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Phase field simulation on the effect of micropore morphology on grain growth in porous ceramics

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ABSTRACT

The properties of the porous ceramics are known not only related to the pore-solid composite model, but also have a significant grain-size effect. In this study, a phase field simulation is carried out to study the effect of different micropores on the grain growth kinetics of porous ceramics, and results indicate that the average grain size and distribution are highly influenced by the topological shape of the second-phase. The efficiency of the grain boundary migration is determined by the pinning forces applied in the interaction of the grains and pores. The pining forces are calculated based on Zener Theory, and results indicate that the maximum pinning force is highly dependent on the second-phase shape, and the contacting mode between the grain boundaries and second-phase pores is the determining factor of the grain boundary migration in porous materials.

1. Introduction

Modern materials have increasingly complex structures at different length scales and are designed for multi-functional applications. Recognized as a promising candidate for a wide range of applications due to their good thermal shock resistance, high strain tolerance, porous ceramics have been widely studied in recent years [1–5]. Although the property-microstructure correlation is complex in detail [6], it is generally accepted that properties of the porous materials are not only related to the pore-solid composite model, but also has an significant grain-size effects [7–9]. Grain growth in porous ceramics is a complex process, since the kinetics of grain growth in porous polycrystalline materials is highly dependent on the interaction between pores and grain boundaries [10]. In particular, the grain size should be considered to be correlated to the second-phase in composites [11–14]. Therefore, it would be of much significance to study the effect of pore phase on grain structure formations in porous materials. Experimental researches have been carried out to study the property-microstructure relation in porous ceramics [15–18], and it is well established that the pore shape and porosity have significant effect on their properties of porous ceramics. Besides experimental investigations, a number of theoretical models were developed to study the kinetics of grain growth in porous ceramics [19–22]. Specially, a phase field approach comprising a system of Cahn–Hilliard and Allen–Cahn equations has been developed to study concurrent evolution of grain size and porosity in solids, involving curvature-driven motion of grain boundaries and the pore motion by surface diffusion [10,23,24].

Though several attempts have been carried to study the interaction between pores and grain, the effect of micropores on grain structure formation and its mechanism are still needed to be discussed in details. Thus. In this study, a phase-field simulation was carried out to investigate the effect of the second-phase on the grain growth kinetics during ceramic microstructure formation. Dragging forces for the grain boundary migration applied by pores of different shapes are calculated based on the Zener theory, which is implemented to explain the shape effect of the pores on grain boundary migration in porous materials.

2. Numerical simulation method

The grain structure is determined by the grain growth kinetics during the synthesis process, and in this study the grain growth in porous materials is investigated via the phase-field method. The phase-field model implemented in this paper was extended from the model for simulating grain growth in materials containing small incoherent second-phase particles with constant properties [13,25]. Here, we consider pores as the second-phase in porous materials and use this model to simulate the effect of pores on the matrix grain growth in porous materials. The free energy of the system is described by [25]

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$$F = \int_V \left(\sum_{i=1}^{p} \left(\frac{\eta_i^4}{4} - \frac{\eta_i^2}{2} \right) + \sum_{i=1}^{p} \sum_{j \neq i}^{p} \eta_i^2 \eta_j^2 + \phi^2 \sum_{i=1}^{p} \eta_i^2 + \frac{\kappa}{2} \sum_{i=1}^{p} (\nabla \eta_i)^2 \right) d^3\mathbf{r} \tag{1}$$

$\eta_1(\mathbf{r},t), \eta_1(\mathbf{r},t), \ldots, \eta_p(\mathbf{r},t)$ are phase-field variables to distinguish the different crystallographic orientations of the grains. The interface between a particle and matrix does not play a significant role in determining the kinetics of grain growth [11], and in this study, the surface of the micropores is treated as a sharp interface of the grain and micropore. φ is a spatially dependent parameter to represent the pore phase distribution which remain static in time. The value of φ in the simulation domains is the controlling parameter in this study, which represents different morphologies of the second-phase. Here we assume micropores introduced into the simulation zone have sharp interface and do not evolve, thus the elastic energy induced by the misplacement at the pore surfaces is a constant, and could be neglected for convenience.

The spatial and temporal evolution of the phase-field variables is governed by the time-dependent Ginzburg-Landau equations:

$$\begin{aligned} \frac{\partial \eta_i(\mathbf{r},t)}{\partial t} &= -L \frac{\delta F}{\delta \eta_i(\mathbf{r},t)} \\ &= L \left(\kappa \nabla^2 \eta_i - \eta_i^3 + \eta_i - 2\eta_i \left(\sum_{j \neq i}^{p} \eta_i^2 + \phi^2 \right) \right), \; i = 1, \ldots, p. \end{aligned} \tag{2}$$

with L a kinetic parameter and κ the gradient energy coefficient. A full description of the model can be found in Ref. [13]. A set of 30 phase field variables is used ($p = 30$) that grains represented by the same phase field variable are far from each other. The phenomenological implemented in the simulations are chosen as: $L = 1.0$, $\kappa = 1.0$, $\phi = 2.0$. The grid spacing Δx and time step Δt are chosen to be 1.0 and 0.25, respectively. Eq. (2) are solved via the Finite-Difference Method, and periodic boundary conditions are applied.

3. Results and discussions

In this section, the grain growth kinetics is studied by the phase-field simulation, and the pore shape effect on the grain size is investigated. All simulations are conducted in a system of 1024×1024 grid points (g.p.), with the same pore volume fraction $f_V = 0.1$. The initial grain structure for Fig. 1 are generated with the same algorithm, which makes sure all simulations start with the same initial grain structure. After initial grain structure are generated, 200 micropores are randomly introduced into the simulation zone directly, and all pores have sharp interfaces since the pore phase is assumed to be unchanged in this study. Micropores of different shapes represent different composite mode of the porous materials.

Fig. 1 gives the microstructure for single phase and porous polycrystalline with pores of different shapes at 100,000 time step. In the case of pure single phase, the larger grains grow at the expense of the smaller ones to reduce the excess free energy associated with grain boundary network, which has been investigated in many other papers [12,14,26]. In the case of spherical pores, grain boundaries are pinned by pores, which slows the grain ripening

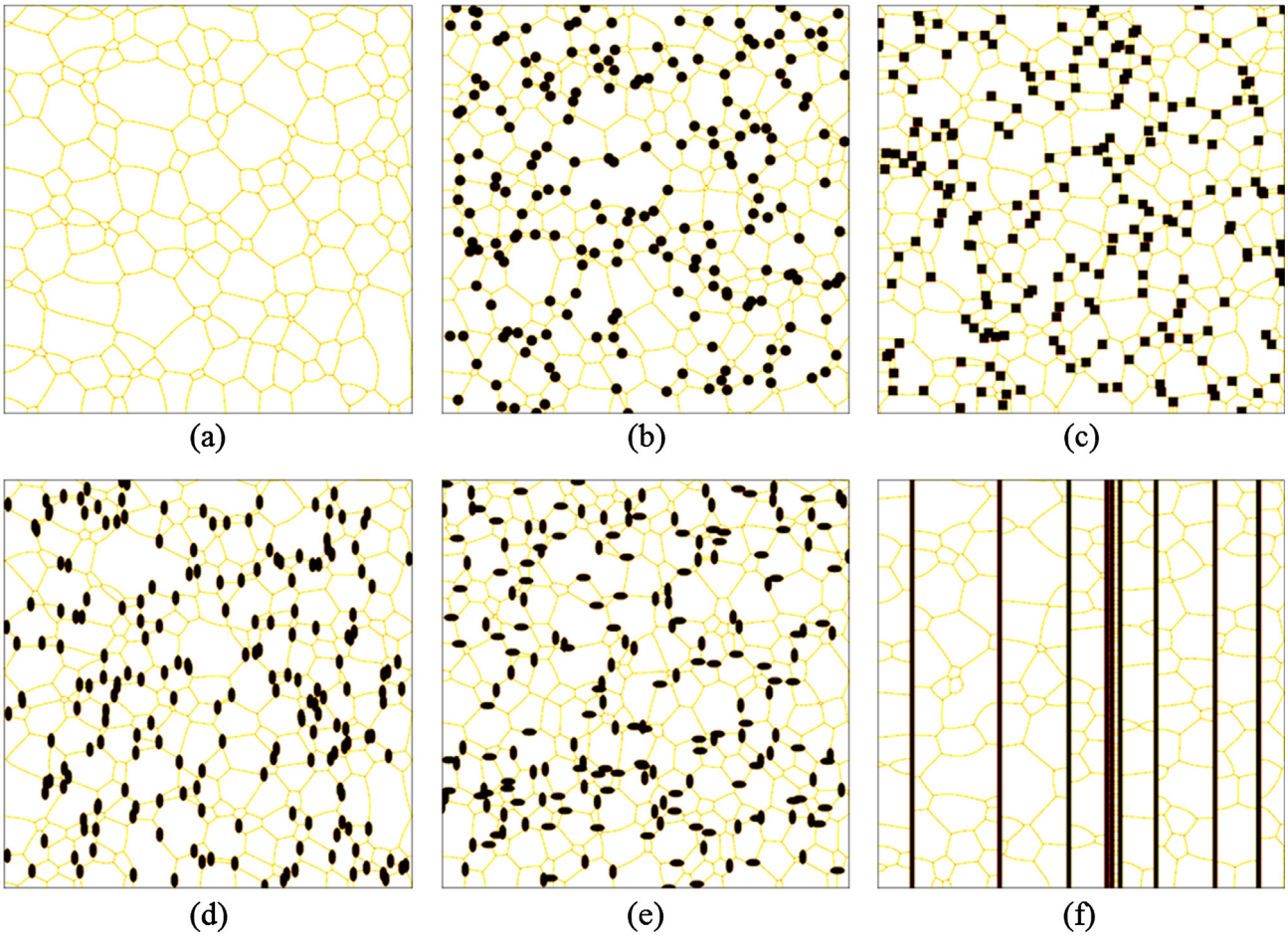

Fig. 1. Snapshots of microstructure evolution of polycrystalline at 100,000Δt. (a) single phase, (b) spherical pores, (c) cubical pores, (d) ellipsoidal pores of one direction, (e) ellipsoidal pores of two directions, (f) 10 straight-through pores.