

Keynote Paper

## **Bioinspired Structural Materials: Virtual Processing and Virtual Testing**

\*Chuin-Shan Chen<sup>1)</sup>, Heng Lee<sup>2)</sup>, Shu-Wei Chang<sup>3)</sup>, Yang-Shan Lin<sup>4)</sup>

<sup>1)2)3)</sup>Department of Civil Engineering, National Taiwan University, TAIWAN  
<sup>1)</sup>[dchen@ntu.edu.tw](mailto:dchen@ntu.edu.tw)

<sup>4)</sup>Industrial Technology Research Institute, TAIWAN

### **ABSTRACT**

Biological structural materials such as nacre and bone have achieved superior mechanical properties as a result of well-designed microstructure with dissimilar, namely soft and bulk, composites. Among all the manufacturing methods to emulate design and assembly principles learned from the nature, freeze casting is a novel and promising way to form a variety of biocomposites with an excellent microstructural control. In this keynote talk, I will present a modeling and simulation framework to perform virtual processing and virtual testing of bioinspired structural materials by freeze casting. For virtual processing, a phase-field model is developed to describe the crystallization in an ice template and the evolution of particles during anisotropic solidification. Under the assumption that ceramic particles can be represented by a concentration field, we derive a sharp-interface model and then transform the model into a continuous boundary value problem via the phase-field method. The adaptive finite-element technique and generalized single-step single-solve time-integration method are employed to reduce computational cost and reconstruct microstructure details. For virtual testing, we adapt the concept of representative volume element and micromechanics to investigate the stress distribution, load transmission as well as crack propagation due to different structural design of soft matrix geometry. We compare different microstructures from freeze casting to explore the relationship between mechanical properties and microstructures of bioinspired structural material. We show that dendritic patterns result in a certain influence on mechanical properties. Finally, we reveal that the design of soft matrix geometry determines the microcrack initiating patterns and impacts the local transmission mechanism of biocomposites.

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<sup>1)</sup> Professor

<sup>2)</sup> Graduate Student

<sup>3)</sup> Assistant Professor

<sup>4)</sup> Research Fellow

## 1. INTRODUCTION

Recently, designing high-strength, high-toughness, and lightweight materials has attracted significant attention [1, 2]. From the investigation of natural materials such as nacre or bone, bioinspired structural materials are found to exhibit excellent mechanical properties, mainly attributed to their complex microstructure [3]. Among all the manufacturing methods to emulate design and assembly principles learned from the nature, freeze casting is a novel and promising way to form a variety of biocomposites with an excellent microstructural control [4–6].

In this paper, we present a modeling and simulation framework to perform virtual processing and virtual testing of bioinspired structural materials by freeze casting. For virtual processing, a phase-field model is developed to describe the crystallization in an ice template and the evolution of particles during anisotropic solidification. For virtual testing, we adapt the concept of representative volume element and micromechanics to investigate the stress distribution, load transmission as well as crack propagation due to different virtual samples produced from virtual processing.

## 2. Virtual Processing: Phase Field Method

Freeze casting exploits the solidification behavior of a solvent in a well-dispersed slurry to form controllably porous ceramics, metals or polymers. By freezing slurry under freezing point, ice crystals nucleate on one side of the slurry and grow along with the external temperature gradient. The ice crystals will redistribute the suspended particles as they grow within the slurry, effectively templating the desirable porous microstructures. A phase-field model is developed to describe the crystallization in an ice template and the evolution of particles during anisotropic solidification [7]. Under the assumption that ceramic particles can be represented by a concentration field, we derive a sharp-interface model and then transform the model into a continuous boundary value problem via the phase-field method. Then the model is solved by using adaptive finite element technique [8] and single-step single-solve (GSSSS) time-integration method [9, 10] to reduce computational cost. In the following, we briefly summarize the phase-field formulation. For details, the readers may refer to [7].

Phase-field method [11, 12, 13] transforms the sharp-interface into continuous partial differential equations. In a phase-field model, a continuous scalar field  $\phi$  is introduced to distinguish between solid ( $\phi = 1$ ) and liquid ( $\phi = -1$ ). The final phase-field model of freeze casting is summarized below:

$$\begin{aligned} \tau_0 [1 - (1 - k_e) \tilde{T}] A^2(\theta) \frac{\partial \phi}{\partial t} = \nabla \cdot [W_0^2 A^2(\theta) \nabla \phi] + \phi - \phi^3 - \lambda (1 - \phi^2)^2 (U + T) \\ + \sum_{k=x,y} \frac{\partial}{\partial k} \left[ |\nabla^2 \phi|^2 A(\theta) \frac{\partial A(\theta)}{\partial \theta_{,k}} \right] \end{aligned} \quad (1)$$

$$\left(\frac{1+k_e}{2}-\frac{1-k_e}{2}\phi\right)\frac{\partial U}{\partial t}=\nabla\cdot\left(D\frac{1-\phi}{2}\nabla U+\frac{1}{2\sqrt{2}}[1+(1-k_e)U]\frac{\partial\phi}{\partial t}\frac{\nabla\phi}{|\nabla\phi|}\right) \\ +[1+(1-k_e)U]\frac{1}{2}\frac{\partial\phi}{\partial t} \quad (2)$$

in which  $\tau_0$  is the temperature-dependent relaxation time  $k_e$  is segregation fields,  $T$  is temperature field,  $A(\theta)$  is the anisotropic function controlling different diffusivity in different nucleation direction,  $W$  is the width of diffusion area,  $\lambda$  is coupling constant,  $U$  is supersaturation and  $D$  is the diffusion coefficient of the particle suspension.

The phase field model is solved by standard Galerkin finite element method combining with adaptive-mesh algorithm and GSSS time-integration method to reduce the computational cost. The simulation is also compared with experiments, and results show a good agreement with experiments, including the tendency of dendrites growing and the effect of concentration. For more details about the derivation and the comparison with experiments, please refer to reference [7].

### 3. Virtual Testing: Micromechanics and Representative Volume Element

Concepts from micromechanics and representative volume element (RVE) are adapted to obtain a mean constitutive response from microstructure for macroscopic behavior. Meshing a microstructure like the result of freeze casting simulation is a complex task. In order to directly employ the model into numerical simulation, methods using Fast Fourier Transform (FFT) are introduced. FFT-based numerical simulation for composite material was first introduced by Moulinec and Suquet [14]. Regular mesh-grids are operated and analyzed. The linear elasticity problem is solved iteratively, which does not require assemblage and storage of a global stiffness matrix in contrary to a standard finite element method. For more details readers may refer to [15].

## 4. RESULTS AND DISCUSSION

Freeze casing simulation is performed for three different concentrations, 20%, 30% and 40%, to generate different microstructures (Fig. 1). We then extract parts of microstructures as RVE to perform further stress analyze. The analysis results are shown in Fig. 2. The area below the stress-strain curve, which partially represents the toughness, shows the toughness from 20% concentration is greater than that of 30% and the toughness from 30% concentration is greater than that of 40%. The results reveal that the level of dendrites is an important controlled parameter of the toughness.

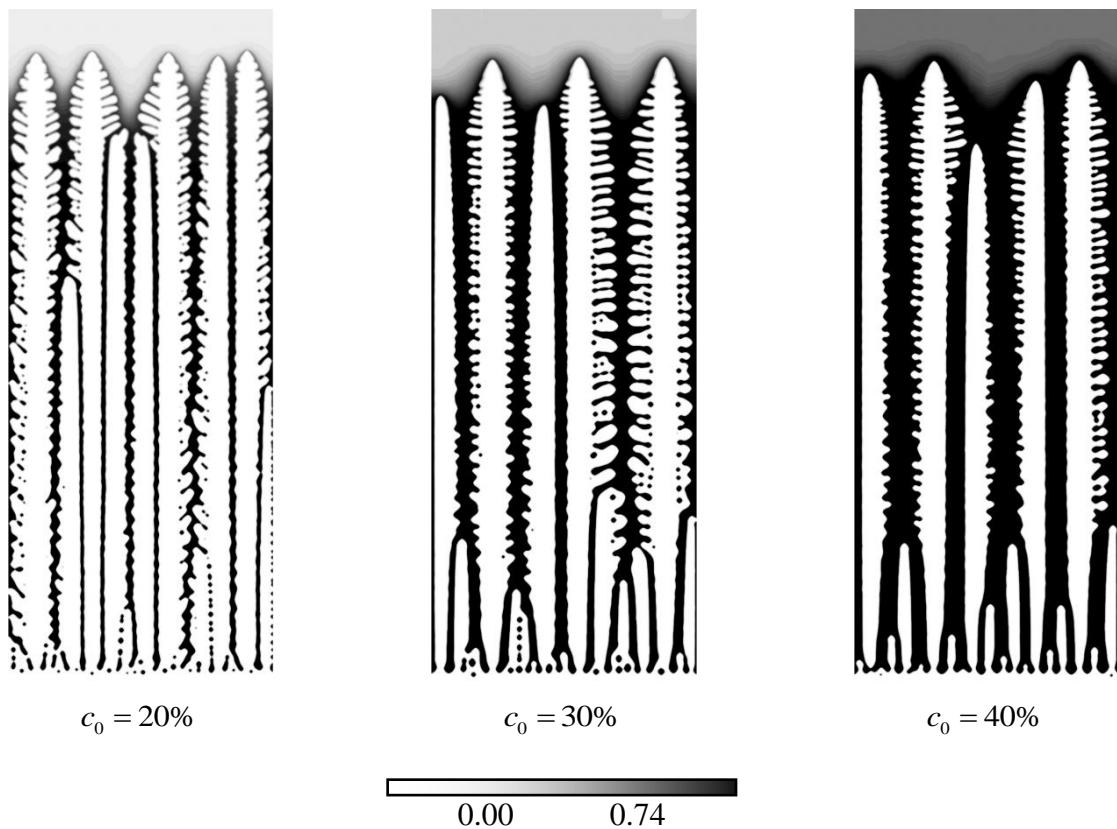


Fig. 1 Results of freeze casting simulation in 20%, 30% and 40% concentrations.

To further study the dendritic patterns on toughness, we choose three cases(case 1 to 3) to compare different shapes of dendrites (Fig. 3).Microstructures in these cases are taken directly from features in freeze casting microstructure to produce the RVE. Notice that, in order to maintain the criterion of these microstructures, the spatial density is kept in the same value.

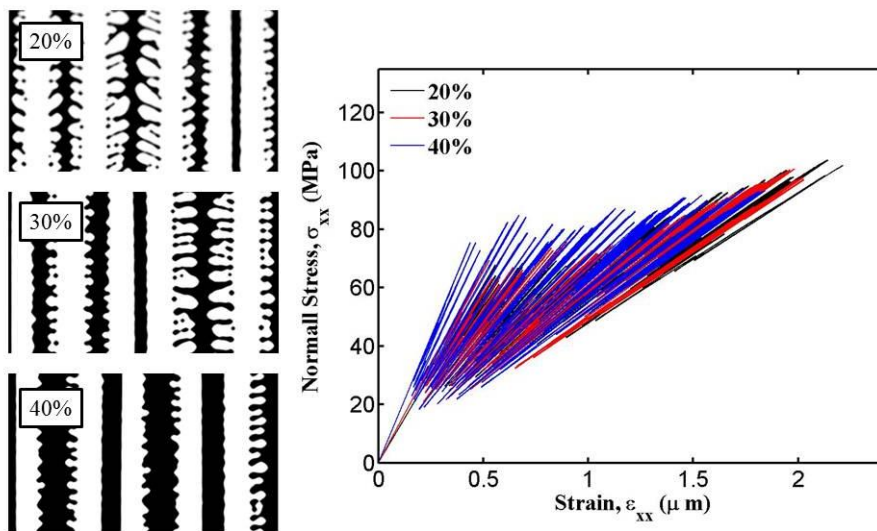


Fig. 2 Stress strain curve for different microstructures

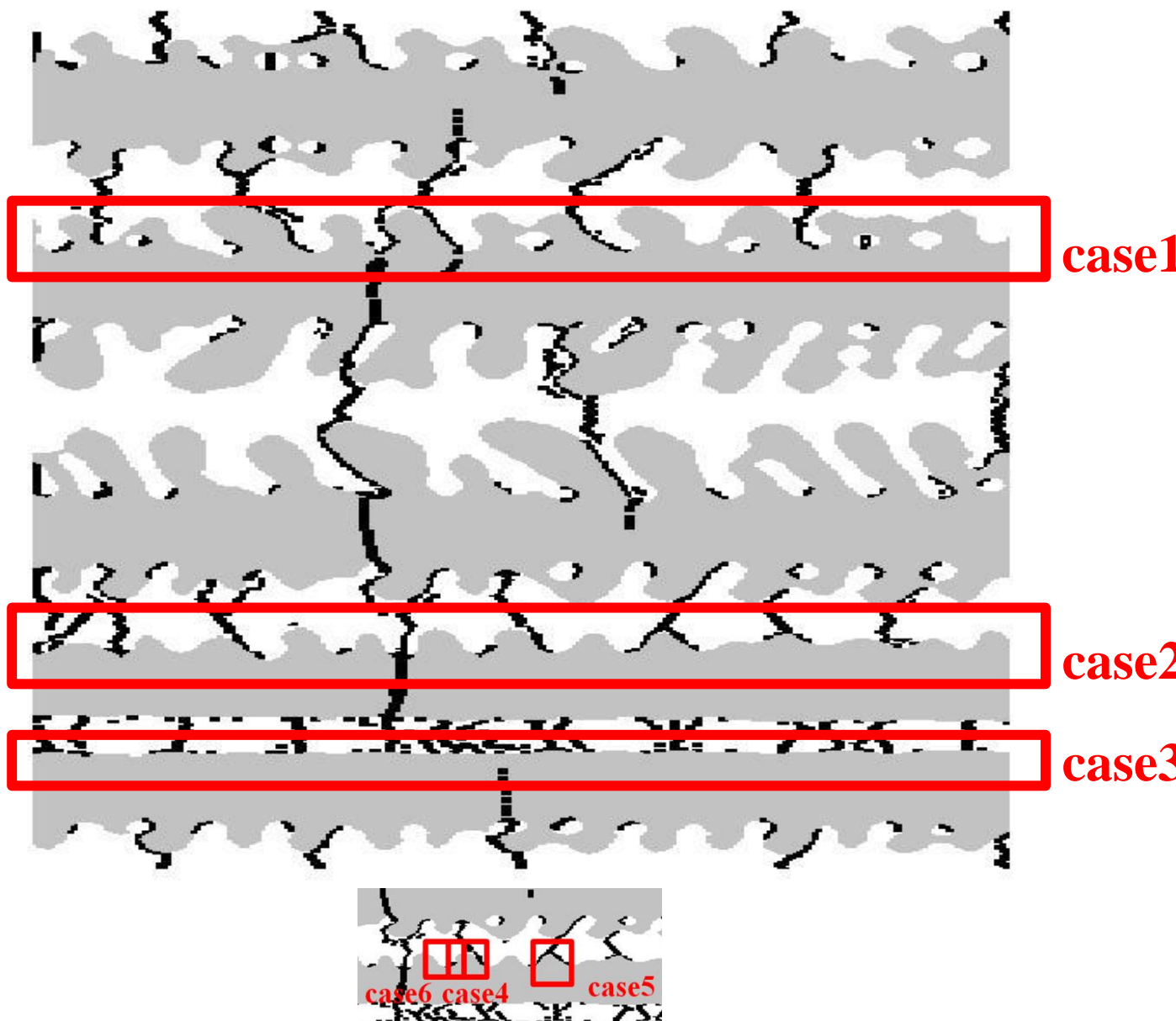
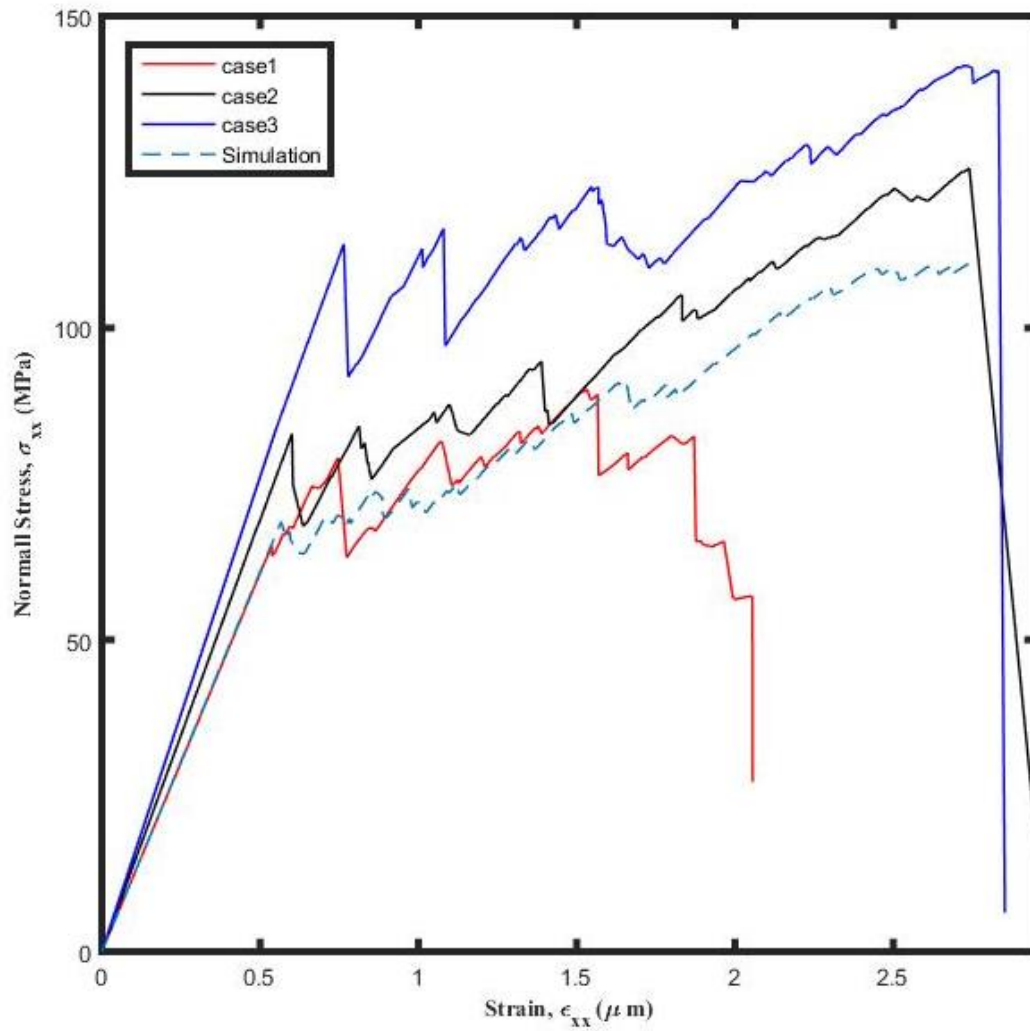


Fig. 3 Damage of the microstructure and the selected cases for further analysis

Left of Fig. 4 compares case 1 to 3 with the original freeze casting microstructure. It shows that dendrites do influence the property, but not all dendrite is beneficial for toughness, like case1. Case 3, which seems to process less dendrite, is actually tougher than the other cases. We notice that the case 2 does not fail at a sudden. It is implied that the shape of dendrites seems to be an important parameter. We thus further extract a single dendrite to explore the impact of shape.

By observing the crack development, we choose three cases (Fig. 3). The analysis results show that the shape of dendrites play an important role of toughness. Case 5 and case 6 process a better toughness comparing to case 3. (Fig. 4). All failure patterns are shown in Fig. 5.

## Case 1 to 3



## Case 3 to 6

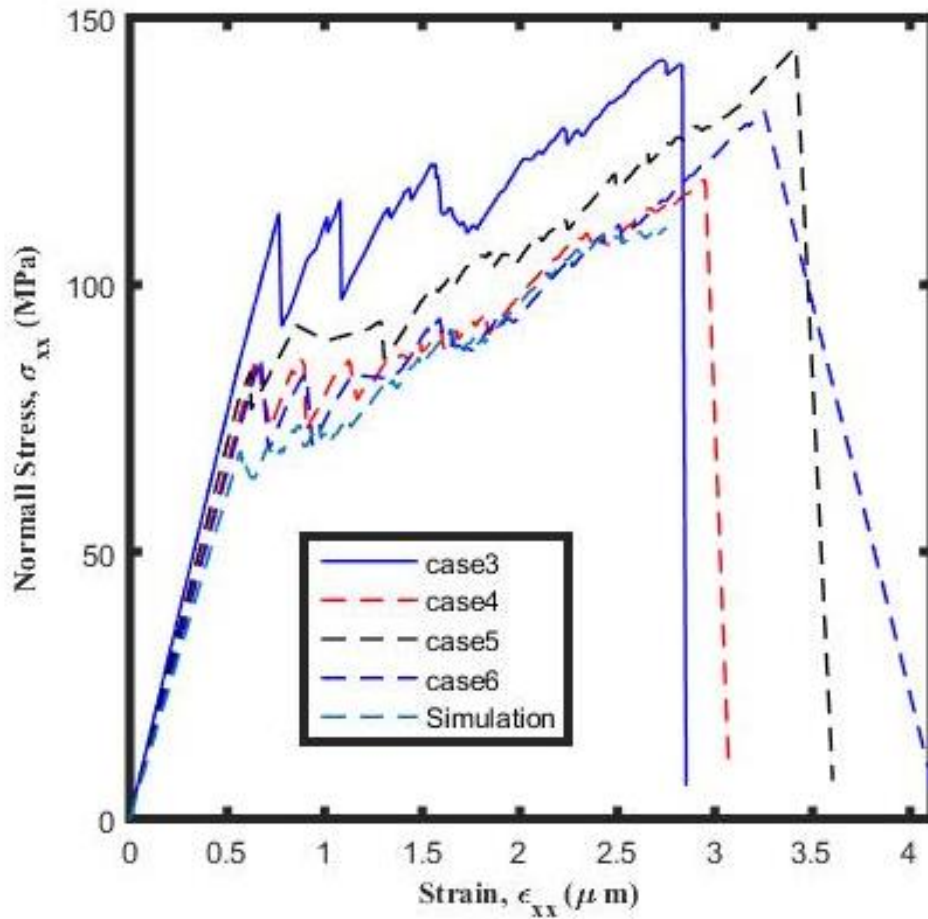


Fig. 4 Stress strain curve for six cases, including comparing first three cases with original freeze casting microstructure (left) and comparing last three cases with case 3.



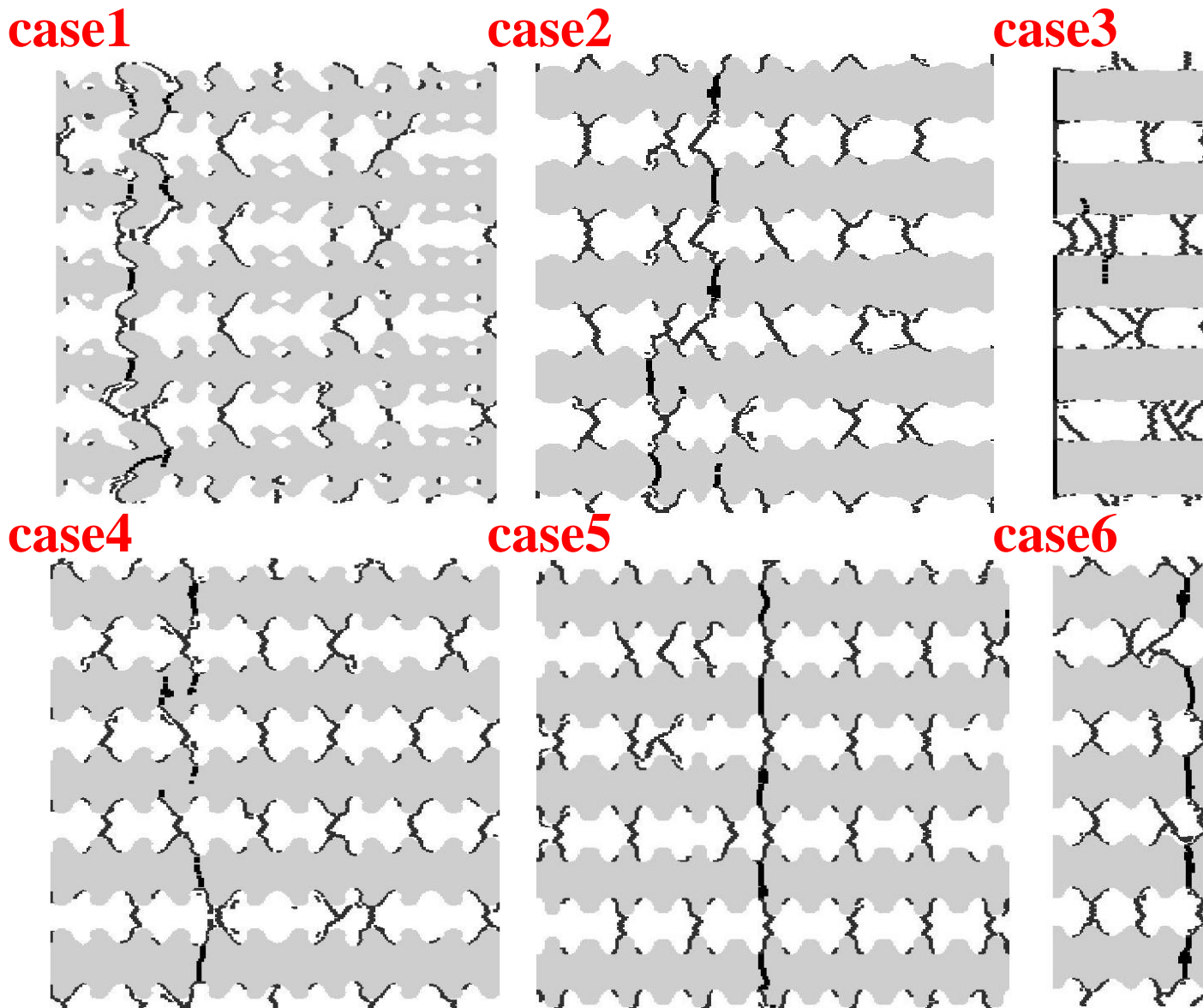


Fig. 5 Failure patterns of all the six cases studied herein.

#### 4. CONCLUSION

In this study, a virtual processing for freeze casting based on a phase-field model is developed. A virtual testing adapting the concept of RVE is developed to investigate the stress distribution, load transmission as well as crack propagation due to different microstructures from freeze casting. We show that the level of dendrites is an important controlled parameter of the toughness. Furthermore, the dendritic patterns play an important role for toughness.



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