Article

Not peer-reviewed version

Modelling and Simulation of Microstructural Evolution in Zr Based Bulk Metallic Glass Matrix Composites (BMGMC) in Additive Manufacturing – A Proposal, Opinion and Prospect

Muhammad Musaddique Ali Rafique *

Posted Date: 10 February 2023

doi: 10.20944/preprints202302.0179.v1

Keywords: transport phenomena; melt pool; dendrite; cellular automaton; MATLAB®, ABAQUS®

 doi:10.20944/preprints202302.0179.v1

Article

Modelling and Simulation of Microstructural Evolution in Zr based Bulk Metallic Glass Matrix Composites (BMGMC) in Additive Manufacturing— A Proposal, Opinion and Prospect

Muhammad Musaddique Ali Rafique [1,2,3,*]

[1] Department of Space Engineering, Massachusetts Institute of technology, Cambridge MA 0213; ali.rafique@easternengineeringcambridge.onmicrosoft.com
[2] National Aeronautics and Space Administration, 39B, Merritt Island, Florida
[3] Eastern Engineering Solutions Inc. Cambridge, MA 02139

Abstract: Despite being well established phenomena, solidification principles are experiencing tough challenges in their application to explain microscale transport phenomena in additive manufacturing melt pool. The problem becomes even more complicated when applied to multicomponent bulk metallic glass matrix composites (BMGMC) whose behavior is dubious and still not fully understood. The aim of the present study is to highlight pathways to overcome these challenges. A comprehensive nucleation and growth model based on original KGT theory and Rappaz modification is proposed encompassing actual transient thermophysical BMGMC data to predict evolving microstructure during additive manufacturing. The model is aimed at pictorial representation of *in-situ* ductile phase dendrite evolution from melt pool during solidification using two-dimensional cellular automaton (CA) methods. It is proposed to be coded in MATLAB® using commercial simulation code ABAQUS® at back end for macroscopic heat transfer model. The results will be compared with experimental values for validation.

Keywords: transport phenomena; melt pool; dendrite; cellular automaton; MATLAB®, ABAQUS®

---

1. Introduction

Solidification phenomena has been comprehensively studied since long (Dantzig and Rappaz 2016; Campbell 2004, 2003; Beeley 2001; Flemings 1974; Chalmers 1964; Kurz and Fisher 1986). In literature, various well-established theories (Vehkamäki 2006; Kalikmanov 2012; Karthika, Radhakrishnan, and Kalaichelvi 2016; Katz 1992) and their experimental verifications exist which explains nucleation and growth mechanisms during solidification of metals, alloys and compounds. These have been successfully applied on various systems (Coquerel 2014; Jones, Evans, and Galvin 1999; Frank et al. 2007; Martin 2000; Pruppacher, Klett, and Wang 1998) and in various processes (Venables, Spiller, and Hanbucken 1984; Baumgartner et al. 2013; Sagui and Grant 1999; Thanh, Maclean, and Mahiddine 2014; Browne, Kovacs, and Mirihanage 2009) to effectively explain their development (CHRISTIAN, J.W' 2002; Gránásy et al. 2006). These range from simple one component pure metals to multicomponent complex alloys ('Front Matter A2 - CHRISTIAN, J.W' 2002; Neilson and Weinberg 1979; Erdemir, Lee, and Myerson 2009). However, their application on new bulk metallic glass matrix composites and additive manufacturing process has faced severe challenges (Cordero et al. 2017; Weissmayer et al. 2015; Smith et al. 2016). Fundamental principles of solidification become difficult to apply on an extremely narrow melt pool region in additive manufacturing (Yap et al. 2015; Cunningham et al. 2017). Various multiphysics and multiscale phenomena simultaneously happening (Dunbar 2016; Lavery et al. 2014) such as convection (Pengpeng and Dongdong 2015), conduction (Buchbinder et al. 2014; Manvatkar, De, and DebRoy

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 10 February 2023 doi:10.20944/preprints202302.0179.v1

2014; King et al. 2014), radiation (King et al. 2014), fluid flow (Qiu et al. 2015; Panwisawas et al. 2015; Lee and Zhang 2015; Khairallah and Anderson 2014), solute diffusion (Roehling et al. 2017; Thijs et al. 2010), thermocapillary effect (Khairallah et al. 2016), and surface tension (Khairallah et al. 2016; Schoinochoritis, Chantzis, and Salonitis 2017) collectively contribute and create a synergic effect which is difficult to model at very small scale (Dunbar 2016; King, Anderson, Ferencz, Hodge, Kamath, and Khairallah 2015; Markl and Körner 2016; Liou et al. 2015; Ganeriwala and Zohdi 2014; King, Anderson, Ferencz, Hodge, Kamath, Khairallah, et al. 2015; Francois et al. 2017). Bulk metallic glass matrix composites (BMGMC) have emerged as new competitive material possessing combination of enormous strength, hardness and elastic strain limit which is not exhibited by any other material known till date (Hofmann 2013; Wu et al. 2014; Ferry et al. 2013). However, they manifest brittleness due to parent glassy structure and suffer from lack of ductility and little or no toughness and fail catastrophically under the action of applied load (Wu et al. 2014; Wu et al. 2011). Various theories and mechanisms have been proposed to counter this effect such as introduction of external foreign particles as obstacle to the motion of shear bands (Siegrist 2007; Siegrist, Amstad, and Löffler 2007; Siegrist and Löffler 2007; Siegrist, Steinlin, and Löffler 2007; Conner, Dandliker, and Johnson 1998), self-multiplication of shear bands at junctions or points of their intersection (Greer, Cheng, and Ma 2013), "*in-situ*" nucleation and growth of ductile phase dendrites from melt in glassy matrix (Hays, Kim, and Johnson 2000) as a result of solute partitioning (Hofmann, Suh, Wiest, Duan, et al. 2008; Jiang et al. 2017; Kim, Kim, and Lee 2003; Cheng et al. 2013; Hofmann, Suh, Wiest, Lind, et al. 2008; Launey et al. 2009; Sarac 2015) but none have proved out to be satisfactory. An effective way to overcome this problem is to utilize one of their intrinsic properties, known as "devitrification". This is structural relaxation in supercooled strained structure of bulk metallic glass upon heating below their glass transition temperature (T_g). This structural relaxation (Hammond, Houtz, and O'Reilly 2003; Li et al. 2003) as well as rejuvenation (Dmowski et al. 2010; Zhang et al. 2017; Ketov et al. 2015) imparts toughness without sacrificing strength. This effect intrinsically exists inside additive manufacturing process. Bulk metallic glass matrix composites (BMGMC) of appropriate composition, if manufactured by additive manufacturing (AM), form in layer – by – layer (LBL) fashion (Li et al. 2016; Sun and Flores 2013, 2011). In this formation, layer preceding fusion layer gets heated automatically to a temperature below glass transition (T_g) thus devitrification occurs. However, the biggest challenge is to tailor the process in such a way as to avoid complete crystallization of glassy structure. This can happen only if the laser scan speed, power, width (spot size) and angle of incidence are controlled in such a way that partial crystallization happens only. This is very big challenge and till date no reported attempt have been witnessed which have successfully produced bulk metallic glass matrix composite components using additive manufacturing. An effective pathway to achieve this is to predict the evolution of microstructure in melt pool during additive manufacturing. Various rigorous multiphysics and multiscale modelling techniques combine the power to do this. Out of these, two main fundamental techniques namely, phase field (Gránásy et al. 2014) and cellular automation (Laurentiu and Doru 1997; Nastac 1999; Lee and Hong 1997; Charbon and Rappaz 1993; Reuther and Rettenmayr 2014) have successfully predicted the microstructure evolution in various alloys systems in various processes such as welding (Wei et al. 2007), joining, rolling (Zhou et al. 2016), batch and continuous casting. Since majority of theory of additive manufacturing comes from welding, same underlying principles can explain microstructural evolution in this unique new technique.

2. Mathematical Model

Model will consist of two parts. first part shall comprise of deterministic modeling (Rafique, Qiu, and Easton; Rafique 2018b; Musaddique Ali Rafique 2018) which is backed by macroscopic heat transfer model for predicting melt pool shape and associated heat transfer (Rafique and Iqbal 2009; Rafique 2015). This will be coupled with a probabilistic model (Rafique 2018c, 2018d) to predict solidification microstructure evolution in these versatile and important class of materials. This aim is to predict microstructure evolution at part scale level in additive manufacturing melt pool. Heat transfer model used to predict melt pool shape is achieved at after application of various point, line and plane source models. Overall, objectives of this research are to investigate and utilize rigor, versatility and power of modeling and simulation techniques to probe into and investigate the effect of different processing techniques on the final microstructure and properties of bulk metallic glass matrix composites (BMGMC). It aims to employ transient nature multiphysics transport processes and arrive at near experimental real values at microscale. These will be applied to predict microstructure evolution in bulk metallic glass matrix composites (BMGMC). Following research **objectives** are aimed to be achieved during research;

OBJECTIVE 1

Macroscopic transient heat transfer model: This consist of development of macroscopic non-linear transient heat transfer model to explain heat flow process during laser matter interaction. The model is based on well-established Beer Lambert Law of light (laser) matter interaction (Khairallah et al. 2016; Gusarov and Kruth 2005; Pengpeng and Dongdong 2015; Zohdi 2014; Chen et al. 2016; Yuan 2013). It is aimed to be programmed in commercial finite element (FE) simulation code ABAQUS® with moving heat source and varying boundary conditions. It is expected to yield temperature profile data at each node of mesh. It is aimed to be simulated with medium size mesh to keep a balance between size of mesh and resulting values. An output of incidence of laser on thin plate and its traverse is represented in Figure 1 below.

Figure 1. Track of incidence of laser on the surface of sample.

1. Hypothesis: Null hypothesis is heat transfer process is difficult to model due to transient nature of process and unavailability of temperature dependent thermophysical data related to bulk metallic glass matrix composites (BMGMC).
2. Experimental procedure: It will consist of use of commercial finite element code ABAQUS® 6.14-3 with the application of user defined subroutines (UTEMP and DFLUX) to simulate moving heat source.
3. Protocols: Step-by-step standard approach of the use of ABAQUS® with user defined subroutines linked in Intel Parallel Studio XE (consisting of Microsoft Visual FORTRAN®) and Microsoft® Visual Studio will be adopted to generate part drawing, property assignment, meshing, optimisation and running of simulation to arrive at results. Special care will be taken in the use of CFD module rather than thermal module. ABAQUS® explicit mode alongside implicit mode with the extraction of thermal data and its usage in third party softwares e-g JAVA® or MATLAB will also be considered (Liu, Kouadri-Henni, and Gavrus 2016).
4. Facilities: A dedicated IBM ThinkPad® P 51 machine with Intel Xeon E3-1505M v6 (Quad Core, 3.0 GHz on the base / up to 4.0 GHz with Intel Turbo, 8MB cache, 2400MHz speed), 32GB DDR4 Memory (upgraded, maximum memory capacity is 64 GB), 512 GB PCIe NVMe M.2 Solid State Drive (SSD), 15.6 Inch IPS FHD (1920x1080) Screen, Anti-glare, NVIDIA Quadro M2200 (4GB)

graphics, 6 Cell Battery and Windows 10 Pro 64-bit is aimed to be employed. Average time taken to run one simulation is expected to be 2 to 2.5 hours.

5. Techniques of analysing data: Parallel processing available as "in built" function in linked Intel® Parallel studio XE, MS visual studio and ABAQUS 6.14-3 will be used to carefully model and simulate heat transfer phenomena occurring during laser matter interaction in additive manufacturing. Use of loops with standard low to medium iteration will be used to arrive at convergence and refined results.
6. Expected results and impact: It is expected that with the use of this protocol a moving heat source with real time temperature dependent data will be generated simulating actual thermofluidic conditions in additive manufacturing melt pool. This will be a value-added contribution towards efforts made to model simultaneous heat and mass transfer phenomena in additive manufacturing melt pool in bulk metallic glass matrix composite (BMGMC) in which, still there is a gap in literature as well as in practice.

As an extended approach, this methodology and code will be employed towards development of commercial software dedicated to solving additive manufacturing problems.

OBJECTIVE 2

Microscopic deterministic microstructure model: This will consist of development of microstructure model which are combination of deterministic and probabilistic models to arrive at physical representation of microstructure in evolving domain. Fundamentally, deterministic model is non-linear one dimensional (1D) open boundary conditions problem solving evolution of microstructure in terms of nuclei of certain density as function of undercooling. This undercooling is measured at three specific locations. (a) bulk liquid (homogeneous nucleation), (b) potent nuclei (heterogeneous nucleation) and (c) mold wall (heterogeneous nucleation). The "growth" of these nucleation sites of certain density is expressed in terms of supersaturation. A unique feature of present approach will be, it expresses supersaturation of individual elements in multicomponent alloy system not adopted previously (Kurz, Giovanola, and Trivedi 1986; Zhang et al. 2013). It will give more accurate and precise measure of dendrite tip radius, its velocity and temperature as a result of contribution from individual elements (Rafique, Qiu, and Easton 2017).

1. Hypothesis: Null hypothesis is measurement of individual elements and their supersaturation is ineffective means of arriving at quantitative prediction of microstructure parameters of multicomponent bulk metallic glass matrix composites (BMGMC).
2. Experimental procedure: Procedure adopted to achieve this objective will employ modifications in original 35 years old solidification theory for rapid solidification (Kurz, Giovanola, and Trivedi 1986) and simulate the resulting model in MATLAB® with open boundary conditions. Aim is to employ temperature dependent thermophysical properties with well-established dimensionless numbers for mass transfer at microscale yielding accurate solidification parameters. MATLAB® programming will be assimilated with use of loops to account for iteration.
3. Protocols: Step-by-step standard approach of the use of MATLAB® with user defined functions which lead to generation of vectors, loops and outputs will be adopted. No inbuilt MATLAB® function will be employed; rather all programming will be done as a standalone code. However, use of its linking with inbuilt libraries in Simulink® will be employed to arrive at refined results. Use of third party software and plug – ins (e-g. Abaqus2Matlab (Papazafeiropoulos, Muñiz-Calvente, and Martínez-Pañeda 2017)) for integration with previous heat transfer model as and when needed will also be employed.
4. Facilities: A dedicated IBM ThinkPad® P 51 machine with Intel Xeon E3-1505M v6 (Quad Core, 3.0 GHz on the base / up to 4.0 GHz with Intel Turbo, 8MB cache, 2400MHz speed), 32GB DDR4 Memory (upgraded to maximum 64 GB), 512 GB PCIe NVMe M.2 Solid State Drive (SSD), 15.6 Inch IPS FHD (1920x1080) Screen, Anti-glare, NVIDIA Quadro M2200 (4GB) graphics, 6 Cell

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 10 February 2023 doi:10.20944/preprints202302.0179.v1

Battery and Windows 10 Pro 64-bit is aimed to be employed. Average time taken to run one simulation is expected to be few minutes as the length of code is compensated for by its bifurcation in parts which ease out processing and decrease computational cost.

5. Techniques of analysing data: Output results will be plotted in various forms using in built graphical functions of MATLAB as well as external software e-g Minitab®, Prism® which will be employed for performing various statistical analysis on generated data. These include, but not limited to ANOVA, standard deviation, standard error, 95% confidence and curve fitting.
6. Expected results and impact: It is expected that with the use of this protocol, a modified solidification microstructure model accounting for numerical determination of solidification parameters will be obtained. This will give quantitative results rather than qualitative output. Its validity will be comprehensively tested for accuracy of simulation results by performing various simulations on different independent computing platforms and comparing results. It will also be tested for various alloys systems for a set of thermophysical properties which are expected to generate different but comparable results.

The robustness of code will also be tested by varying number of iterations and their effect on resulting outputs.

OBJECTIVE 3

Microscopic probabilistic microstructure model: This part will consist of development of probabilistic model which gives physical representation of microstructure in evolving domain. This involve use of well-defined 2D Cellular Automaton (CA) theory (Shiffman 2012; Wei et al. 2007; Gu et al. 2017; Wei et al. 2011; Zhou et al. 2016) to describe evolution of solid fraction in a carefully selected cellular domain as a function of time. This method relies on selection of cellular automaton domain typically defined by number of cells selected for performing analysis and generating output. This number, which typically ranges from 30,000 – 50,000 (Rafique, Qiu, and Easton 2017) gives a measure of refined outputs. After selection of number of cells to define simulation domain, a random number (p_r) (Jabbareh and Assadi 2013; Dezfoli et al. 2017; Charbon and Rappaz 1993) will be assigned which determines the probability of selection of next cell after first cell as its solid content is achieved and its phase state changes. This is very important and must be determined with care. As with the previous case, grain growth will be determined at three separate locations, (a) bulk liquid (homogeneous nucleation), (b) potent nuclei (heterogeneous nucleation) and (c) mold wall (heterogeneous nucleation). A detailed model accounting for application of this cellular automaton (CA) theory to explain evolution of solid fraction of ductile phase dendrites in BMGMC during solidification in additive manufacturing melt pool is described. Another feature of this model will be; it is computationally less expensive as compared to its counterpart phase field models (Gránásy et al. 2006; Gránásy et al. 2014), gives quick results and easy to apply to evolution of dendrites, their branching, spacing (DAS) and multiplication as compared to single dendrite growth in phase field approach.

1. Hypothesis: Null hypothesis is measurement of solid fraction of individual elements is ineffective means of arriving at physical microstructure which is true representation of actual solidification process in multicomponent bulk metallic glass matrix composites (BMGMC).
2. Experimental procedure: Procedure adopted to achieve this objective will consist of use of cellular automaton theory to account for measurement of solid faction caused by individual elements rather than measurement of solid fraction of predetermined simulation-based phases from pseudo binary phase diagrams. Then solid fraction of individual elements will be grouped into different categories to give an estimate of evolved phases. The resulting microstructure will also depend on cellular automata transition rules. Various previously tested rules will be employed to arrive at highly optimised rule which gives physical picture resembling actual microstructure of alloy cross section under optical light microscopy. Again, temperature based thermophysical properties with well-established dimensionless numbers for mass transfer at

microscale will be employed yielding best possible picture of physical processes happening at microscale for multicomponent alloys. MATLAB® programming will be assimilated with use of loops to account for iteration.

3. Protocols: Step-by-step standard approach of the use of MATLAB® with user defined functions which lead to generation of vectors, loops and outputs will be adopted as was done for previous objective. Inbuilt MATLAB® functions which assign colour to evolving domain will be employed to represent microstructure consisting of different elements. Programming itself will be done as standalone code on a dedicated machine. Its linking with inbuilt libraries in Simulink® will also be employed. Use of third party softwares and plug – ins (e-g. Abaqus2Matlab (Papazafeiropoulos, Muñiz-Calvente, and Martínez-Pañeda 2017)) for integration with previous heat transfer model as and when needed will also be employed to explain real time additive manufacturing process.
4. Facilities: A dedicated IBM ThinkPad® P 51 machine with Intel Xeon E3-1505M v6 (Quad Core, 3.0 GHz on the base / up to 4.0 GHz with Intel Turbo, 8MB cache, 2400MHz speed), 32GB DDR4 Memory (upgraded to maximum 64 GB), 512 GB PCIe NVMe M.2 Solid State Drive (SSD), 15.6 Inch IPS FHD (1920x1080) Screen, Anti-glare, NVIDIA Quadro M2200 (4GB) graphics, 6 Cell Battery and Windows 10 Pro 64-bit is aimed to be employed.. Average time taken to run one simulation was observed to be few minutes as the length of code is compensated for by its divisions in parts which make it computationally inexpensive.
5. Techniques of analysing data: Output results will be plotted in the form of evolving dendrite using inbuilt plot and surf functions of MATLAB®. Their input will be based on matrix values.
6. Expected results and impact: It is expected that with the use of this protocol a detailed 2D physical solidification microstructure of bulk metallic glass matrix composites will be obtained. It will be tested by varying (a) composition, (b) thermophysical properties and (c) iteration cycles. It is expected that variation in these values will result in varied microstructures which will yield a detailed and in depth understanding of solidification phenomena of BMGMC.

4. Research Approach and Methods

Quantitative research methodology will be adopted for solving this problem which consists of (1) formulation of hypothesis / research questions, (2) defining of variables for addressing research questions and (3) using quantitative / analytical techniques employing variables to solve problems. Here, the problem is sought after by modelling and simulation. The model is combined deterministic and probabilistic model. Below some of the salient features and significant points of research approach are enlisted;

1. **Quantitative / Deterministic part**: Model is significant modification of existing KGT theory of alloy solidification. It consists of nucleation and growth of ductile phase dendrites.

Nucleation: Nucleation is based on Oldfield's theory of heterogeneous nucleation which describes a relationship between undercooling and grain density at each segment of interest. Two parameters namely, maximum nucleation density (n_{maxi}) and grain density (n(ΔT) are sought after to be determined. Maximum nucleation density may be determined by

$$n_{max_i} = \int_0^\infty \frac{dn}{d\Delta T\prime} \Delta T' \tag{1}$$

while grain density is given by

$$n(\Delta T) = \int_0^\infty \frac{n_{max}}{\Delta T_\sigma \sqrt{2\pi}} exp\left[-\frac{1}{2}\left(\frac{\Delta T' - \Delta T_N}{\Delta T_\sigma}\right)\right] d\Delta T' \tag{2}$$

where ΔT_n and ΔT_σ are mean undercooling and standard deviation of grain density distribution respectively.

With this, probability of happening of one event (nucleation) is given by nucleation probability (p_v) as described by Prof. Rappaz in his famous article (Rappaz and Gandin 1993).

$$p_v \geq r \quad (3)$$

i-e if at any instant of time t, p_v exceeds r, nucleation will occur. $p_v = \delta n_v . V_{CA}$ where δn_v = grain density increases and V_{CA} = one cell volume (measure by noting all dimensions of cell assuming it to have square shape).

Growth: This section concerns the determination of supersaturation of individual elements in multicomponent alloy (BMGMC) systems. This supersaturation Ω_i is a function of Peclet number, Pe_i

$$\Omega = I_v(\text{Pe}) \quad (4)$$

Solving a set of equations yields relationships for R = Dendrite tip radius, V = Dendrite tip velocity and Dendrite tip temperature. A schematic flow chart describing the working of model and interdependence of parameters is presented in Figure 1 below.

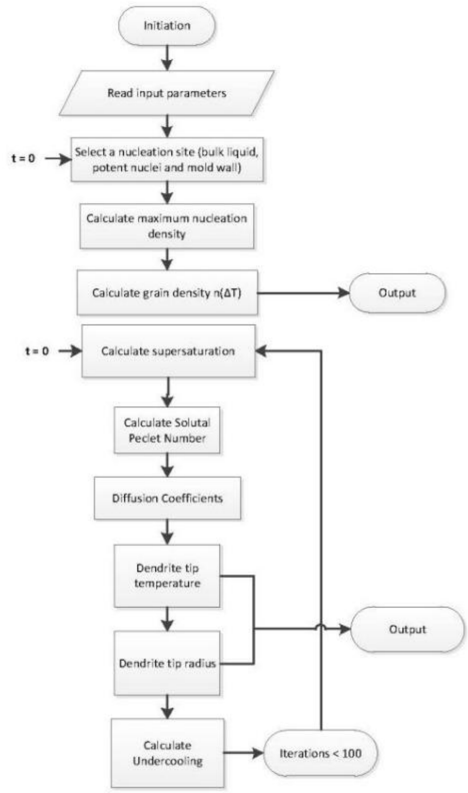


Figure 1. Schematic flow chart describing working of model.

Its salient features are;

a. Supersaturation of individual elements is aimed to be measured to account for overall behavior of multicomponent system – an approach missing previously.
b. It comprises of effort to remove / reduce error by use of iteration-based approach for model refinement.
c. Programming of model will be done in MATLAB® – not done elsewhere previously.
d. Temperature dependent properties (transient heat and mass transfer conditions) will be used.
e. A unique approach based on segregation coefficient (k) as a function of temperature was adopted (Previously (Kurz, Giovanola, and Trivedi 1986), it was only velocity dependent).
f. Slope of liquids (m) is taken to be concentration (C*) dependent.
g. Peclet number (Pe) & ξ are not taken as constant like previous studies [Bobadilla, M., J. Lacaze, and G. Lesoult, Journal of Crystal Growth, 1988. 89(4): p. 531-544] in which it is assumed;

i. $\xi = 1$ (low growth rate) (low Pe)
ii. $\xi = 0$ (very fast cooling rate – typical Additive Manufacturing conditions)
iii. $2\Gamma / R = 1$ (high velocity AM conditions).

h. New relation for dendrite tip temperature was developed.

In **summary**, KGT model is aimed to be extended for multicomponent systems beyond BLL model employing real time temperature dependent conditions in Additive Manufacturing. One step towards this approach has already been established by principle investigator (Rafique, Qiu, and Easton 2017).

2. **Probabilistic Part:** It consists of making a detailed probabilistic model explaining two dimensional (2D) evolution of dendritic microstructure (e-g. B2 in CuZrAlCo and β-Zr in CuZrAlNi alloys) in a carefully selected simulation domain based on cellular automaton (CA) method (Wei et al. 2007; Gu et al. 2017; Dezfoli et al. 2017).

Method consists of discretising simulated area into finite cells while time into small time steps. Then at a particular time state of a cell is determined. Mostly it depends on (a) temperature and (b) solute concentration. State of cell is determined by state of its nearest neighbours by a transition rule known as neighbourhood transition rule. Two types of rules are used which are Moore's law (8 neighbourhood) and Von Neuman's Law (4 neighbourhood). Solute diffusion happens in two steps (a) Solute diffusion in a single cell and (b) Solute diffusion between cells. Most important steps are determination of fraction solid in a single cell, calculation of solid fraction increment, solute diffusion between cells, interpolation and calculation of nucleation density of new cells and assigning p number (Rafique 2018c, 2018d).

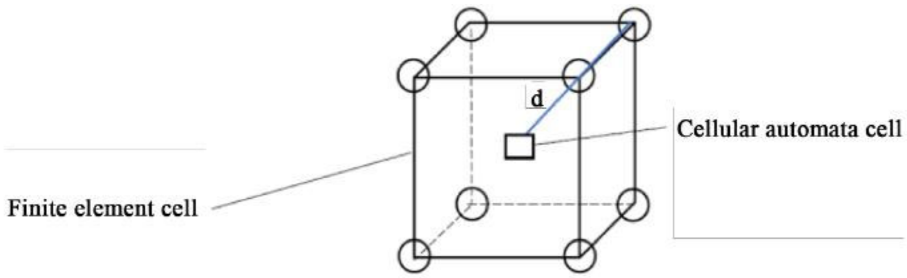


Figure 2. Representation of interpolation in one cell.

Its features are;

a. It accounts for transient thermal parameters (temperature, density, specific heat capacity (C_P), thermal conductivity (k)) from detailed heat transfer model in ABAQUS® (Zhou et al. 2016; Hussein et al. 2013; Dong et al. 2009). CA process adopted is;

i. Determine phases to be evolved in a typical selected alloy system (based on literature).
ii. Determine their volume fraction (Vf) (based on literature).
iii. Select Representative Volume Element (RVE) in a test piece / coupon (in mm).
iv. Select simulation domain (cartesian or point based grid) (e-g. 300 x 300). This will be done in MATLAB®.
v. Select cell shape (square, hexagon, rectangle (based on literature)). This will be done in MATLAB®.
vi. Select parameters to account for mesh anisotropy. This can be done by any of following;

1. Selection of modified square cell (decentred square algorithm (DCSA) (Zhang et al. 2013; Chen, Xu, and Liu 2014; Tan and Shin 2015)) (most popular approach).

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 10 February 2023 doi:10.20944/preprints202302.0179.v1

2. Refining of square cells e.g. limited angle method (Chen, Xu, and Liu 2015).
3. Refining of mesh (by decreasing it physical size from micron to nm) (computationally inefficient).

vii. Select neighborhood transition rules based on well-established CA pattern selected in step v above (These rules are well defined in literature e.g. Von Numen rules, Moore rules (popular, accurate but computationally expensive) (Wei et al. 2011), Solid / Liquid Interface generation and energy at tip (Sharifi and Larouche 2014; Hamid and Daniel 2015)).

viii. Scan whole simulation domain for n number of cells and assign a random number r ($0 < r < 1$) to each cell.

ix. Select physical appearance of next cells based on neighborhood transition rules of step vii above.

NOTE: Cellular Automaton model is a 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, and it depends on previous deterministic and heat transfer model.

5. Research Significance

Present project has its significance stemmed from the fact that a comprehensive solidification model specially tailored to multicomponent bulk metallic glass matrix composites (BMGMC) is need of the hour to predict microstructure and properties of these diversified class of materials without recurring to expensive, exhaustive and time-consuming experimentation. Although, accurate and reliable way to understand the properties, experimental approach has its biggest drawbacks in being time consuming and expensive. Modelling and simulation approach on the other hand, if done properly, yields same results in much quicker time, with higher accuracy and versatility. Thus, not only path is shortened but researcher also has more control, flexibility and power in his hands to manoeuvre the values to generate a range of simulation results without labour and fatigue which is significant advancement in field.

6. Enhancement of Career Development

Mr. Rafique believes, inclusion in this research program will be a great asset for him to improve his skills and develop a better and deeper understanding of subject. His research work, under the directions of Prof. Stephen Niezgoda will focus on studying nucleation and growth of ductile phase dendrites from melt of bulk metallic glass matrix composites (BMGMC) during solidification in additive manufacturing as affected by intrinsic (alloy chemistry and thermophysical properties) and extrinsic (melt pool velocity, depth, width and temperature) parameters. This work will allow him to apply the research & analytical techniques developed in both materials sciences and engineering classes, laboratories, research organizations and practical training to find a solution of a practical problem. His duties in this research project will include devising a scheme for identifying problematic factors in processing and alloy development, formulation of model, gathering of thermophysical properties, their insertion, simulation of model, generation of results, applying different model refinement techniques, testing to quantify and recheck results, examining & evaluating the results for reaching conclusion and suggesting remedies to problems. These duties will help him a great deal in improving his skills and knowledge to an advanced degree. In addition to this, working in internationally renowned laboratories of The Ohio State University, collaborative national laboratories, private laboratories, participation in training courses, conferences, symposia, workshops and meetings with peers, experts and researchers will help him improve his skills and knowledge, develop contacts and research network which will be great valuable platform to flourish future research and cultivate infant minds.

7. Relationship to The Ohio State University

Despite having strong back ground, history (Fullwood et al. 2010) and infrastructure (Palma et al. 2008) for applied research on modelling and simulation of alloy solidification (Fullwood et al. 2008), microstructure modelling (Niezgoda, Yabansu, and Kalidindi 2011; Niezgoda et al. 2010; Fullwood, Niezgoda, and Kalidindi 2008), welding engineering, additive manufacturing and physical and transport phenomena (Niezgoda et al. 2014; Arul Kumar et al. 2015; Zong et al. 2014), The Ohio State University still lacks a comprehensive program in the part scale thermal and CFD modelling to describe melt pool and probabilistic simulation to describe microstructure evolution in bulk metallic glass matrix composites (BMGMC). Despite efforts of years, still there is dearth of knowledge about these alloy systems especially in context to how they form and solidify? No real effort exists to address this problem by modelling and simulation approach. Present project aims to address this gap by making certain fundamental mathematical modifications to original well established alloy solidification KGT (Kurz, Giovanola, and Trivedi 1986) / LGK (Lipton, Glicksman, and Kurz 1984) theories to account for the effect of multicomponent alloy systems under transient conditions. The biggest gap in this field exists in terms of unavailability of actual thermophysical data pertinent to BMGMCs. Present project aims to bridge this gap by not relying on prior simulation generated input values for another simulation, but rigorously using experimental data already present in Center for Information and Numerical Data Analysis and Synthesis (CINDAS), Purdue University (Valencia and Quested 2001; Ho and Li 1986; Ho and Li 1993), University of Michigan (Pehlke, Jeyarajan, and Wada 1982) and Thermodynamic Research Centre (TRC), National Institute of Standards and Technology (NIST) (Wilthan et al. 2017; Pfeif and Kroenlein 2016) which will also help in resource development at department of Materials Science and Engineering..

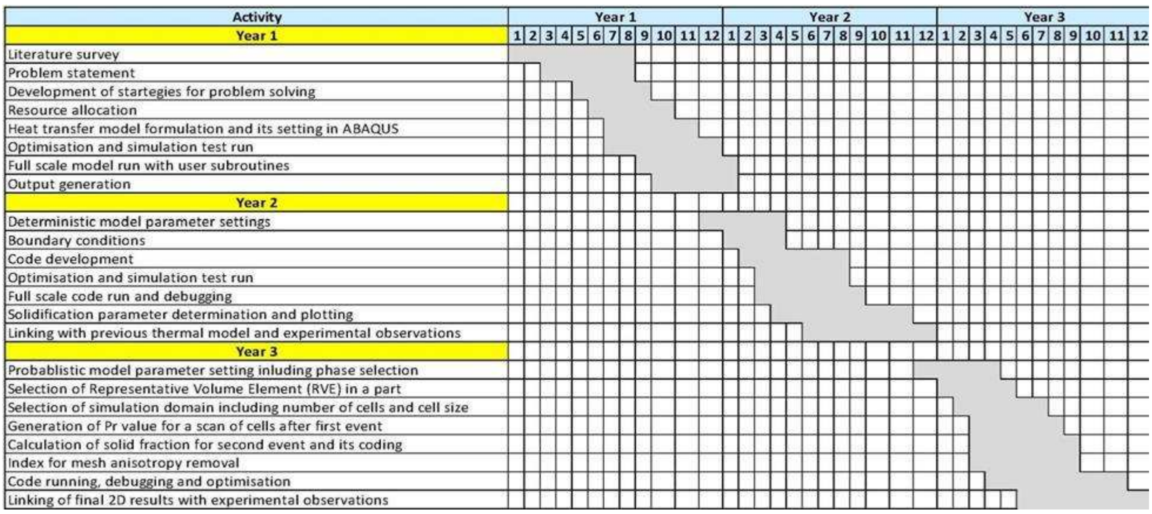
8. Broader Impact of Proposed Activities

Establishment of well-defined refined theorems and their simulation results will serve as source of inspiration for future research activities. It will not only fuel but trigger new research in scientific community, academia, laboratories and industry. It will also provide and ready-made source of properties pertinent to these metal matrix composites. An inset of activities in this material will also serve as tool for economic prosperity and growth. A quick and efficient way of handling varied alloy systems in complicated additive manufacturing will generate tools which will provide base of market development in literature, software, hardware and machinery for robotics.

a. Year–by–year deliverables

Year by year deliverables for whole three-year project are described in detailed Gantt chart which gives

Gantt chart



References

1. Arul Kumar, M., A. K. Kanjarla, S. R. Niezgoda, R. A. Lebensohn, and C. N. Tomé. 2015. 'Numerical study of the stress state of a deformation twin in magnesium', *Acta Materialia*, 84: 349-58.
2. Baumgartner, Jens, Archan Dey, Paul H. H. Bomans, Cécile Le Coadou, Peter Fratzl, Nico A. J. M. Sommerdijk, and Damien Faivre. 2013. 'Nucleation and growth of magnetite from solution', *Nat Mater*, 12: 310-14.
3. Beeley, P. 2001. *Foundry Technology* (Elsevier Science).
4. Browne, David J., Zsolt Kovacs, and Wajira U. Mirihanage. 2009. 'Comparison of nucleation and growth mechanisms in alloy solidification to those in metallic glass crystallisation — relevance to modeling', *Transactions of the Indian Institute of Metals*, 62: 409-12.
5. Buchbinder, Damien, Wilhelm Meiners, Norbert Pirch, Konrad Wissenbach, and Johannes Schrage. 2014. 'Investigation on reducing distortion by preheating during manufacture of aluminum components using selective laser melting', *Journal of Laser Applications*, 26: 012004.
6. Campbell, J. 2003. *Castings* (Elsevier Science).
7. ———. 2004. Castings Practice: The Ten Rules of Castings (Elsevier Science).
8. Chalmers, B. 1964. *Principles of solidification* (Wiley).
9. Charbon, C., and M. Rappaz. 1993. '3D probabilistic modelling of equiaxed eutectic solidification', *Modelling and Simulation in Materials Science and Engineering*, 1: 455.
10. Chen, Qiang, Gildas Guillemot, Charles-André Gandin, and Michel Bellet. 2016. "Finite element modeling of deposition of ceramic material during SLM additive manufacturing." In *MATEC Web of Conferences*, 08001. EDP Sciences.
11. Chen, Rui, Qingyan Xu, and Baicheng Liu. 2014. 'A Modified Cellular Automaton Model for the Quantitative Prediction of Equiaxed and Columnar Dendritic Growth', *Journal of Materials Science & Technology*, 30: 1311-20.
12. ———. 2015. 'Cellular automaton simulation of three-dimensional dendrite growth in Al–7Si–Mg ternary aluminum alloys', *Computational Materials Science*, 105: 90-100.
13. Cheng, Jia-Lin, Guang Chen, Chain-Tsuan Liu, and Yi Li. 2013. 'Innovative approach to the design of low-cost Zr-based BMG composites with good glass formation', *Scientific Reports*, 3: 2097.
14. Conner, R. D., R. B. Dandliker, and W. L. Johnson. 1998. 'Mechanical properties of tungsten and steel fiber reinforced Zr41.25Ti13.75Cu12.5Ni10Be22.5 metallic glass matrix composites', *Acta Materialia*, 46: 6089-102.
15. Coquerel, Gerard. 2014. 'Crystallization of molecular systems from solution: phase diagrams, supersaturation and other basic concepts', *Chemical Society Reviews*, 43: 2286-300.
16. Cordero, Zachary C., Ralph B. Dinwiddie, David Immel, and Ryan R. Dehoff. 2017. 'Nucleation and growth of chimney pores during electron-beam additive manufacturing', *Journal of Materials Science*, 52: 3429-35.
17. Cunningham, Ross, Andrea Nicolas, John Madsen, Eric Fodran, Elias Anagnostou, Michael D. Sangid, and Anthony D. Rollett. 2017. 'Analyzing the effects of powder and post-processing on porosity and properties of electron beam melted Ti-6Al-4V', *Materials Research Letters*: 1-10.
18. Dantzig, J.A., and M. Rappaz. 2016. *Solidification: 2nd Edition - Revised & Expanded* (Taylor & Francis Group).
19. Dezfoli, Amir Reza Ansari, Weng-Sing Hwang, Wei-Chin Huang, and Tsung-Wen Tsai. 2017. 'Determination and controlling of grain structure of metals after laser incidence: Theoretical approach', 7: 41527.
20. Dmowski, W., Y. Yokoyama, A. Chuang, Y. Ren, M. Umemoto, K. Tsuchiya, A. Inoue, and T. Egami. 2010. 'Structural rejuvenation in a bulk metallic glass induced by severe plastic deformation', *Acta Materialia*, 58: 429-38.
21. Dong, L., A. Makradi, S. Ahzi, and Y. Remond. 2009. 'Three-dimensional transient finite element analysis of the selective laser sintering process', *Journal of Materials Processing Technology*, 209: 700-06.
22. Dunbar, Alexander Jay. 2016. Analysis of the laser powder bed fusion additive manufacturing process through experimental measurement and finite element modeling (The Pennsylvania State University).
23. Erdemir, Deniz, Alfred Y. Lee, and Allan S. Myerson. 2009. 'Nucleation of Crystals from Solution: Classical
24. and Two-Step Models', *Accounts of Chemical Research*, 42: 621-29.
25. Ferry, M., K. J. Laws, C. White, D. M. Miskovic, K. F. Shamlaye, W. Xu, and O. Biletska. 2013. 'Recent developments in ductile bulk metallic glass composites', *MRS Communications*, 3: 1-12.
26. Flemings, M.C. 1974. *Solidification Processing* (McGraw-Hill).
27. Francois, M. M., A. Sun, W. E. King, N. J. Henson, D. Tourret, C. A. Bronkhorst, N. N. Carlson, C. K. Newman, T. Haut, J. Bakosi, J. W. Gibbs, V. Livescu, S. A. Vander Wiel, A. J. Clarke, M. W. Schraad, T. Blacker, H. Lim, T. Rodgers, S. Owen, F. Abdeljawad, J. Madison, A. T. Anderson, J. L. Fattebert, R. M. Ferencz, N. E. Hodge, S. A. Khairallah, and O. Walton. 2017. 'Modeling of additive manufacturing processes for metals: Challenges and opportunities', *Current Opinion in Solid State and Materials Science*.
28. Frank, Xavier, Nicolas Dietrich, Jing Wu, Renaud Barraud, and Huai Z. Li. 2007. 'Bubble nucleation and growth in fluids', *Chemical Engineering Science*, 62: 7090-97.

29. 'Front Matter A2 - CHRISTIAN, J.W.' in. 2002. *The Theory of Transformations in Metals and Alloys* (Pergamon: Oxford).
30. Fullwood, D. T., S. R. Kalidindi, S. R. Niezgoda, A. Fast, and N. Hampson. 2008. 'Gradient-based microstructure reconstructions from distributions using fast Fourier transforms', *Materials Science and Engineering: A*, 494: 68-72.
31. Fullwood, David T., Stephen R. Niezgoda, Brent L. Adams, and Surya R. Kalidindi. 2010. 'Microstructure sensitive design for performance optimization', *Progress in Materials Science*, 55: 477-562.
32. Fullwood, David T., Stephen R. Niezgoda, and Surya R. Kalidindi. 2008. 'Microstructure reconstructions from 2-point statistics using phase-recovery algorithms', *Acta Materialia*, 56: 942-48.
33. Ganeriwala, Rishi, and Tarek I. Zohdi. 2014. 'Multiphysics Modeling and Simulation of Selective Laser Sintering Manufacturing Processes', *Procedia CIRP*, 14: 299-304.
34. Gránásy, L., T. Pusztai, T. Börzsönyi, G. Tóth, G. Tegze, J. A. Warren, and J. F. Douglas. 2006. 'Phase field theory of crystal nucleation and polycrystalline growth: A review', *Journal of Materials Research*, 21: 309-19.
35. Gránásy, László, László Rátkai, Attila Szállás, Bálint Korbuly, Gyula I. Tóth, László Környei, and Tamás Pusztai. 2014. 'Phase-Field Modeling of Polycrystalline Solidification: From Needle Crystals to Spherulites—A Review', *Metallurgical and Materials Transactions A*, 45: 1694-719.
36. Greer, A. L., Y. Q. Cheng, and E. Ma. 2013. 'Shear bands in metallic glasses', *Materials Science and Engineering: R: Reports*, 74: 71-132.
37. Gu, C., Y. Wei, X. Zhan, and Y. Li. 2017. 'A three-dimensional cellular automaton model of dendrite growth with stochastic orientation during the solidification in the molten pool of binary alloy', *Science and Technology of Welding and Joining*, 22: 47-58.
38. Gusarov, A. V., and J. P. Kruth. 2005. 'Modelling of radiation transfer in metallic powders at laser treatment', *International Journal of Heat and Mass Transfer*, 48: 3423-34.
39. Hamid, Sharifi, and Larouche Daniel. 2015. 'An automatic granular structure generation and finite element analysis of heterogeneous semi-solid materials', *Modelling and Simulation in Materials Science and Engineering*, 23: 065013.
40. Hammond, Vincent H., Marlene D. Houtz, and James M. O'Reilly. 2003. 'Structural relaxation in a bulk metallic glass', *Journal of Non-Crystalline Solids*, 325: 179-86.
41. Hays, C. C., C. P. Kim, and W. L. Johnson. 2000. 'Microstructure Controlled Shear Band Pattern Formation and Enhanced Plasticity of Bulk Metallic Glasses Containing in situ Formed Ductile Phase Dendrite Dispersions', *Physical Review Letters*, 84: 2901-04.
42. Ho, C. Y., and H. H. Li. 1986. 'Computerized comprehensive numerical data system on the thermophysical and other properties of materials established at CINDAS/Purdue University', *International Journal of Thermophysics*, 7: 949-62.
43. Ho, CY, and HH Li. 1993. 'Numerical databases on materials property data at CINDAS/Purdue University', *Journal of chemical information and computer sciences*, 33: 36-45.
44. Hofmann, Douglas C. 2013. 'Bulk Metallic Glasses and Their Composites: A Brief History of Diverging
45. Fields', Journal of Materials, 2013: 8.
46. Hofmann, Douglas C., Jin-Yoo Suh, Aaron Wiest, Gang Duan, Mary-Laura Lind, Marios D. Demetriou, and William L. Johnson. 2008. 'Designing metallic glass matrix composites with high toughness and tensile ductility', *Nature*, 451: 1085-89.
47. Hofmann, Douglas C., Jin-Yoo Suh, Aaron Wiest, Mary-Laura Lind, Marios D. Demetriou, and William L. Johnson. 2008. 'Development of tough, low-density titanium-based bulk metallic glass matrix composites with tensile ductility', *Proceedings of the National Academy of Sciences*, 105: 20136-40.
48. Hussein, Ahmed, Liang Hao, Chunze Yan, and Richard Everson. 2013. 'Finite element simulation of the temperature and stress fields in single layers built without-support in selective laser melting', *Materials & Design (1980-2015)*, 52: 638-47.
49. Jabbareh, Mohammad Amin, and Hamid Assadi. 2013. 'Modeling of Grain Structure and Heat-Affected Zone in Laser Surface Melting Process', *Metallurgical and Materials Transactions B*, 44: 1041-48.
50. Jiang, Yunpeng, Longgang Sun, Qingqing Wu, and Kun Qiu. 2017. 'Enhanced tensile ductility of metallic glass matrix composites with novel microstructure', *Journal of Non-Crystalline Solids*, 459: 26-31.
51. Jones, S. F., G. M. Evans, and K. P. Galvin. 1999. 'Bubble nucleation from gas cavities — a review', *Advances in Colloid and Interface Science*, 80: 27-50.
52. Kalikmanov, V. 2012. *Nucleation Theory* (Springer Netherlands).
53. Karthika, S., T. K. Radhakrishnan, and P. Kalaichelvi. 2016. 'A Review of Classical and Nonclassical Nucleation Theories', *Crystal Growth & Design*, 16: 6663-81.
54. Katz, J. L. 1992. "Homogeneous nucleation theory and experiment: A survey." In *Pure and Applied Chemistry*, 1661.
55. Ketov, S. V., Y. H. Sun, S. Nachum, Z. Lu, A. Checchi, A. R. Beraldin, H. Y. Bai, W. H. Wang, D. V. Louzguine-Luzgin, M. A. Carpenter, and A. L. Greer. 2015. 'Rejuvenation of metallic glasses by non-affine thermal strain', *Nature*, 524: 200-03.

56. Khairallah, Saad A., Andrew T. Anderson, Alexander Rubenchik, and Wayne E. King. 2016. 'Laser powder-bed fusion additive manufacturing: Physics of complex melt flow and formation mechanisms of pores, spatter, and denudation zones', *Acta Materialia*, 108: 36-45.
57. Khairallah, Saad A., and Andy Anderson. 2014. 'Mesoscopic simulation model of selective laser melting of stainless steel powder', *Journal of Materials Processing Technology*, 214: 2627-36.
58. Kim, Yu Chan, Do Hyang Kim, and Jae-Chul Lee. 2003. 'Formation of Ductile Cu-Based Bulk Metallic Glass Matrix Composite by Ta Addition', *MATERIALS TRANSACTIONS*, 44: 2224-27.
59. King, W., A. T. Anderson, R. M. Ferencz, N. E. Hodge, C. Kamath, and S. A. Khairallah. 2015. 'Overview of modelling and simulation of metal powder bed fusion process at Lawrence Livermore National Laboratory', *Materials Science and Technology*, 31: 957-68.
60. King, W. E., A. T. Anderson, R. M. Ferencz, N. E. Hodge, C. Kamath, S. A. Khairallah, and A. M. Rubenchik. 2015. 'Laser powder bed fusion additive manufacturing of metals; physics, computational, and materials challenges', *Applied Physics Reviews*, 2: 041304.
61. King, Wayne E., Holly D. Barth, Victor M. Castillo, Gilbert F. Gallegos, John W. Gibbs, Douglas E. Hahn, Chandrika Kamath, and Alexander M. Rubenchik. 2014. 'Observation of keyhole-mode laser melting in laser powder-bed fusion additive manufacturing', *Journal of Materials Processing Technology*, 214: 2915-25.
62. Kurz, W., and D.J. Fisher. 1986. *Fundamentals of solidification* (Trans Tech Publications).
63. Kurz, W., B. Giovanola, and R. Trivedi. 1986. 'Theory of microstructural development during rapid solidification', *Acta Metallurgica*, 34: 823-30.
64. Launey, Maximilien E., Douglas C. Hofmann, William L. Johnson, and Robert O. Ritchie. 2009. 'Solution to the problem of the poor cyclic fatigue resistance of bulk metallic glasses', *Proceedings of the National Academy of Sciences*, 106: 4986-91.
65. Laurentiu, Nastac, and M. Stefanescu Doru. 1997. 'Stochastic modelling of microstructure formation in solidification processes', *Modelling and Simulation in Materials Science and Engineering*, 5: 391.
66. Lavery, Nicholas P, Stephen GR Brown, Johann Sienz, John Cherry, and Fawzi Belblidia. 2014. 'A review of Computational Modelling of Additive Layer Manufacturing–multi-scale and multi-physics', *Sustainable Design and Manufacturing*: 651-73.
67. Lee, Kyong-Yee, and Chun P Hong. 1997. 'Stochastic modeling of solidification grain structures of Al-Cu crystalline ribbons in planar flow casting', *ISIJ international*, 37: 38-46.
68. Lee, YS, and W Zhang. 2015. "Mesoscopic simulation of heat transfer and fluid flow in laser powder bed additive manufacturing." In *International Solid Free Form Fabrication Symposium, Austin*, 1154-65.
69. Li, Gong, Liling Sun, Jun Zhang, Riping Liu, Qin Jing, Wenkui Wang, Yunpeng Gao, and Dan Chen. 2003. 'Structural relaxation of Zr41Ti14Cu12.5Ni10Be22.5 bulk metallic glass under high pressure', *Science in China Series G: Physics, Mechanics and Astronomy*, 46: 468-73.
70. Li, X. P., M. P. Roberts, S. O'Keeffe, and T. B. Sercombe. 2016. 'Selective laser melting of Zr-based bulk metallic glasses: Processing, microstructure and mechanical properties', *Materials & Design*, 112: 217-26.
71. Liou, Frank, Joseph Newkirk, Zhiqiang Fan, Todd Sparks, Xueyang Chen, Kenneth Fletcher, Jingwei Zhang, Yunlu Zhang, Kannan Suresh Kumar, and Sreekar Karnati. 2015. 'Multiscale and Multiphysics Modeling of Additive Manufacturing of Advanced Materials'.
72. Lipton, J, ME Glicksman, and W Kurz. 1984. 'Dendritic growth into undercooled alloy metals', *Materials Science and Engineering*, 65: 57-63.
73. Liu, Shibo, Afia Kouadri-Henni, and Adinel Gavrus. 2016. "Modeling grain orientation of DP600 steel by Nd: YAG laser." In *MATEC Web of Conferences*, 02010. EDP Sciences.
74. Manvatkar, V., A. De, and T. DebRoy. 2014. 'Heat transfer and material flow during laser assisted multi-layer additive manufacturing', *Journal of Applied Physics*, 116: 124905.
75. Markl, Matthias, and Carolin Körner. 2016. 'Multiscale Modeling of Powder Bed–Based Additive Manufacturing', *Annual Review of Materials Research*, 46: 93-123.
76. Martin, Scot T. 2000. 'Phase Transitions of Aqueous Atmospheric Particles', *Chemical Reviews*, 100: 3403-54.
77. Musaddique Ali Rafique, Muhammad. 2018. Simulation of Solidification Parameters during Zr Based Bulk Metallic Glass Matrix Composite's (BMGMCs) Additive Manufacturing.
78. Nastac, L. 1999. 'Numerical modeling of solidification morphologies and segregation patterns in cast dendritic alloys', *Acta Materialia*, 47: 4253-62.
79. Neilson, G. F., and M. C. Weinberg. 1979. 'A test of classical nucleation theory: crystal nucleation of lithium disilicate glass', Journal of Non-Crystalline Solids, 34: 137-47.
80. Niezgoda, Stephen R., Anand K. Kanjarla, Irene J. Beyerlein, and Carlos N. Tomé. 2014. 'Stochastic modeling of twin nucleation in polycrystals: An application in hexagonal close-packed metals', *International Journal of Plasticity*, 56: 119-38.
81. Niezgoda, Stephen R., David M. Turner, David T. Fullwood, and Surya R. Kalidindi. 2010. 'Optimized structure based representative volume element sets reflecting the ensemble-averaged 2-point statistics', *Acta Materialia*, 58: 4432-45.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 10 February 2023 doi:10.20944/preprints202302.0179.v1

82. Niezgoda, Stephen R., Yuksel C. Yabansu, and Surya R. Kalidindi. 2011. 'Understanding and visualizing microstructure and microstructure variance as a stochastic process', *Acta Materialia*, 59: 6387-400.
83. Palma, J.M.L.M., P. Amestoy, M. Daydé, M. Mattoso, and J.C. Lopes. 2008. High Performance Computing for Computational Science - VECPAR 2008: 8th International Conference, Toulouse, France, June 24-27, 2008. Revised Selected Papers (Springer).
84. Panwisawas, C., C. L. Qiu, Y. Sovani, J. W. Brooks, M. M. Attallah, and H. C. Basoalto. 2015. 'On the role of thermal fluid dynamics into the evolution of porosity during selective laser melting', *Scripta Materialia*, 105: 14-17.
85. Papazafeiropoulos, George, Miguel Muñiz-Calvente, and Emilio Martínez-Pañeda. 2017. 'Abaqus2Matlab: suitable tool for finite element post-processing', *Advances in Engineering Software*, 105: 9-16. Pehlke, Robert Donald, A Jeyarajan, and H Wada. 1982. 'Summary of thermal properties for casting alloys and mold materials', *NASA STI/Recon Technical Report N*, 83.
86. Pengpeng, Yuan, and Gu Dongdong. 2015. 'Molten pool behaviour and its physical mechanism during selective laser melting of TiC/AlSi10Mg nanocomposites: simulation and experiments', *Journal of Physics D: Applied Physics*, 48: 035303.
87. Pfeif, E. A., and K. Kroenlein. 2016. 'Perspective: Data infrastructure for high throughput materials discovery', *APL Materials*, 4: 053203.
88. Pruppacher, Hans R., James D. Klett, and Pao K. Wang. 1998. 'Microphysics of Clouds and Precipitation', *Aerosol Science and Technology*, 28: 381-82.
89. Qiu, Chunlei, Chinnapat Panwisawas, Mark Ward, Hector C. Basoalto, Jeffery W. Brooks, and Moataz M. Attallah. 2015. 'On the role of melt flow into the surface structure and porosity development during selective laser melting', *Acta Materialia*, 96: 72-79.
90. Rafique, M. M. A., and J. Iqbal. 2009. 'Modeling and simulation of heat transfer phenomena during investment casting', *International Journal of Heat and Mass Transfer*, 52: 2132-39.
91. Rafique, Muhammad Musaddique Ali. 2015. 'Modeling and Simulation of Heat Transfer Phenomena'.
92. ———. 2018a. 'Effect of Inoculation on Phase Formation and Indentation Hardness Behaviour of Zr_{47.5}Cu_{45.5}Al₅Co₂ and Zr₆₅Cu₁₅Al₁₀Ni₁₀ Bulk Metallic Glass Matrix Composites', *Engineering*, Vol.10No.08: 30.
93. ———. 2018b. 'Modelling and Simulation of Solidification Phenomena during Additive Manufacturing of Bulk Metallic Glass Matrix Composites (BMGMC)¡ªA Brief Review and Introduction of Technique', *Journal of Encapsulation and Adsorption Sciences*, Vol.08No.02: 50.
94. ———. 2018c. "Probabilistic Modeling and Simulation of Microstructural Evolution in Zr Based Bulk Metallic Glass Matrix Composites During Solidification." In, 305-09. Cham: Springer International Publishing.
95. ———. 2018d. 'Probabilistic Modelling of Microstructural Evolution in Zr Based Bulk Metallic Glass Matrix Composites during Solidification in Additive Manufacturing', *Engineering*, Vol.10No.04: 12.
96. Rafique, Muhammad Musaddique Ali, Dong Qiu, and Mark Easton. 'Modeling and simulation of microstructural evolution in Zr based Bulk Metallic Glass Matrix Composites during solidification', *MRS Advances*, 2: 3591-606.
97. ———. 2017. 'Modeling and simulation of microstructural evolution in Zr based Bulk Metallic Glass Matrix Composites during solidification', *MRS Advances*: 1-16.
98. Rappaz, M., and Ch A. Gandin. 1993. 'Probabilistic modelling of microstructure formation in solidification processes', *Acta Metallurgica et Materialia*, 41: 345-60.
99. Reuther, K., and M. Rettenmayr. 2014. 'Perspectives for cellular automata for the simulation of dendritic solidification – A review', *Computational Materials Science*, 95: 213-20.
100. Roehling, Tien T., Sheldon S. Q. Wu, Saad A. Khairallah, John D. Roehling, S. Stefan Soezeri, Michael F. Crumb, and Manyalibo J. Matthews. 2017. 'Modulating laser intensity profile ellipticity for microstructural control during metal additive manufacturing', *Acta Materialia*, 128: 197-206.
101. Sagui, Celeste, and Martin Grant. 1999. 'Theory of nucleation and growth during phase separation', *Physical Review E*, 59: 4175.
102. Sarac, B. 2015. Microstructure-Property Optimization in Metallic Glasses (Springer International Publishing).
103. Schoinochoritis, Babis, Dimitrios Chantzis, and Konstantinos Salonitis. 2017. 'Simulation of metallic powder bed additive manufacturing processes with the finite element method: A critical review', *Proceedings of the Institution of Mechanical Engineers, Part B: Journal of Engineering Manufacture*, 231: 96-117.
104. Sharifi, Hamid, and Daniel Larouche. 2014. 'A Numerical Method for Microstructure Generation of a Binary Aluminum Alloy and Study of Its Mechanical Properties Using the Finite Element Method', *Metallurgical and Materials Transactions A*, 45: 5866-75.
105. Shiffman, D. 2012. *The Nature of Code* (D. Shiffman).

106. Siegrist, Marco E. 2007. 'Bulk metallic glass composites'.
107. Siegrist, Marco E., Esther D. Amstad, and Jörg F. Löffler. 2007. 'Tribological properties of graphite- and ZrC-reinforced bulk metallic glass composites', *Intermetallics*, 15: 1228-36.
108. Siegrist, Marco E., and Jörg F. Löffler. 2007. 'Bulk metallic glass–graphite composites', *Scripta Materialia*, 56: 1079-82.
109. Siegrist, Marco E., David P. Steinlin, and Jörg F. Löffler. 2007. 'Processing of diamond-reinforced bulk metallic glass composites', *Materials Science and Engineering: A*, 447: 298-302.
110. Smith, Jacob, Wei Xiong, Wentao Yan, Stephen Lin, Puikei Cheng, Orion L. Kafka, Gregory J. Wagner, Jian Cao, and Wing Kam Liu. 2016. 'Linking process, structure, property, and performance for metal-based additive manufacturing: computational approaches with experimental support', *Computational Mechanics*, 57: 583-610.
111. Sun, Hongqing, and Katharine M. Flores. 2011. 'Spherulitic crystallization behavior of a metallic glass at high heating rates', *Intermetallics*, 19: 1538-45.
112. ———. 2013. 'Spherulitic crystallization mechanism of a Zr-based bulk metallic glass during laser processing', *Intermetallics*, 43: 53-59.
113. Tan, Wenda, and Yung C. Shin. 2015. 'Multi-scale modeling of solidification and microstructure development in laser keyhole welding process for austenitic stainless steel', *Computational Materials Science*, 98: 446-58.
114. Thanh, Nguyen T. K., N. Maclean, and S. Mahiddine. 2014. 'Mechanisms of Nucleation and Growth of Nanoparticles in Solution', *Chemical Reviews*, 114: 7610-30.
115. Thijs, Lore, Frederik Verhaeghe, Tom Craeghs, Jan Van Humbeeck, and Jean-Pierre Kruth. 2010. 'A study of the microstructural evolution during selective laser melting of Ti–6Al–4V', *Acta Materialia*, 58: 3303-12.
116. Valencia, Juan J, and PN Quested. 2001. 'Thermophysical properties', *Modeling for Casting and Solidification Processing*: 189.
117. Vehkamäki, H. 2006. *Classical Nucleation Theory in Multicomponent Systems* (Springer Berlin Heidelberg). Venables, J. A., G. D. T. Spiller, and M. Hanbucken. 1984. 'Nucleation and growth of thin films', *Reports on Progress in Physics*, 47: 399.
118. Wei, Lei, Xin Lin, Meng Wang, and Weidong Huang. 2011. 'A cellular automaton model for the solidification of a pure substance', *Applied Physics A*, 103: 123-33.
119. Wei, Y. H., X. H. Zhan, Z. B. Dong, and L. Yu. 2007. 'Numerical simulation of columnar dendritic grain growth during weld solidification process', *Science and Technology of Welding and Joining*, 12: 138-46.
120. Weissmayer, Lisa, Tim Schubert, Timo Bernthaler, and Gerhard Schneider. 2015. 'Applications of Microscopy in Additive Manufacturing', *Optik & Photonik*, 10: 44-46.
121. Wilthan, Boris, Erik A. Pfeif, Vladimir V. Diky, Robert D. Chirico, Ursula R. Kattner, and Kenneth Kroenlein. 2017. 'Data resources for thermophysical properties of metals and alloys, Part 1: Structured data capture from the archival literature', *Calphad*, 56: 126-38.
122. Wu, Y., H. Wang, X. J. Liu, X. H. Chen, X. D. Hui, Y. Zhang, and Z. P. Lu. 2014. 'Designing Bulk Metallic Glass Composites with Enhanced Formability and Plasticity', *Journal of Materials Science & Technology*, 30: 566-75.
123. Wu, Y., H. Wang, H. H. Wu, Z. Y. Zhang, X. D. Hui, G. L. Chen, D. Ma, X. L. Wang, and Z. P. Lu. 2011. 'Formation of Cu–Zr–Al bulk metallic glass composites with improved tensile properties', *Acta Materialia*, 59: 2928-36.
124. Yap, C. Y., C. K. Chua, Z. L. Dong, Z. H. Liu, D. Q. Zhang, L. E. Loh, and S. L. Sing. 2015. 'Review of selective laser melting: Materials and applications', *Applied Physics Reviews*, 2: 041101.
125. Yuan, Mengqi. 2013. 'Additive manufacturing of laser sintered polyamide optically translucent parts'.
126. Zhang, Jingwei, Frank Liou, William Seufzer, Joseph Newkirk, Zhiqiang Fan, Heng Liu, and Todd E Sparks. 2013. "Probabilistic simulation of solidification microstructure evolution during laser-based metal deposition." In *Proc. Int. Solid Freeform Fabr. Symp., 24th*, 739-48.
127. Zhang, M., Y. M. Wang, F. X. Li, S. Q. Jiang, M. Z. Li, and L. Liu. 2017. 'Mechanical Relaxation-to-Rejuvenation Transition in a Zr-based Bulk Metallic Glass', *Scientific Reports*, 7: 625.
128. Zhou, Xiangman, Haiou Zhang, Guilan Wang, Xingwang Bai, Youheng Fu, and Jingyi Zhao. 2016. 'Simulation of microstructure evolution during hybrid deposition and micro-rolling process', *Journal of Materials Science*, 51: 6735-49.
129. Zohdi, T. I. 2014. 'Additive particle deposition and selective laser processing-a computational manufacturing framework', *Computational Mechanics*, 54: 171-91..
130. Zong, Hongxiang, Turab Lookman, Xiangdong Ding, Cristiano Nisoli, Don Brown, Stephen R. Niezgoda, and Sun Jun. 2014. 'The kinetics of the ω to α phase transformation in Zr, Ti: Analysis of data from shock-recovered samples and atomistic simulations', *Acta Materialia*, 77: 191-99.