

Heterogenous nucleation and microstructure formation—a scale- and system-bridging approach

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FOREWORD

Heterogenous nucleation and microstructure formation—a scale- and system-bridging approach

Guest Editor

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Scope and aim of this volume.

Nucleation and initial microstructure formation play an important role in almost all aspects of materials science [1, 2, 3, 4, 5]. The relevance of the prediction and control of nucleation and the subsequent microstructure formation is fully accepted across many areas of modern surface and materials science and technology. One reason is that a large range of material properties, from mechanical ones such as ductility and hardness to electrical and magnetic ones such as electric conductivity and magnetic hardness, depend largely on the specific crystalline structure that forms in nucleation and the subsequent initial microstructure growth. A very demonstrative example for the latter is the so called *bamboo* structure of an integrated circuit, for which resistance against electromigration [6], a parallel alignment of grain boundaries vertical to the direction of electricity, is most favorable. Despite the large relevance of predicting and controlling nucleation and the subsequent microstructure formation, and despite significant progress in the experimental analysis of the later stages of crystal growth in line with new theoretical computer simulation concepts [7], details about the *initial* stages of solidification are still far from being satisfactorily understood. This is in particular true when the nucleation event occurs as heterogenous nucleation.

The Priority Program SPP 1296 '*Heterogenous Nucleation and Microstructure Formation—a Scale- and System-Bridging Approach*' [8] sponsored by the German Research Foundation, DFG, intends to contribute to this open issue via a six year research program that enables approximately twenty research groups in Germany to work interdisciplinarily together following this goal. Moreover, it enables the participants to embed themselves in the international community which focuses on this issue via internationally open joint workshops, conferences and summer schools. An outline of such activities can be found in [8]. Furthermore, the honorable invitation to publish a special issue in *Journal of Physics: Condensed Matter* dedicated to the Priority Program's topic allows the obtained results to be communicated to relevant international colleagues, which stimulates further interest and encourages future collaborations.

The issue comprises the research results of the participants during the first two year period of the Priority Program as well as that of the international referees of the program.

Now, what precisely is the research concept of the Priority Program and thus, what are the articles in this special issue dedicated to?

Ever since the pioneering work of Volmer and Weber [9], Becker and Döring [10], as well as Turnbull and Fisher [11] nucleation has been modelled more or less phenomenologically. These traditional models describe nucleation by stochastic processes of single atoms, respectively, molecules, which attach at primary droplets. Those thereby growing droplets become stable by reaching a critical size. This concept has largely been employed to model thermal activated

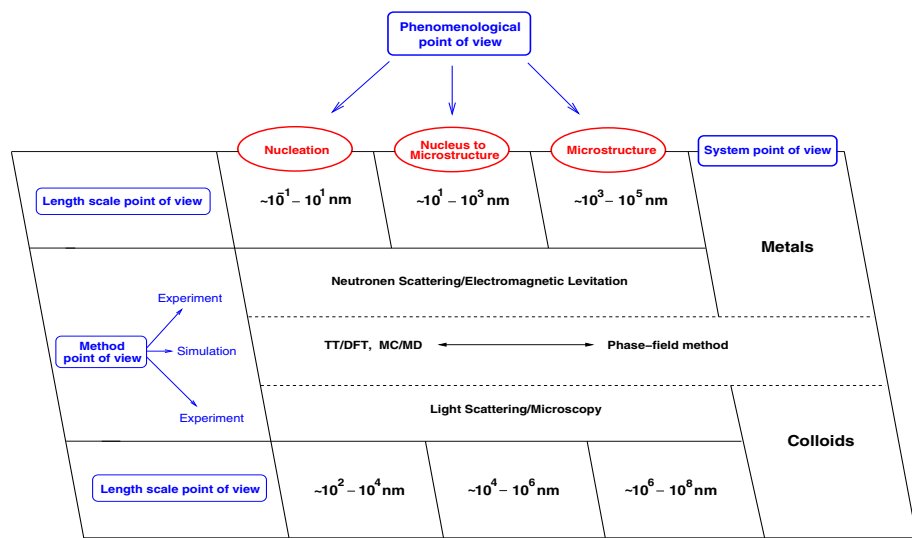


Figure 1. Illustration of the interdisciplinary approach in the Research Priority Program ‘Nucleation and Growth Kinetics in Colloids and Metals—Steps towards a Scale- and System-Bridging Understanding’ [8]: to advance towards a system- and scale-bridging detailed understanding of the energetics and kinetics of heterogeneous nucleation and micro-structure formation, two different experimental (binary colloids and binary metallic alloys) model systems are investigated jointly by experimental scientists working with different experimental techniques together with theoreticians, whose expertise is likewise diverse, ranging from density functional theory (DFT), over molecular simulations (MC/MD) to the phase-field method and who at the same time aim at a rigorous connection of these methods. This sketch illustrates the different ‘dimensions’ of the interdisciplinary research setting of the Priority Program and thus underlying the articles in this issue.

first-order phase transformations. However it contains basic weak points, which raises the question of its physical justification. For instance, the dependence of the interfacial free energy on the critical size of a nucleus is—from the point of view of recent experiments—not considered adequately. In the past years, several advances have been performed to put the modelling of nucleation and microstructure formation on a wider base [12–15].

Still the comparison of these new approaches with experimental results leads to controversial conclusions [12, 16]. Hence the study and development of theoretical models for the understanding and in particular for the quantitative description of the heterogeneous nucleus- and microstructure-formation processes remains an open but successively more and more quantitatively approachable issue. The development of physically relevant models for nucleus- and initial microstructure-formation is based on reliable knowledge of key parameters as the interfacial energy between crystal nucleus and melt. The latter is still experimentally difficult to access in metallic systems due to limitations arising e.g. from non-transmittance of optical light. To accelerate the development of more quantitative models capable of addressing the open issues of heterogenous nucleation and microstructure formation further, it is therefore essential to find complementary experimental systems which are less limited in accessing the above key parameters than metals.

For this reason, within the Priority Program 1296 ‘Heterogenous Nucleation and Microstructure Formation—a Scale- and System-Bridging Approach’ [8], the

emphasis is to investigate the energetics and kinetics of heterogeneous nucleation and microstructure-formation processes experimentally jointly with metals as well as colloids as mesoscopic model systems for these processes. Thereby the most comprehensive experimental picture shall be obtained. The research on colloidal systems is now at a point, at which it promises, in a symbiotic approach with metal physics, to make significant contributions to the identification of the above key parameters. So it has e.g. become possible to tune the interaction potential in colloids and thus to adjust it to display generic mechanisms of heterogeneous nucleation and microstructure-formation [17]. This offers several advantages compared to experimental investigations in metals: the crystallization of fluidic colloidal systems is much slower than the crystallization of metals. Moreover colloids are transparent in the field of optical light, so it is possible to study nucleation *in situ* by using novel optical research methods (confocal light microscopy)—thus, determining the above key parameters.

For this reason the DFG Research Priority Program 1296 employs a system- and scale-bridging interdisciplinary scientific approach intended to thereby contribute to a comprehensive multiscale understanding of the basic mechanisms determining heterogeneous nucleation and initial microstructure formation, which might successively be an applicable material system-independently.

Initially its focus—and thus the focus of this issue—will be on the simplest types of model systems for heterogeneous crystalline orders, on pure metals, binary metal alloys, and colloids. Theoretically and simulation based these systems are jointly studied based on density functional theory (DFT), molecular simulation methods (MC/MD) and the phase-field method at the same time aiming at a rigorous connection of these methods. The joint approach comprising theory and experiment is depicted in figure 1.

More specifically the following questions are addressed and the first advances on these can be found in this issue:

- Heterogeneous nucleation: what does a critical nucleation grain look like? Does the classical concept of a contact angle make sense for heterogeneous nucleation? Can claims made about the dominant contributions to the nucleation barrier for heterogeneous nucleation, as they can be obtained from molecular simulations, be reconciled with results obtained via the phase-field method? What is the relation between interaction potentials and the relevant boundary energies?
- Transition from nucleus to microstructure: how does a microstructure develop out of a nucleus in the interplay between crystallization and segregation depending on the precise reference point in the phase diagram? How stable are those scenarios with respect to changes of that reference point? How well can these scenarios be reproduced via binary colloidal model systems?
- Microstructure development: what kind of consequences result from the new understanding of nucleation for the initial development of the microstructure? What kind of kinetic rules does the initial growth of the solidifying microstructure follow? Is it possible to identify conditions under which several microscopic morphologies of the same alloy composition are kinetically stable?

This issue is organized as follows: it starts with three sections, where the main focus is on theoretical and simulation based advances beginning with the methods at the lowest scale, i.e. with a section on density functional theory and phase-field crystal method based contributions. This section is succeeded by a section devoted to the investigations of the molecular modelling groups inside the Priority Program, and a subsequent one on phase-field simulation. Sections 4, 5 and 6 are devoted to articles with a main focus on experimental contributions for the metallic and the colloidal systems and finally a section on applications. It is important to have in mind the term ‘main focus’ with an emphasis on *main* when

reflecting this deviation due to the interdisciplinary nature of the research reported here, which can already be seen in the articles as well.

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