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Modelling and simulation of microstructural evolution for extra-terrestrial planetary chemistry mapping using artificial intelligence – a NASA Mars rover study

Muhammad Musaddique Ali Rafique[1,2]

[1]Eastern Engineering Solutions LLC, Detroit MI, 48202 USA (https://easternengineering.org)
[2]Law Chamber, Muhammad Rafique (Advocate High Court Lahore, Supreme Court of Pakistan), H 15/B, St 23, Nizamabad Kot Khawaja Saeed, Lahore 54920, Pakistan

Abstract

Development of rovers and development of infrastructure which enables them to probe other planets (such as Mars) have sparked a lot of interest recently specially with increasing public attention in Moon and Mars program by National Aeronautics and Space Administration. This is designed to be achieved by various means such as advanced spectroscopy and artificial intelligent techniques such as deep learning and transfer learning to enable the rover to not only map the surface of planet but to get a detailed information about its chemical makeup in layers beneath (deep learning) and in areas around point of observation (transfer learning). In this work, which is part of a proposal, later approach is explored. A systematic strategy is presented which make use of aforementioned techniques developed for metallic glass matrix composites as benchmark and helps develop algorithms for chemistry mapping of actual Martian surface on Perseverance Rover launching shortly.

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1. Introduction

Like other inorganic compounds, bulk metallic glasses [1-3] and their composites [4-8] have attracted the attention of scientific community recently due to their high strength [9-14], hardness [15, 16] and large elastic strain limit [17, 18]. However, they lack ductility and toughness. This problem could be overcome by forming a metal matrix composite [19]. In present study an effort is made to address this problem and understand this phenomenon by modelling and simulation which is used as benchmark for chemical composition mapping of other inorganic compounds present in extra-terrestrial planetary surfaces. Carefully selected alloy chemistry is used to form two model systems ($Zr_{47.5}Cu_{45.5}Al_5Co_2$ and $Zr_{65}Cu_{15}Al_{10}Ni_{10}$) by vacuum arc melting and suction casting and additive manufacturing [8, 20, 21]. The formation, development and evolution of melt pool (a function of heat transfer [22] and fluid dynamics (solved by computational fluid dynamics (CFD)) as well as microstructure in the melt pool (a function of mass transfer (solute diffusion and capillary action)) [23-25] is modelled using MATLAB Simulink® and ABAQUS®. First step resembles striking of sun rays on surface causing any chemical compositional changes on daily basis. This is optional and will be utilized intermittently as a function of other factors and parameters such as planet's atmospheric condition (wind direction, speed, dust storm formation, gravity and volcanic activity). It involves solving moving heat source equations [26, 27] and post processing them in MATLAB to generate a physical picture of changes in heat transfer pattern of surface. Changes in melt pool may be solved by understanding fluid dynamics inside it and solving computational fluid dynamics equations. The aim is to generate thermal history and temperature profile (including histograms) of test piece (sample surface) as heat source (sunlight) traverses across it. Second step involves writing code in MATLAB Simulink® and interfacing it with ABAQUS® [28] or write new subroutines in FORTRAN compiler of ABAQUS® to perform part scale modelling and simulation. Next (third step) is microstructure modeling. So far, Cellular Automaton method (a well-established probabilistic method [29, 30]) has been used to model nucleation and growth of alloy systems as far as 25 years ago.

2. Study

In the present study, for NASA Entrepreneurs Challenge 2020 due to probabilistic nature of nucleation and growth process during chemical composition change, same CA algorithm is used with MATLAB. Only nucleation and growth of crystalline phase(s) is modelled [23] as glassy phase cannot be modelled (represented by empty cells / background). Equations written in MATLAB are used to construct alloy / compound solidification on a sample part geometry. Based on knowledge gained by earlier missions to mars or direct data from spectrophotometer installed on rover arm, initial chemical composition and parameters for individual elements is determined and used as initial input to model. This is further represented as physical displacement (tip velocity and radius) by solving motion displacement equations. It is first step toward physical pattern generation. Heat transfer and CFD calculation are performed in this selected part at the same time when microstructure is evolving. This finally constitutes Finite Element (FE) analysis coupled [31-33] with CA forming CAFE approach [34].

Part geometry selection, meshing, optimization, and determination of heat transfer coefficients

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(heat transfer part) constitutes major activities of step 1 and 2 of project. Heat flow during conventional solidification is three dimensional in nature while in additive manufacturing / rapid cooling it is primarily one dimensional from bottom. This will be taken care of, and accounted for, in the model based on prior studies. Effect of turbulence caused by very high power of initial sunrays during very early part of day, midday and sunset cause and spatter in liquid pool will also be taken care of in this work. (If permitted, effect of thermo-capillary convection (Marangoni Convection [35, 36]) will also be modelled). Primarily, our model is formulated as a result of combination of following five studies.

1. Gandin, C.-A., M. Rappaz, and R. Tintillier, Three-dimensional probabilistic simulation of solidification grain structures: Application to superalloy precision castings. Metallurgical Transactions A, 1993. 24(2): p. 467-479.
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3. Rappaz, M., et al., Development of microstructures in Fe−15Ni−15Cr single crystal electron beam welds. Metallurgical Transactions A, 1989. 20(6): p. 1125-1138.
4. Kurz, W., B. Giovanola, and R. Trivedi, Theory of microstructural development during rapid solidification. Acta Metallurgica, 1986. 34(5): p. 823-830.
5. Zhang, J., et al. Probabilistic simulation of solidification microstructure evolution during laser-based metal deposition. in Proc. Int. Solid Freeform Fabr. Symp., 24th. 2013.

Its (**deterministic model**) salient features are.

1. Supersaturation of individual elements was measured to account for overall behaviour of multicomponent system – an approach missing in previous studies
2. Due to scarcity, dispersion and unavailability of data, a correlation from nearest possible element in same group in periodic table was used.
3. An effort was made to remove / reduce error by use of iteration-based approach to refine model.
4. Programming of model was done in MATLAB® – not done elsewhere previously.
5. Temperature dependent properties (transient heat transfer conditions) were used.
6. A unique approach based on segregation coefficient (k) as a function of temperature was adopted (Previously [37], it was only velocity dependent)
7. Slope of liquids (m) is taken to be concentration (C*) dependent.
8. Peclet number (P_e) & 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
    a. $\xi = 1$ (low growth rate) (low P_e)
    b. $\xi = 0$ (very fast cooling rate – typical Additive Manufacturing conditions)
9. $2\Gamma / R = 1$ (high velocity AM / rapid solidification / rapid quench conditions)
10. New relation for dendrite tip temperature was developed

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In summary, KGT model was extended for multicomponent systems beyond BLL model employing real time temperature dependent conditions in AM / rapid solidification / rapid quench.

NOTE: No physical microstructure was either reported previously or tried in present step. Physical simulation is "not possible" at deterministic stage as it is analytical model which defines parameters for next stage only.

Its (**probabilistic model**) salient features are.

It consists of making a detailed probabilistic model explaining two-dimensional evolution of dendritic microstructure (e-g B2 in $Zr_{47.5}Cu_{45.5}Al_5Co_2$ and β-Zr in $Zr_{65}Cu_{15}Al_{10}Ni_{10}$) in a carefully selected simulation domain based on cellular automaton method. Its features are;

1. A detailed CA based model is developed taking transient thermal parameters (temperature, density, specific heat capacity, thermal conductivity) from detailed heat transfer model in ABAQUS. In summary CA process
    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 my case wedge / rectangular block).
    d. Selection of simulation domain (Cartesian or point based grid) (e-g 300 x 300). Performed in MATLAB.
    e. Select cell shape (square, hexagon, rectangle (based on literature)). Performed in MATLAB.
    f. Select parameters to account for mesh anisotropy. This may be performed by any of following.
        i. Selection of modified square cell (decentred square algorithm (DCSA)) (most popular approach).
        ii. Refining of square cells e.g. limited angle method.
        iii. Refining of mesh (by decreasing it physical size from micron to nm) (usually not adopted – leads to increase of computational time).
    g. Select neighbourhood transition rules 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 (popular, accurate but computationally expensive), Solid / Liquid Interface generation and energy at tip).
    h. Scan whole simulation domain / grid for n number of cells (300 x 300) and assign a random number r ($0 < r < 1$) to each cell.
    i. Select physical appearance of next cells based on neighbourhood transition rules of step g above.

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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 and heat transfer model.

3. Deep learning

Deep learning has emerged as a promising mathematical method to develop computational models comprising of multiple processing layers. It convolutes intricate structure in large data sets by using backpropagation algorithms rather than forward propagation algorithms. It dictates a machine to compute representation in each layer from representation in previous layer. It has greatly improved our understanding of the layered data / nets. Two of its most important variants namely, convolutional nets have brought about improvements in processing images, video, speech and audio while recurrent nets have furthered the understanding of sequential data such as text and speech [38]. It has proved its grounds in many fields and has solved problems in materials, processes and structures engineering [39], instrumented engineering [40], and quantification of mechanical properties [41] and microstructure [42]. However, it has not been applied on bulk metallic glass matrix composites and inorganic substances and compounds. Only one study is carried out in which, its variant, machine learning is applied [43]. In the present study, researcher, using his background and understanding [21, 44] is developing rigorous layered mathematical models – convolution nets which will be solved using backpropagation algorithms.

Information generated during modeling of microstructure evolution is used to develop understanding of chemical makeup (chemistry, composition, phases, and elemental distribution) of primary rocks, secondary rocks, deposits, sediments, igneous rocks, and metamorphic signatures on extra-terrestrial surfaces. Deep learning is used to study not only surface chemistry but chemical composition of underneath layers using rigorous layered mathematical models – convolution nets which will be solved using backpropagation algorithms in deep learning algorithms.

4. Transfer learning

This information is used in transfer learning algorithms [45-47] to develop knowledge of surrounding rocks and their chemical makeup in upcoming Mars missions (Mars Perseverance Rover, its probes and helicopter) and in future outer and deep space missions (satellites, helicopters and rovers). Further, transfer learning will be used to effectively process source logic networks to target domain and then revises the mapped structure to further improve its accuracy [48]. As probabilistic modeling and simulation is based on neighborhood transition rules (John Von Neuman and Moore neighborhood), it will also serve as basis for development of self-evolving robots.

5. Conclusions

1. Algorithms developed for modelling and simulation of microstructure evolution in ordinary inorganic materials such as metallic glass matrix composites are adopted to be used to study in depth surface and below surface chemistry of extra-terrestrial environments.
2. Layered mathematical models – convolution nets are solved using backpropagation algorithms – deep learning.
3. Information and pattern generated in step 1 above is used to study chemical makeup of areas around point of observation – transfer learning. It is a strong function of complexity and type of convolution net and computing power of hardware machinery.

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