

# Probabilistic Modeling and Simulation of Microstructural Evolution in Zr Based Bulk Metallic Glass Matrix Composites During Solidification

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**Abstract** Bulk metallic glass and their composites are unique new materials which have superior mechanical and structural properties as compared to existing conventional materials. However, their mechanical behavior is dubious, unpredictable and requires extensive experimentation to draw conclusive results. In present study, which is continuation of previous work of author, a non-linear one-dimensional iterative deterministic model is combined with two-dimensional probabilistic cellular automaton method to describe nucleation and growth of primary ductile phase from melt in glassy matrix during solidification. Preliminary methodology and philosophy of model making is described with an aim to explain the grounds on which this approach is adopted. MATLAB<sup>®</sup> is chosen as programming platform. Results indicate that the effect of incorporating all heat transfer, mass transfer and diffusion coefficients with appropriate interpolation play a vital role in refining the model and bringing it closer to actual experimental observations. Two types of hypo and hyper eutectic systems were studied with different inoculants.

**Keywords** Cellular automaton • Solidification • Mass transfer coefficients  
Interpolation

## Introduction

Bulk Metallic Glass Matrix Composites (BMGMC) have emerged as new materials of future bearing unique properties of strength, hardness and elastic strain limit [1] which are not observed in other conventional engineering materials. However, they suffer from lack of ductility and toughness which make them impracticable to be used in any structural engineering application [2]. They fail catastrophically under

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the application of external load without yielding. Due to this they have not been able to gain enough popularity and are still being investigated at laboratory scale. Various theories and thoughts exist which reinforce or cast doubts about their large scale manufacturing. Recently, a lot of attention has been diverted at making them useful for outer space and extreme environment conditions [3–6] such as windows of international space station (ISS) [5], gears of outer and deep space exploration missions and rovers [7, 8]. However, an in depth understanding of their microstructure evolution is still a gap in field of research. Various efforts have been made to address this problem such as use of container less levitation techniques [4], experiments in micro and zero gravity [4, 9] and use of synchrotron light [10, 11] but none has proved out to be satisfactory. In present study, an effort has been made to address this problem from modeling and simulation perspective. A detailed probabilistic iterative model is developed based on well-known theory of self-reproducing automata [12] which is based on authors earlier work [3] describing deterministic modeling and simulation in Zr based BMGMCs. Some of the salient features of model and approach are described below.

## Model

It consists of making a detailed probabilistic model explaining two dimensional evolution of dendritic microstructure (e.g. B2 in CuZrAlCo and  $\beta$ -Zr CuZrAlNi) in a carefully selected simulation domain based on cellular automaton method [13]. Its features are:

1. It takes into account the use of transient thermal parameters (temperature, density, specific heat capacity, thermal conductivity) of actual Zr based BMGMCs [14], incorporate them in detailed heat transfer model in ABAQUS, generate temperature profile at each node of mesh in ABAQUS simulation geometry and finally use this temperature as input for CA simulation domain inside ABAQUS finite element (FE) grid [15]. In summary CA process [13] adopted here is:
  - a. Determine phases to be evolved in a typical selected alloy system (based on literature).
  - b. Determine their volume fraction ( $V_f$ ) (based on literature).
  - c. Select Representative Volume Element (RVE) in a test piece/coupon (in mm) (actual part—in present case rectangular block).
  - d. Selection of simulation domain (Cartesian or point based grid) (e-g  $300 \times 300$  [15]). This is performed in MATLAB.
  - e. Select cell shape (square, hexagon, rectangle (based on literature)). This is done in MATLAB.

- f. Select parameters to account for mesh anisotropy. This can be done by any of following
  - i. Selection of modified square cell (decentred square algorithm (DCSA [16–19])) (most popular approach).
  - ii. Refining of square cells e.g. limited angle method [15]
  - iii. Refining of mesh (by decreasing its physical size from micron to nm) (usually not adopted—leads to increase of computational time and makes process inefficient).
- g. Select neighborhood transition rules [20] based on well-established CA pattern selected in step e above (These rules are well defined in literature e.g. Von Numen rules, Moore rules [21] (popular, accurate but computationally expensive), Solid/Liquid Interface generation and energy at tip) [22, 23].
- h. Scan whole simulation domain/grid for “ $n$ ” number of cells ( $300 \times 300$  [15]) and assign a random number  $r$  ( $0 < r < 1$ ) to each cell [24–26].
- i. Select physical appearance of next cells based on neighborhood transition rules of step g above.

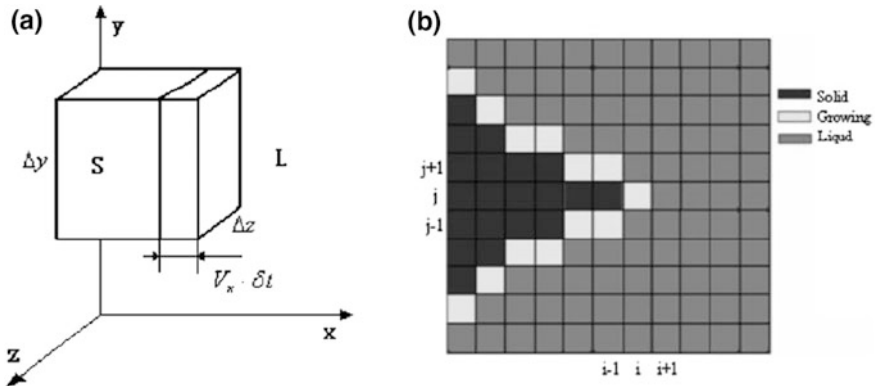
**Note:** CA model is physical model as it gives interface curvature physically and plot it in a cell in terms of solid fraction in a 2D simulation domain/grid thus a visual/physical picture is obtained. (However, it depends on previous deterministic [3] and heat transfer model (as described above)).

## Explanation

In essence, the model consists of calculating solid fraction in defined cell as a function of time. Once this solid fraction is calculated at a particular time, a random number is generated which is assigned to next growing grain/cell. Life or death of next cell is determined on the basis of this number. Similarly, growth (solid fraction) in next cell (Fig. 1a and b) is determined on the basis of its life/existence and the process continues.

It is primarily based on following fundamental studies [24, 27–29] whose origins go back to welding process owing to similarities in features and characteristics as additive manufacturing process.

1. Nastac, L., *Numerical modeling of solidification morphologies and segregation patterns in cast dendritic alloys*. Acta Materialia, 1999. 47(17): p. 4253–4262
2. Wei, Y.H., et al., *Numerical simulation of columnar dendritic grain growth during weld solidification process*. Science and Technology of Welding and Joining, 2007. 12(2): p. 138–146



**Fig. 1** a Schematic of growth in one cell b Schematic diagram of movement of dendrite tip in a grid of cells represented by change of state index of each cell [27]. (Reprinted with permission from Taylor and Francis Group)

3. Zhou, X., et al., *Simulation of microstructure evolution during hybrid deposition and micro-rolling process*. Journal of Materials Science, 2016. **51**(14): p. 6735–6749
4. Dezfoli, A.R.A., et al., *Determination and controlling of grain structure of metals after laser incidence: Theoretical approach*. Sci. Rep. 2017. **7**: p. 41527

Present study is focused on development of detailed theoretical model for BMGMCs. Coding, simulation results and their comparison with experimental values will be described in subsequent studies.

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