Modelling of grain boundary dynamics using amplitude equations

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Abstract We discuss the modelling of grain boundary dynamics within an amplitude equations description, which is derived from classical density functional theory or the phase field crystal model. The relation between the conditions for periodicity of the system and coincidence site lattices at grain boundaries is investigated. Within the amplitude equations framework, we recover predictions of the geometrical model by Cahn and Taylor for coupled grain boundary motion, and find both ⟨100⟩ and ⟨110⟩ coupling. No spontaneous transition between these modes occurs due to restrictions related to the rotational invariance of the amplitude equations. Grain rotation due to coupled motion is also in agreement with theoretical predictions. Whereas linear elasticity is correctly captured by the amplitude equations model, open questions remain for the case of nonlinear deformations.

Keywords Amplitude equations · Grain rotation · Coupled motion · Nonlinear elasticity

1 Introduction

The phase field method has a long track of remarkable success in various branches of applied and theoretical physics and engineering. Generally speaking, it is an approach tailored to interfacial pattern formation problems, which arise in various classical phase transformations that are formulated as free boundary problems. The phase field method introduces an additional variable to describe the phase state. This variable, the phase field
or order parameter, yields a smooth transition between the phases on an artificial length scale [40]. From a historical perspective, next to Landau theory [38], the work of Cahn [12] on discrete and diffusive interfaces in phase transitions, which introduces the scaling for the length scale associated with a finite interface thickness, is probably the most influential preliminary work. These publications are fundamental to the seminal developments by Fix [22] and Langer [39], who presented the method originally. Right from the start, the new approach led to several milestones of solid-state simulation. We just name Hillert’s discrete model for spinodal decomposition [29], the continuous model of Cahn and Hilliard for the same problem [10,11], which uses the alloy concentration as order parameter, and Khachaturyan’s theory of micro-elasticity [36] which is fundamental to a group of phase field models which focus on the application to microstructure evolution [16,55,56].

Among this wide range of interesting topics, very prominent examples of successful combinations with complementary methods are the solidification of pure materials or alloys and various solid-state transformations, see the reviews of Karma and Boettinger et al. [5,34]. In particular, the combination with boundary integral descriptions [5,7,8,30,31] proved to be very successful. Together, a comprising understanding of the fundamental aspects of such phase transitions, covering both the aspects of stability and dynamics as well as asymptotic behaviour and basic scaling laws, could be obtained.

As the phase field community grew with increasing success of the method, the theory evolved mainly in two branches, the order-parameter and the indicator-field interpretation, see also the reviews of Chen and Steinbach [16,52]. The indicator-field models assign to thermodynamically distinguishable phases the material data and are often used for coupled dynamics of e.g. elasticity and diffusion, while the physical order-parameter models are mostly used to describe order-disorder transitions, phase separations or martensitic transformations [18,35,43,54]. While the developed phase field models could be modified to describe even atomistic scale effects, such as premelting [4,53], the phase field crystal (PFC) method which was introduced quite recently by Elder et al. [20] provides a natural description of such effects. Specifically, the phase field crystal theory describes the phenomena on atomic length and diffusive timescales. The former naturally yields elastic and plastic deformation, and the latter allows simulations on timescales much larger than comparable atomic methods. The PFC model was shown to be consistent with predictions for the grain boundary energy and misfit dislocations in epitaxial growth, showing the capacity to describe atomistic scale phenomena. The remaining drawback of the PFC method is the required spatial discretisation on atomistic or even sub-atomic length scales.

In this article, we present results on an approach for materials science modelling based on amplitude equations which compensates this limitation of the PFC method. Amplitude equations are well known in pattern formation modelling, especially in hydrodynamics [17]. The transfer to cubic crystal systems [49,59] showed the potential of this elegant and computationally efficient method. The amplitude equations model might be considered as “phase field with atoms”, while the involved coarse-graining process allows a quantitative link to atomistic modelling methods such as molecular dynamics and classical density functional theory [27,28,37,44-46]. In combination with recent studies on premelting and atomistic effects in grain boundary melting [32,33,47], this demonstrates the capacity of amplitude equations to provide insights which were previously not accessible by continuum approaches. At the same time, it offers the possibility to describe large-scale coarsening phenomena with elastic effects which were previously studied using scaling analyses [9].

In particular we investigate in the present paper grain boundary dynamics during coupled motion and grain rotation to show the abilities and limitations of the amplitude equations description.

The article is organised as follows: first, in Sect. 2, we introduce the amplitude equations model and discuss its relation to classical phase field modelling and the density functional theory of freezing. In particular, we show that the fact that many elements in the periodic table crystallize in a body-centred cubic (bcc) structure first when solidified from the melt phase is reflected also in this model. In Sect. 3, we discuss the role of periodic boundary conditions, as they are frequently used for spectral implementations of the model. Here we discuss in detail how the constraints on the system size in order to fulfil all periodicity conditions are related to coincidence site lattices (CSLs). Section 4 is devoted to the coupling dynamics, as modelled by the amplitude equations. Here we consider two scenarios which are important for many metallurgical applications, namely the coupled motion of grain boundaries, which are subjected to a shear force, and grain rotation. In Sect. 5, we discuss nonlinear elastic deformations, and how they are represented in the amplitude equations model. Finally, the results are summarised in Sect. 6.

2 Model description

In this section, we introduce the amplitude equation model which is also called Ginzburg–Landau model. It can be derived rigorously via a multiscale expansion from the phase field crystal model, and it can also be