

**HELMHOLTZ** RESEARCH FOR  
GRAND CHALLENGES

**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**

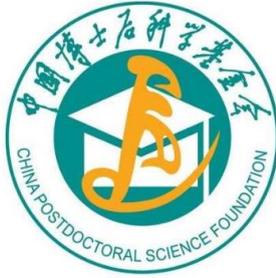
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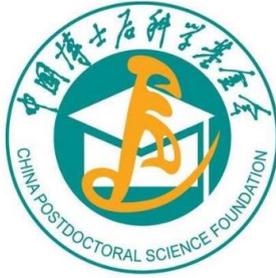
## Description of the project:

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.

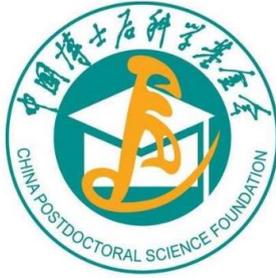


## References

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- [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.



**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