Helmholtz - OCPC - Programme 2017-2021

for the Involvement of Postdocs in Bilateral Collaboration Projects with China

PART A

Title of the project

Multiphase-field simulation of grain growth and statistical analysis of its multi-dimensional dataset using data-mining techniques

Helmholtz Centre and institute

Karlsruhe Institute of Technology (KIT), Institute of Applied Materials (IAM)

Project leaders

Dr. P. G. Kubendran Amos, IAM, KIT
MSc. P. Altschuh, IAM, KIT
Prof. Dr. B. Nestler, IAM, KIT

Web-address

www.iam.kit.edu/cms/

Description of the project:

Desired properties in a polycrystalline material are achieved by appropriately modifying its grain size. Grain growth, which facilitates in establishing required grain size, is primarily governed by the ability of the system to reduce its interfacial energy per volume, and thus, is observed in wide-range of materials including metals, alloys, ceramics, and polycrystalline glasses. Despite being directed by a rather straightforward thermodynamic principle, the current understanding of grain growth in three-dimensional systems is far from comprehensive [1]. Two reasons predominantly contribute to the difficulty in investigating grain growth. One pertains to the intricacy of a microstructure, which demands three-dimensional characterisation to physically discern its evolution [2,3]. The other is associated with the analysis of the huge 'four-dimensional' dataset that comprises of temporally evolving information of three-dimensional grains *(4D = 3D+Time)* [4,5].

Given that convoluted experimental procedures are a requisite for convincing analysis of grain growth, theoretical techniques have increasingly been adopted to complement current understanding [6,7,8]. Correspondingly, multiphase-field approach largely proves to be a potent numerical tool for modelling grain growth [9,10]. Moreover, by comparative study, it has been demonstrated that the outcomes of this technique corroborate with experimental observations [11]. Therefore, as an alternate to arduous experimental techniques, a multiphase-field model can be employed to simulate grain growth in three-dimensional systems, and to render the required datasets for subsequent analysis [12].

During grain growth, the temporal evolution of a grain is dictated numerous factors including size, face-class, surface area, number of vertices and junctions, which are categorised as geometrical and topological features [13]. Four – dimensional datasets associated with grain growth comprises of the geometrical and topological features of all the grains in a three – dimensional setup, and their corresponding changes with time. Owing to the enormity of the information, often, influence of one of these factors on grain growth is exclusively analysed. This is an intrinsic limitation of adopting conventional techniques to analyse the dataset. In other words, in order to understand the cumulative effect of the geometrical and topological features on grain growth, state-of-the-art data-mining techniques must be employed [14,15].

In view of the above delineation, the proposed research is intended to render an extensive investigation of grain growth by adopting sophisticated statistical techniques. Accordingly, the candidate is expected to perform numerical simulations of normal and abnormal grain growth exhibited by three-dimensional systems in a well-established phase-field package [16,17]. The simulations will be followed by comprehensive analysis with statistical functions, and subsequent reduction of the resulting multi-dimensional data to a low-dimensional feature space. To that end, the candidate should develop appropriate statistical tools, and a definite framework for its implementation, which ultimately would render critical insights on the evolution of three-dimensional grains.

References:

[1] P R Rios and D Zoellner, Critical assessment: Grain growth – unresolved issues, Material Science and Technology, 34(6): 629 – 638, 2018.

[2] C Zhang, M Enomoto, A Suzuki and T Ishimaru, Characterization of three-dimensional grain structure in polycrystalline iron by serial sectioning, Metallurgical and Materials Transaction A, 35(7): 1927 – 1933, 2004.

[3] J Baruchel, J Y Buffiere, P Cloetens, M D Michiel, E Ferrie, W Ludwig, E Maire and L Salvo, Advances in synchrotron radiation microtomography, Scripta Materialia, 55(1): 41 – 46, 2006.

[4] D J Jensen, E M Lauridsen, L Margulies, H F Poulsen, S Schmidt, H O Sorensen and G B M Vaughan, X – ray microscopy in four dimensions, Materials Today, 9(1): 18 – 25, 2006.

[5] E Miyoshi, T Takaki, M Ohno, Y Shibuta, S Sakane, T Shimokawabe and T Aoki, Ultra – large – scale phase – field simulation study of ideal grain growth, NPJ Computational Materials, 3(1): 1 – 6, 2017.

[6] P R Rios, T G Dalpian, V S Brandai, J A Castro and A C L Oliveira, Comparison of analytical grain size distribution with three-dimensional computer simulation and experimental data, Scripta Materialia, 54(9): 1633 – 1637, 2006.

[7] K Fuchizaki, T Kusaba and K Kawasaki, Computer modelling of three-dimensional cellular pattern growth, Philosophical Magazine B, 71(3), 333 – 357, 1995.

[8] D Weygand, Y Brechet, J Lepinoux and W Gust, Three – dimensional grain growth: A vertex dynamics simulation, Philosophical Magazine B, 79(5): 703 – 716, 1999.

[9] R Perumal, P G Kubendran Amos, M Selzer and B Nestler, Phase – field study on the formation of first — neighbour topological clusters during isotropic grain growth, Computational Material Science, 140: 209 – 223, 2017.

[10] R Perumal, P G Kubendran Amos, M Selzer and B Nestler, Phase – field study of the transient phenomena induced by 'abnormally' large grains during 2 – dimensional isotropic grain growth, Computational Material Science, 147: 227 – 237,2018.

[11] I M Mckenna, S O Poulsen, E M Lauridsen, W Ludwig and P W Voorhees, Grain growth in four dimensions: A comparison between simulation and experiment, Acta Materialia, 78: 125 – 134, 2014.

[12] P G Kubendran Amos, R Perumal, M Selzer and B Nestler, Multiphase – field modelling of concurrent grain growth and coarsening in complex multicomponent system, Journal of Material Science and Technology, in-press, 2020.

[13] H V Atkinson, Theories of normal grain growth in pure single-phase systems, Acta Metallurgica, 36(3): 469 – 491, 1988.

[14] P Altschuh, C Y Yuksel, J Hoetzer, M Selzer, B Nestler and S R Kalidindi, Data science approach for microstructure quantification and feature identification of porous membrane, Journal of Membrane Science, 540: 88 – 97, 2017.

[15] F Wang, P Altschuh, L Ratke, H Zhang, M Selzer and B Nestler, Progress report on phase separation in polymer solutions, Advanced Materials, 31(26), 2019.

[16] B Nestler, H Garcke and B Stinner, Multicomponent alloy solidification: phase-field modeling and simulations, Physical Review E, 71(4), 2005.

KIT – International Affairs (INTL) Contact: Oliver Kaas Phone: +49 721 608 45323 Email:

[17] J Hoetzer, A Reiter, H Hierl, P Steinmetz, M Selzer and B Nestler, The parallel multi-physics phase-field framework Pace3D, Journal of Computational Science, 26: 1—12, 2018.

Description of existing or sought Chinese collaboration partner institute:

This proposal is not designated to any specific partner institute but is rather intended as a public call wherein interested PhD scholars can apply, and the subsequent shortlisting will be done based on their research experience.

Required qualification of the post-doc:

- PhD in Material Science, Mechanical Engineering, Physics or any related fields with thesis directed towards data science and/or numerical modelling and/or statistical analysis
- Experience in developing and/or employing statistical tools in Python, R, JASP or any related packages is highly desired.
- Additional skills include convincing communication skills, and ability to work Independently towards the proposed goal.

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team

KIT – International Affairs (INTL) Contact: Oliver Kaas Phone: +49 721 608 45323 Email: