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Microstructure Design for Ken-Materials Using Computer Simulation

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We have successfully developed the computer simulation technique of microstructural design for Ken-materials with multi-phases and integrated functions. The Monte Carlo (MC) and the molecular dynamic (MD) methods have been used for the simulations of the microstructures with particle-size level and atomic revel, respectively. The MC simulations were performed at the array of two or three dimensional lattices. Plural mechanisms of mass transport were introduced in the MC simulations of sintering and grain growth in composites and ceramics systems which involve a liquid phase and a second solid phase. The MD simulation was applied into the grain boundary formation of ionic ceramics and showed the characteristic structures and excess energy at the boundaries and interfaces. The MC and MD simulations for sintering process are useful for microstructural design for Ken-materials.

Key words: microstructure, computer simulation, sintering, grain growth, percolation, grain boundary, interface, composites, ceramics

1. INTRODUCTION

Materials produced and used in industries, machines, buildings and our daily life are required to have some intelligent function by means of interaction among different properties in a material. We need optimize microstructures of a material to have well interacted and integrated functions at its application. The computer simulation is a promising technique to design microstructures suitable for required performances in materials. The studies of material design using computer simulation can give us not only basic understanding about the microstructural development but also new important directions for material technologies.

We have successfully developed the computer simulation techniques by Monte Carlo and molecular dynamics methods for some characteristic microstructures in Ken-materials with multi-phases and integrated functions. This paper is aimed to study the simulations of various microstructures by the MC and MD methods useful for the Ken-materials developments.

2. METHOD

Figure 1 shows the construction of the simulation system for microstructure design in ceramic materials which has been developed in our research group.

The Monte Carlo (MC) simulation for grain growth is a probability type method in which sequences proceed to the direction of decreasing the total grain boundary energy. The MC simulation can be applied into some important processes of microstructural development in ceramics such as grain growth through liquid (Ostwald ripening), sintering of solid state and sintering under the existence of liquid (liquid phase sintering)[1-3].

The array of MC simulation in this study is the two dimensional and triangular lattices which consist of a matrix solid phase with different crystal orientations, a liquid phase, a second solid phase and a pore (or void) phase. There are different energy values depending on of grain boundaries, interfaces and surfaces. When a solid lattice is selected in the array, it tries the mass transfer through grain boundaries and a liquid phase. When a pore lattice is selected, the pore lattice moves due to the four diffusion routes; volume, grain boundary, pore-surface and outside-surface routes. If the total energy change ≤ 0, this try is in practice.

The software of MASPHYC (Fujitsu Co.) is used to perform the molecular dynamics (MD) simulations in the three dimensional array under the ensemble of NTP. Alumina and Zirconia base systems are studied for the simulations of atomic structures and energies at gain boundaries or interfaces.

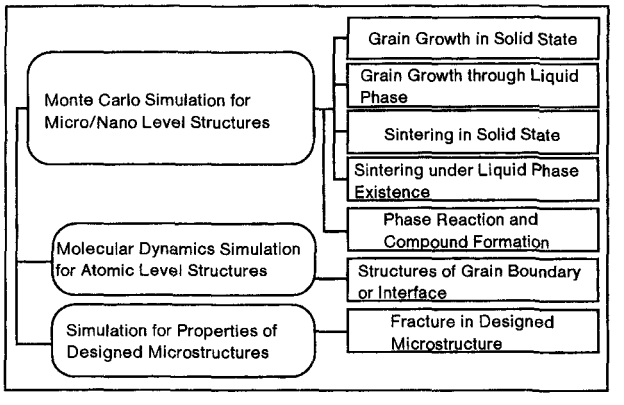

Fig. 1 Construction of the simulation program developed for ceramic microstructure design.

1. SIMULATION RESULTS AND DISCUSSION

3-1 Grain Growth Simulations

Figure 2 shows the three examples of microstructural design by using the grain growth simulation[2,3]. The case of (a) shows the simulation for arranged coarse grains in fine grains rustling in the unique microstructure with texture. The result of (b) demonstrates the layer structure caused by pinning effect of regularly arranged dispersoids. The case of (c) indicates a more characteristic microstructure caused by the arrangement of coarse grains and second phase particle (dispersoid) having the pinning effect on grain growth. It is noted that such MC simulations enables the design for unique microstructures in grain growth process under the combined effects.

Figure 3 demonstrates MC simulations of grain growth under the presence of a large amount of liquid phase[4-6]. This type of grain growth is called Ostwald ripening by the mass transfer mechanism through solution and reprecipitation of solid element in liquid phase. These results are simulated commonly at a constant fraction of a liquid phase, 20%, to examine the influence of the interfacial energy between solid and liquid (γ_{SL}). The simulation can indicate the two different mass transfer mechanisms; the movement of solid boundary (grain growth at solid state) and that of solid/liquid interface (solution/reprecipitation through a liquid phase, Ostwald ripening). The result of (a) is the case of high γ_{SL} which demonstrates the dominant mechanism of solid state growth in the microstructure with isolated liquid phase. The result of (b) is the simulation with low γ_{SL} indicating the activated movement of solid/liquid interface and thin film formation of liquid phase. The case of (c) shows the effect of anisotropy of γ_{SL} by which directional growth behavior or unique microstructure with texture can designed in many real ceramic or cermet systems.

3-2 Sintering Simulations

Figure 4 shows the two results of MC simulation of sintering at solid state[2,3]. The case of (a) has the initial configuration of single phase particles with different sizes. The simulation shows distinctly the behavior of shrinkage accompanied by grain growth. The results simulated for 10^4MCS is the microstructure including coarse grains and a residual pore caused by grain growth during sintering. The result of (b) is the simulation of the initial configuration that second phase particles are distributed in the same initial microstructure of matrix

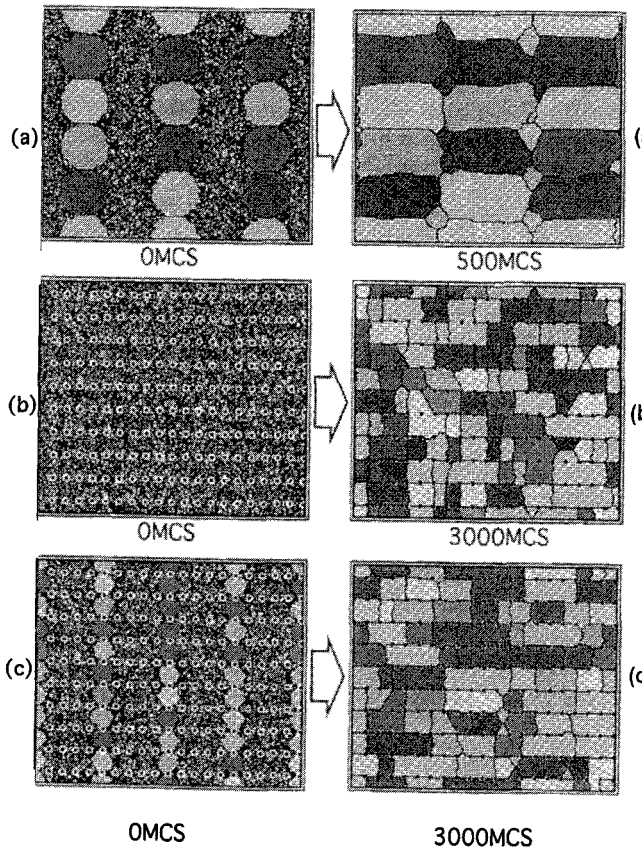

Fig. 2 Examples of microstructural design by using grain growth simulations. (a) arranged coarse grains, (b) arranged dispersoids, (c) arranged coarse grains and dispersoids.

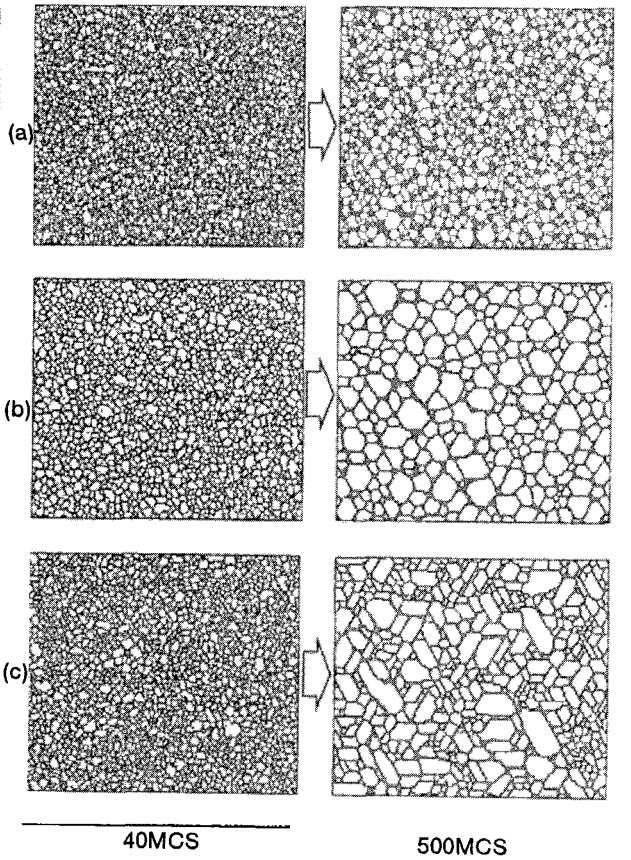

Fig. 3 MC simulations of grain growth under the presence of a liquid phase affected by the interface energy between solid and liquid (γ_{SL}). (a) high γ_{SL}, (b) low γ_{SL}, (c) anistropic γ_{SL}.

phase particles as the case of (a). This simulation can treat such a more complicated feature of microstructure development under the interaction of three phases of matrix, dispersoid and pore. The second phase particles play not only the inhibiting effect of grain growth but also delaying effect of shrinkage. The final simulated structure illustrates finer grain structure and a little more residual pores comparing the case of (a). The MC simulation possesses many other possibilities of the design for complex microstructures.

3-3 Percolation Structure Simulations

Figure 5 indicates the simulated percolation structures of particles with different aspect ratios[7]. The percolation structure that means the continuous network formation of particles (dispersoids) in a material is of great importance to get the paths of electrical conductivity for self-diagnosis function in FRP and CMC composites[8]. The higher aspect ratio can generate the low critical content for the percolation structure with conductive paths.

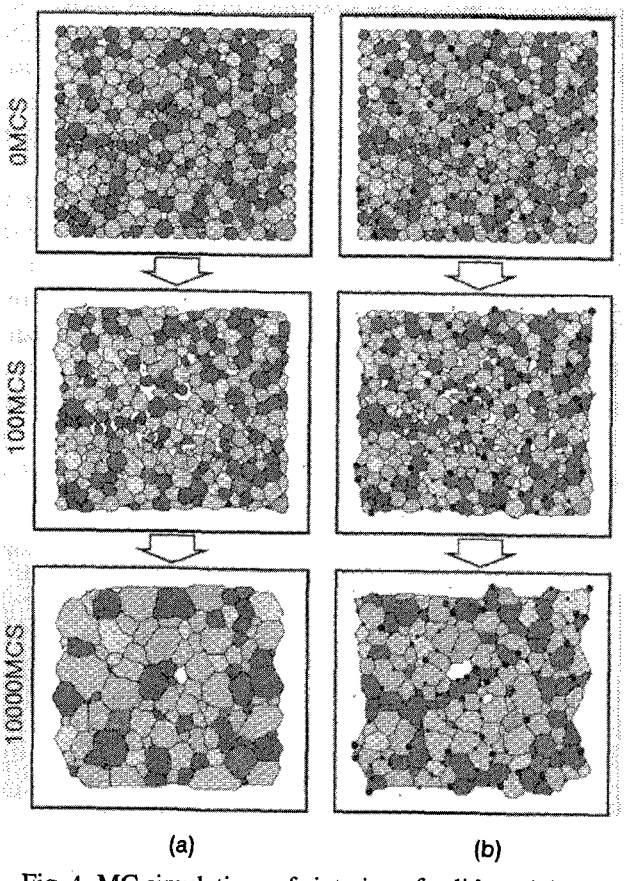

Fig. 4 MC simulations of sintering of solid particles. (a) single phase, (b) tow phases involving dispersoids.

3-4 Atomistic Structure Simulations

Figure 9 shows an example of MD simulation results of atomistic structure for cubic Zirconia-Yttria[2,3]. The starting configuration is that the two super fine grains with 20nm diameter and cylinder shape have a space of one atomic length and the orientation relationship of Σ 5 between two grains. The material consist of approximately 4000 atoms of Zr, Y and O ions of ZrO_2-8mol%Y_2O_3 composition and involves the amount of O ion vacancies corresponding to the composition. Temperature is 1300K and time is up to 6 pico second. The two fine particles join immediately for before. At the same time, the crystal structure remarkably deforms into amorphous-like structure. Such a behavior is considered to be due to a extremely strong attractive force between super fine particles.

Figure 6 demonstrates the grain boundary formation in pure alumina by the MD simulation at a high temperature as a function of time[9]. It is possible to calculate grain boundary energies by the MD

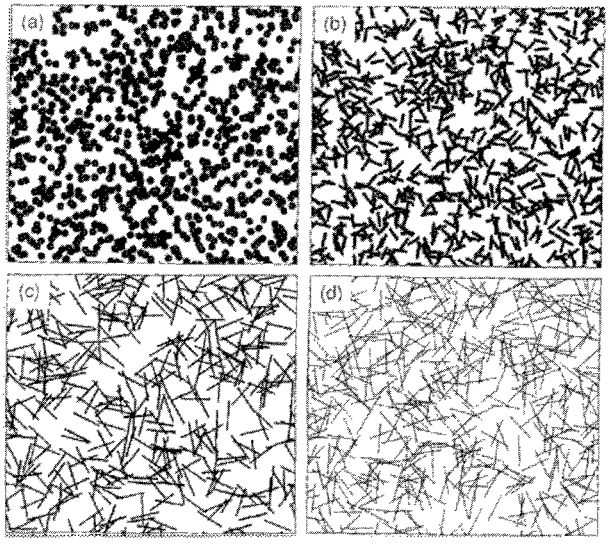

Fig. 5 Computer graphics of the simulation allowing the over lap among second phases with various aspect ratios (a.r.). (a) a.r.=1, f=44%, (b) 5, 36%, (c) 20, 20%, (d) 100, 5.6%.

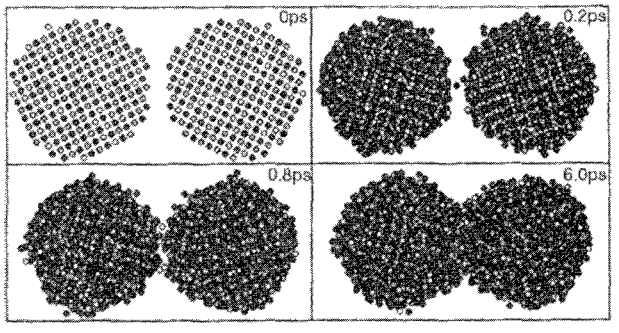

Fig. 6 MD simulation of nano-size particles ZrO 2-8mol%Y 2O3 as a function of time (pico second).

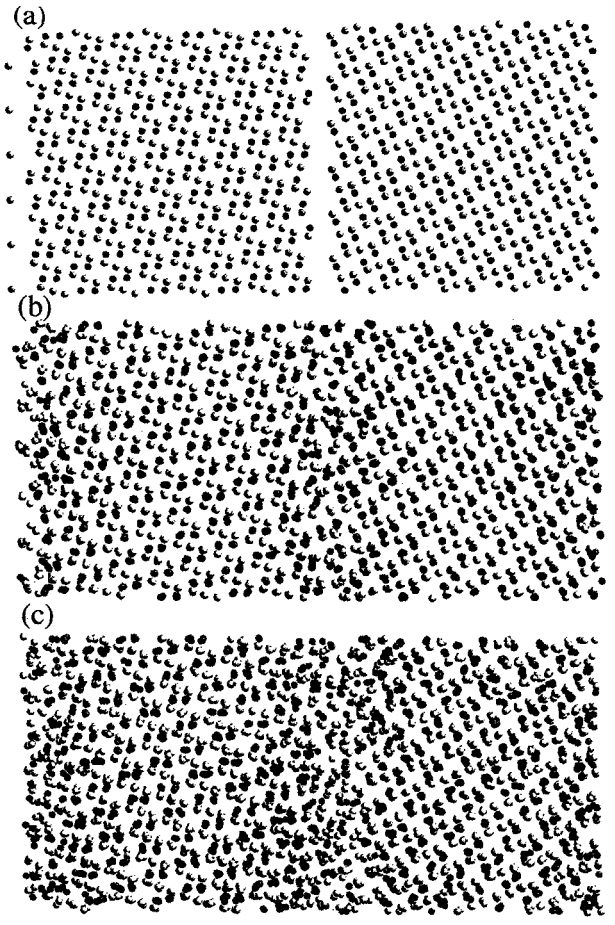

Fig. 7. Structural changes of near Σ11 grain boundary at 1700 K. (a) initial, (b) 0.4 ps, (c) 1.0 ps.

simulations, which are useful data for MC simulation for sintering and grain simulations. Such a treatment is available in the systems including inclusion or sintering additive[10]. The MD simulations can be very interesting method for microstructural design at atomistic level.

4. CONCLUSION

The computer simulations of sintering and grain growth processes for ceramics were studied by the methods of Monte Carlo and molecular dynamics.

(1) The plural mechanisms of mass transfer were designed in the MC simulation of grain growth and sintering processes at micron size grain and particle; grain growth at solid state, solution-reprecipitation through liquid phase, the transfer of pore lattices for shrinkage.

(2) The MC simulations provided the microstructural design for the effects of initial configuration, liquid phase content, energy balance, particle size and second particle inclusion on grain growth and sintering processed.

(3) The microstructures which are designed by MC simulation for sintering and grain growth can be developed to the simulations for crack propagation path and phase reaction in multi-phase systems.

(4) The MD simulation was performed in the case of nano size particles of ionic ceramic and showed the characteristic features in sintering process at atomic levels.

(5) The MC and MD simulations for grain growth and sintering process are useful for microstructural design for ceramics.

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