraction of oriented grains and lower porosity. It is important to compare the simulation and experimental results and to extend the approach to other systems (*e.g.*, anisotropic growth and liquid-phase sintering) in future studies.

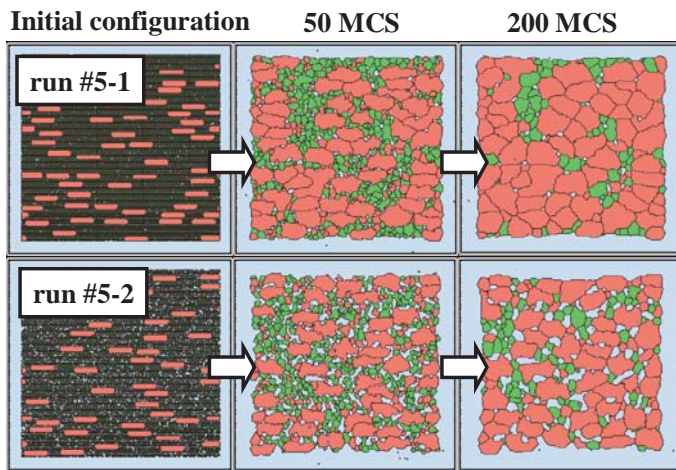


Fig. 9 Development of microstructure for cases with different initial porosities; run #5-1: initial porosity = 10.4 % and run #5-2: 30.8 %. (see, run #1 in Fig. 3 as a comparison: initial porosity = 19.9 %).

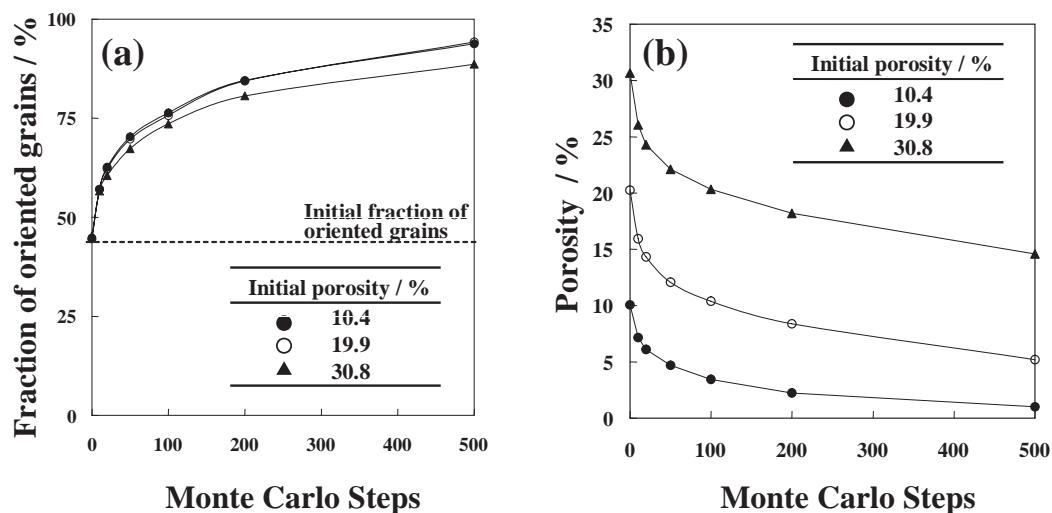


Fig. 10 (a) Change in the fraction of oriented grains with time as a function of initial porosity; run #5-1(●): initial porosity = 10.4 %, run #1(○): 19.9 % and run #5-2(▲): 30.8 %.
(b) Change in porosity with time as a function of initial porosity; run #5-1(●): initial porosity = 30.8 %, run #1(○): 19.9 % and run #5-2(▲): 10.4 %.

4. Conclusions

Computational study was carried out for the design of textured functional ceramics prepared by the templated grain growth (TGG) method. The current simulation was found to well express the microstructural development in ceramics that grow isotropically without a liquid phase. Then, the effect of typical initial parameters of the TGG method on the fabrication of ceramics having both a high fraction of oriented grains and low residual porosity were examined.

- (1) An increase in the initial mixing ratio of template to matrix particles (template/matrix mixing ratio) resulted in an increased number of matrix particles entrapped by template particles, thereby increasing the fraction of oriented grains. On the other hand, an increase in the initial template/matrix mixing ratio increased the average particles size so that it became to be difficult to sinter (residual porosity was increased).
- (2) An increase in template particle size resulted in a decreased number of template particles and thus a decreased fraction of oriented grains. Residual porosity was increased with increasing template particle size by the same reason explained in (1).
- (3) The aspect ratio of the template particles had a significant effect on the production of textured microstructures even for materials that grow isotropically. An increase in aspect ratio resulted in an increased fraction of oriented grains.
- (4) An increase in initial porosity resulted in a decreased fraction of oriented grains and increased residual porosity. This is because pores suppressed the growth of template particles and disturbed the densification of the ceramic body.

In conclusion, the current simulation would be useful for specifying the optimal initial conditions in order to design the complicated microstructures and attain enhanced properties of functional ceramics.

Acknowledgment

This work was carried out in the Computational Materials Design Forum organized by the Japan Fine Ceramics Center.

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