Helmholtz - OCPC - Programme 2017-2021

for the Involvement of Postdocs in Bilateral Collaboration Projects with China

PART A

Title of the project

Multiphase-field modelling of Asaro – Tiller – Grinfeld instability in Allen – Cahn framework

Helmholtz Centre and institute

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

Project leaders

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Description of the project:

In the fabrication of nanostructured semiconductors, which are the integral part of modern lasers and diodes, molecular beam epitaxy (MBE) plays a critical role [1]. MBE involves vaporising the source material, and conscientiously depositing it onto a substrate in the form a 'beam'. Even though a precise control on the chemical composition of the processed material is rendered by MBE, an elastic instability is frequently associated with it [2]. This instability is referred to as Asaro – Tiller – Grinfeld (ATG) instability [3,4].

The difference in lattice parameters of the source material and substrate, along with disparity in the temperature, introduces non-hydrostatic loading as misfit strain and thermal expansion. Relaxation of this strain induces morphological changes which alter the configuration of the interface. Accordingly, *ATG instability* is characteristically associated with the morphological evolution of the interface under the combined influence surface – and elastic – energy, which is introduced by non-hydrostatic loading.

Owing to its noticeable effect on the processing of multi-layered semiconductors, *ATG instability* is extensively analysed [5]. In addition to experimental techniques, theoretical treatments have been adopted to understand interplay of surface – and elastic – energy in governing the configuration of the interface. Recently, morphological evolution of the interface associated with *ATG instability* has been modelled in phase-field framework [6,7,8]. Despite several advancements, this instability in phase-field approach is invariably modelled by treating the order parameter as a conserved variable, and consequently, solving its temporal evolution in Cahn – Hilliard framework. This treatment, in addition to being numerically arduous, is also computationally expensive. Alternatively, *ATG instability* can efficiently be modelled by solving the evolution of order-parameter in Allen – Cahn framework, by separately imposing the necessary constraints. Correspondingly, the proposed work aims to develop a computationally – efficient approach for phase-field modelling of morphological changes accompanying *ATG instability.*

In the proposed research, the candidate will investigate *ATG instability* in two separate frameworks. One would involve coupling elastic energy-density with redistribution energy [9,10,11], while the other would replace the redistribution energy with a volume – preserving bulk contribution [12]. While both these techniques treat order parameter as a non – conserved variable, the latter adopts a quasi – Allen – Cahn framework [13]. By examining these different techniques for thermodynamic consistency, and computational efficiency, this work would ultimately indicate an efficient approach for phase-field modelling of *ATG instability.* Furthermore, effects of different modes of mass transfer including surface and volume diffusion on the morphological evolution will be encompassed in this research.

References

[1] W P McCray, MBE deserves a place in the history books, Nature nanotechnology, 2(5):259, 2007.

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[4] M A Grinfeld, Instability of the interface between a non-hydrostatically stressed elastic and a melt, DoSSR, 290(6): 1358 – 1363, 1986.

[5] A Krost, C Berger, P Moser, J Blasing, A Dadgar, C Hums, T Hempel, B Bastek, P Veit and J Christen, Stranski – Krastnov transition and self – organized structures in low – strained AlInA/GaN multilayer structures, Semiconductor science and technology, 26(1), 2010.

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[8] B G Chirranjeevi, T A Abinandanan and M P Gururajan, A phase – field study of morphological instabilities in multilayer thin film, Acta Materialia, 57(4): 1060 – 1067, 2009.

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[11] B Nestler, F Wendler, M Selzer, B Stinner and H Garcke, Phase – field model for multiphase systems with preserved volume fractions, Physical Review E, 78(1), 2008.

[12] P G K Amos, L T Mushongera and B Nestler, Phase – field analysis of volume – diffusion-controlled shape – instabilities in metallic systems – I: 2 – dimensional plate – like structures, Computational Material Science, 144: 363 – 373, 2018.

[13] P G Kubendran Amos, E Schoof, J Santoki, D Schneider and B Nestler, Limitations of preserving volume in Allen – Cahn framework for microstructural analysis, Computational Material Science, 173, 2020.

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 whereby interested PhD scholars can apply, and the subsequent shortlisting will be done based on their research experience.

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Required qualification of the post-doc:

- PhD in Material Science, Mechanical Engineering, Physics or any related fields with thesis involving phase – field or other analogous numerical modelling techniques
- Experience in developing and implementing numerical models preferably in C, C++ or Python 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

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