Computational Materials Science 69 (2013) 289–298

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Competitive stochastic growth model for the 3D morphology of eutectic Si in Al–Si alloys

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ARTICLE INFO

Article history:
Received 4 September 2012
Received in revised form 23 October 2012
Accepted 25 November 2012
Available online 8 January 2013

Keywords:
Al–Si alloys
Coral-like eutectic Si
Stochastic growth model
Multivariate time series
FIB-SEM tomography
Birth-and-death process

ABSTRACT

A competitive stochastic growth model is developed for the simulation of the 3D morphology of eutectic silicon in Al–Si alloys, which represents the colonies of pairwise disconnected Si corals in an Al matrix. The model is based on ideas from stochastic geometry and multivariate time series analysis. The 3D model is validated by comparing morphological characteristics computed for experimental 3D FIB-SEM data, and for realizations drawn from the model. Good agreement between the simulation model and the experimental image data is shown confirming the efficiency of using the competitive stochastic growth model for the generation of virtual eutectic silicon morphologies.

1. Introduction

A competitive stochastic growth model is developed for the simulation of the 3D morphology of eutectic silicon in Si–Al alloys, where hypoeutectic Al–Si alloys contain less than 12% of Si and present a two-phase material, consisting of primary α-Al dendrites and Al–Si eutectic [1]. The Si particles consist of pairwise disconnected Si corals in an Al matrix.

Combination of good castability and corrosion resistance of Al–Si alloys with good mechanical properties makes these alloys very attractive for applications in automotive industry. In Al–Si alloys, there is a strong relationship between morphology of eutectic Si and their mechanical properties. Commercially used modification of the microstructure morphology with Sr addition changes the morphology of Si from a coarse plate-like into refined fibrous structure, significantly improving mechanical properties of the alloy, particularly tensile strength and elongation [2–6]. The results reported by Shin et al. [6] have shown that Sr-modification of Al–10.5Si–2.0Cu recycled alloy leads to an increase of the elongation by a factor of two (from 2.0% to 4.1%) and tensile strength by more than 10% (from 209 to 237 MPa), which is reflected by a higher quality index of the material.

Stochastic models – in the context of materials science – can be used to elucidate the relationship between morphology and functional properties [7]. Such a design of virtual materials can be obtained by generating a broad range of virtual morphologies according to the stochastic model (using different values for the model parameters) and analyzing their functional properties by numerical calculations. Thus, it is possible to detect morphologies with improved materials properties using computer experiments. This reduces the amount of real experiments which are much more cost- and time-consuming.

In this paper, we present a stochastic model for the morphology of eutectic Si corals in Al–Si alloys. It is organized in a three-stage approach: In a first step, we introduce a model for single corals, where every single coral is represented by a connected system of line segments (which are dilated later). We use multivariate time series to accurately describe the complex spatial correlations of the branches within single corals [8,9]. Secondly, based on the single-coral model we present a competitive growth model which regulates the growth of neighboring corals according to a 'birth-and-death' process. More precisely, if two corals are competing for space, i.e., if the smallest Euclidean distance between two corals falls below a certain threshold, one coral will stop growing ('death') and the other one can continue to grow and expand in space ('birth'). The starting points for the competitive growth model are chosen according to an isotropic and stationary Matérn hard-core point process in 3D. In a third and final step, the aggregation of disconnected corals (i.e., aggregation of line segments) is dilated

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http://dx.doi.org/10.1016/j.commatsci.2012.11.051

in 3D to match the volume fraction of Si. The stochastic model for Al–Si alloys is validated by comparing morphological characteristics computed for a 3D image gained by FIB-SEM tomography, and for realizations of the Al–Si model.

The paper is organized as follows. Section 2 introduces the material and describes imaging of Al–Si alloys. Section 3 establishes the 3D Al–Si model which is given in terms of a competitive growth model. Furthermore, model fitting and model validation are discussed. Section 4 summarizes the results and provides a short outlook regarding possible future research.

2. Materials and imaging

We have performed a tomographic reconstruction and analysis of morphological parameters (volume fraction, particle density, connectivity, etc.) for several samples of Al–Si alloys. Usually, an addition of 0.03 wt.% of Sr is already enough to change an eutectic Si morphology [6]. The Al–Si7 alloy investigated in the present paper contains 150 ppm of Sr and has typical morphological characteristics of this type of alloys. Thus, it can be considered as representative. The alloy is produced by directional solidification leading to a formation of the described coral-like structure of Si particles with major orientation in the direction of the temperature gradient. The main goal is to develop a flexible stochastic simulation model which allows to describe this kind of structural morphologies (coral like, directionally solidified). After having developed a model for a typical experimental structure, it can be used for the (virtual) generation of other similar structures by fitting the model parameters to another experimental data sets, which is described in Section 3.3. The reconstructed volume of modified eutectic and an example of unmodified eutectic are shown in Fig. 1, where the stochastic model describes the modified eutectic Si corals.

The reconstruction of the Al–Si eutectic has been done by using FIB-SEM dual beam tomography. The technique provides a high resolution of less than 50–60 nm [10] and allows imaging of microstructure morphology constituents with a good contrast. FIB-SEM tomography reconstruction consists of iterative milling of the sample with ion beam and imaging of the sectioned planes with electron beam after removing a slice of a certain thickness from the sample. Resolution in milling direction is defined as a thickness of the layer of material removed with an ion beam and depends on the precision of ion beam cuts. The resolution in the imaging plan depends on the resolution of SEM images. The angle between FIB and SEM columns is 52°, so that the sample surface is perpendicular and the imaging plan is parallel to the ion beam. Due to such an experimental setup the voxel of the reconstructed data volume is anisotropic and is bigger in the milling direction. For a detailed exposition of the technique see [11,12]. When a stack of 2D SEM images is collected, 3D reconstruction of the morphology is processed by interpolation in *Avizo 6.3* software. The voxel resolution of the reconstructed 3D image is $46 \times 180 \times 59$ nm. The size of the considered image is $790 \times 195 \times 285$ voxel.

3. Stochastic model for Al–Si

In this section, we introduce a stochastic model describing the morphology of eutectic Si in Al–Si alloys. Eutectic Si in this kind of material bears a coral-like structure, i.e., it consists of aggregates of Si corals which are pairwise disconnected, see Fig. 1 (left). The stochastic model for the morphology of Si corals is organized in a three-stage approach, see also the *flow chart* in Fig. 2.

In a first step, we introduce a model for single corals, where every single coral is represented by connected line segments, which form a stem and branches. Both components, the stem and the branches are modeled using multivariate time series to take into account the complex spatial correlations of the line segments within single corals. A ‘win/lose’ criterion is introduced to control the spatial expansion of the branches and the distances between neighboring branches.

Secondly, based on the single-coral model, a competitive growth model is introduced which regulates the growth of neighboring corals. We introduce some kind of a ‘birth-and-death’ process to control the distances between neighboring corals. More precisely, if two corals are competing for space, i.e., if the smallest Euclidean distance between two corals falls below a certain threshold, one coral will stop growing (‘death’) and the other one can continue to grow and expand in space (‘birth’). In a third and final step, the aggregation of disconnected corals (i.e., aggregation of line segments) is dilated in 3D to match the volume fraction of Si as observed in the experimental image data.

3.1. Data preprocessing

As described in Section 2, the FIB-SEM image of Al–Si alloys is given as binary image with anisotropic voxel. We consider a cutout of the image and rescale the image to isotropic voxel using bilinear interpolation and subsequent global thresholding. The image size is $548 \times 761 \times 357$ (isotropic) voxel with voxel size of 46 nm, see also Fig. 3 (left). Thus, throughout the manuscript, we consider this 3D image of Al–Si alloys with isotropic voxels. In order to describe the single corals by line segments whose

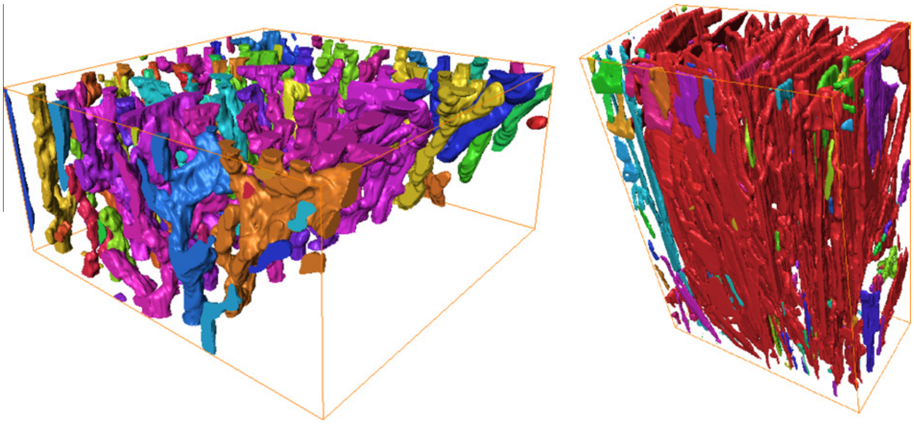

Fig. 1. Left: 3D image of modified coral-like eutectic silicon; right: an example of unmodified lamellar or plate-like eutectic silicon; connected component are displayed by the same color.