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Reconstruction of co-continuous ceramic composites three-dimensional microstructure solid model by generation-based optimization method

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ABSTRACT

It is difficult for co-continuous metal/ceramic composite with complex spatial topology to establish three-dimensional (3D) solid model. A generation-based optimization method is proposed to reconstruct 3D solid model. Firstly, pre-processing of the composite SEM image is applied to obtain two-dimensional (2D) digital matrix using a maximum between-cluster variance method, metallic and ceramic phases are segmented accurately. 2D generation core field is obtained following the principles proposed in the paper. Secondly, an optimization method is proposed and applied for the randomly distributed 3D cores to match the core distribution characteristics. Thirdly, a modified real-time changing directional growth probability is applied to form a smooth interface between the two phases. Finally, volume fractions and 2-point correlation functions of the reconstructed model and a micro-CT model are compared to verify the accuracy. This method can be used to reconstruct the 3D model of other materials with different microstructures such as titanium alloy.

1. Introduction

Co-continuous metal/ceramic composites are consist of two networks, metallic phase as matrix and ceramic phase as reinforcement [1,2]. Other than the particle-reinforced composites [3], both of the two phases are interpenetrating and continuous [4–6]. Volume fraction, types of materials and morphology of each phase significantly affect the composite properties. Along with research and development of composites, co-continuous metal/ceramic composites gradually show its unique properties and are thus applied in many fields, such as automotive, aerospace and packaging and thermal management in electronic devices [7–9].

In the cycle processes of "design-preparation-performance test" for co-continuous metal/ceramic composites, performances could be obtained through experiments directly and reliably. But these investigations are restricted by experimental period, apparatus and other factors which are time-consuming and overspending [10,11]. In recent years, numerical simulation has become an efficient way to guide composite design and performance prediction in the wake of computer technology rapid development. Modeling is the first step in the process of numerical simulation, and its quality is an important influential factor to numerical simulation accuracy, especially for the complex topological structure of the composites. Researchers have accomplished an enormous amount of studies about the analogue microstructure. Sufficient literatures can be found for the research of co-continuous metal/ceramic composites with interpenetrating structure. The current 3D reconstruction research method can be mainly divided into two aspects as following [12–15]:

(1) *Physical experiment method*: As one of the two aspects of solid model reconstruction methods, physical experiment methods, which contain X-ray tomography [16] and serial sectioning method [17,18], can directly reconstruct composite solid model by combining serial sections obtained by X-ray tomography or grinding the material in a certain direction. Węglewski et al. [19] reconstructed a solid analysis model combined by images of the real material microstructure obtained from micro-computed tomography (micro-CT). McLean et al. [20] obtained large 3D microstructural datasets from a morphologically complex multiphase W–Cu composite material system using the Tri-Beam system via in situ femtosecond laser sectioning in a scanning electron microscope (SEM), and sample volumes were extracted from the full-size datasets over a wide range of sizes to determine the relevant volume element size. Singh and Gokhale [21] applied montage serial sectioning

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technique for reconstruction of large-volume high-resolution 3D microstructures of two composites that have different degrees of spatial clustering of SiC reinforcement particles distributed in an Al-alloy matrix. Li et al. [22] built 3D microscopic structural solid model of interpenetrating SiC/Al composites based on X-ray tomography and analysis investigate the dynamic compression response of the 3D model using solid methods. According to above researches, physical experimental methods subject to be limited by the experimental conditions of micro-CT or other instruments. Phases in composites are distinguished by X-ray. For some finer microstructures, some tiny characters could be lost, and in some instances some kinds of material microstructure may change through the sectioning process or the image contrast is not likely to be obvious under X-ray. So the physical method is sometimes confined in modeling process.

(2) *Numerical method* [23,24]: solid model can be reconstructed based on the material real image by numerical modeling methods, such as Gaussian method, simulated annealing method, and quartet structure generation set (QSGS) method. For the Gaussian method, Joshi [25] proposed Gaussian method firstly to research reconstruction problem of porous media, a two-dimensional model was obtained; Quiblier [26] modified Gaussian method to get 3D porous media model. For the simulated annealing method, Wu and Jiang [27] adapted the simulated annealing approach for reconstruction of the 3D microstructure of a $LiCoO_2$ cathode from a commercial Li-ion battery, and characterization of the reconstructed cathode gave important structural and transport properties; Hazlett [28] applied simulated annealing method to reconstruct 3D model of reservoir rock, and flow properties were computed from an accurate depiction of the porosity network in three dimensions. For the QSGS method, Wang et al. [29] had proposed the method based on the stochastic cluster growth theory for generating more realistic microstructures of porous media, and predicted the effective thermal conductivities of porous media with multiphase structure and stochastic complex geometries. Li et al. [30] introduced quartet structure generation set method to model the microstructure of clay, and the corresponding procedures were compiled with Matlab and AutoCAD. From what is discussed above, Gaussian method proposes a complex computation procedure which efficiency is affected by the computer performance. Statistical characteristic consistency between reconstructed model and real material structure mainly depends on whether the kind of material can be described only by the two statistical parameters of phase volume fraction and 2-point correlation function in Gaussian method. Simulated annealing method requires vast and time-consuming cycle computation. The QSGS method can reconstruct the 3D solid model which morphology is determined by the generation parameters. It can generate models with different distribution characteristics by changing the value of these parameters. But QSGS method reconstructed model may have problem with co-continuous metal/ceramic composite interpenetrating characteristic. The reconstructed model quality relies on the assessment of generation parameters. For the co-continuous metal/ceramic composites, these 3D model reconstruction methods cannot sufficiently describe the continuous morphology.

In this study, a generation-based optimization method is proposed to reconstruct 3D solid model based on one single section image of co-continuous metal/ceramic composites. Appropriate parameters choosing by section image analysis are applied in the reconstruction method. By comparisons between the reconstructed model and micro-CT reconstructed model by two geometry characterization parameters which containing volume fraction and 2-point correlation function, the generation-based optimization method can be verified to reconstruct co-continuous metal/ceramic composite solid model which matches the complex distribution characteristics of two phases.

2. Pre-processing

The generation-based optimization method involves two stages: (1) Image pre-processing. Composite SEM image will be transformed into composite 2D digital matrix via binarization. Then generation cores are distributed in the matrix to obtain 2D generation core distribution field which following two distribution principles. 2-point correlation functions and volume fractions are calculated by statistical analysis the matrix and the field. (2) Core distribution, optimization and generation. Generation cores, whose volume fraction remains the same with 2D generation core distribution field, are distributed in composite 3D generation core distribution field randomly. Then the 3D random generation core distribution field is optimized by simulated annealing method, in order to reach distribution uniformity with the 2D core field. Eventually, a 3D model, which is in accordance with the real composites, can be reconstructed by the generation process of 3D generation core distribution field. The details are shown in Fig. 1.

2.1. Image pre-processing

Composite image pre-processing is the first stage of generation-based optimization method. The quality of image pre-process is one of the important factors that affect the reconstructed 3D model precision. In this study, co-continuous metal/ceramic composite microstructure image taken by S4800 Field-Emission Scanning Electron Microscope is adopted as 2D real composite image. As shown in Fig. 2, the darker area and the brighter area are ceramic and metallic phases respectively. The 2D real composite image, whose two phases are continuous for each other in 3D space, can be transformed into 2D digital matrix via binarization. This study reconstructs 1 mm×1 mm×1 mm size 3D reconstructed model according to the 1 mm×1 mm size SEM image in Fig. 2.

By SEM tomography principle, there is a certain image contrast between ceramic and metallic phases in the SEM image. That is, pixel gray levels vary between areas contained by ceramic and metallic phases in computer graphics. So SEM image is equivalent to 2D digital matrix $g(x,y)$, in which each element values are different gray level. Then the SEM image can be divided into binaried ceramic and metallic phases by applying an appropriate threshold T to the 2D digital matrix $g(x,y)$ as Eq. (1) which 1 represents ceramic phase and 0 represents metallic phase.

$$f(x,y) = \begin{cases} 1, & g(x,y) < T \\ 0, & g(x,y) \geqslant T \end{cases} \tag{1}$$

It can be seen that an appropriate threshold T is the key point to divide the two phases in SEM image accurately. The maximum between-cluster variance method is adapted to obtain the appropriate threshold for the SEM image.

Maximum between-cluster variance method (Otsu method for an alternate name), is an adaptive threshold determining method. The Otsu method [31] segments image into background class and target class by gray levels. In binarization of co-continuous metal/ceramic composites, metallic phase is defined as background class and ceramic phase is defined as target class. In a $M \times N$ pixels size image, the supposes are following: