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A novel homogenization method for phase field approaches based on partial rank-one relaxation

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ABSTRACT

This paper deals with the analysis of homogenization assumptions within phase field theories in a finite strain setting. Such homogenization assumptions define the average bulk's energy within the diffusive interface region where more than one phase co-exist. From a physical point of view, a correct computation of these energies is essential, since they define the driving force of material interfaces between different phases. The three homogenization assumptions considered in this paper are: (a) Voigt/Taylor model, (b) Reuss/Sachs model, and (c) Khachaturyan model. It is shown that these assumptions indeed share some similarities and sometimes lead to the same results. However, they are not equivalent. Only two of them allow the computation of the individual energies of the co-existing phases even within the aforementioned diffusive interface region: the Voigt/Taylor and the Reuss/Sachs model. Such a localization of the averaged energy is important in order to determine and to subsequently interpret the driving force at the interface. Since the Voigt/Taylor and the Reuss/Sachs model are known to be relatively restrictive in terms of kinematics (Voigt/Taylor) and linear momentum (Reuss/Sachs), a novel homogenization approach is advocated. Within a variational setting based on (incremental) energy minimization, the results predicted by the novel approach are bounded by those corresponding to the Voigt/Taylor and the Reuss/Sachs model. The new approach fulfills equilibrium at material interfaces (continuity of the stress vector) and it is kinematically compatible. In sharp contrast to existing approaches, it naturally defines the mismatch energy at incoherent material interfaces. From a mathematical point of view, it can be interpreted as a partial rank-one convexification.

1. Introduction

Phase field models have become an indispensable tool in materials science and physics in order to analyze the evolution of complex microstructures, cf. Khachaturyan (1983) and the more recent review, Steinbach (2013). Such microstructures are the source of many interesting and important phenomena defining the properties of materials. Typical examples are TRIP steels (TRansformation Induced Plasticity) and TWIP steels (TWinning Induced Plasticity). These materials are known

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to have a high strength (TRIP) and a high ductility (TWIP) due to transformations of the microstructure. Within a viewpoint of materials science or metal physics, phase field models go back, at least, to the pioneering work of Cahn and Hilliard (1958) and that of Allen and Cahn (1979). Focusing on the latter, the essential idea is to assign an order parameter to each phase which is similar to the mathematical indicator function. In line with the standard definition of the indicator function, the sum of all order parameters has to be equal to one at any point (partition of unity). However, and in contrast to the classical indicator function being either zero or one, the order parameters can also attain values in-between. Such points are associated with interfaces that separate different phases from each other. Physically speaking, a material point can therefore be related to more than one phase, i.e., phase field theory can be understood as a certain mixture theory.

Although phase field models have their roots in materials science, they can also be interpreted from a purely mathematical point of view, whereby phase field models represent sufficiently smooth approximations of the underlying sharp interface problems, i.e., the sharp transition from one phase to another phase is regularized by a smooth function showing a high gradient. In the limiting case, this smooth function converges to the indicator function, cf. Modica and Mortola (1977). An important advantage of phase field models compared to sharp interface representations is that tracking of material interfaces is not required. This tracking is a common numerical problem for most free boundary value problems.

Clearly, the idea to approximate a sharp interface in a smeared fashion can also be found in other types of models. A probably well known example is gradient-enhanced damage theory. By assigning two different order parameters to the virgin material and to the fully damaged state (the crack), such models fall into the range of phase field approaches. More details on the connection between phase field models and gradient-extended continua are discussed in Bourdin et al. (2000), and Miehe et al. (2010).

Although phase field models have nowadays indeed reached a certain maturity, some fundamental problems remain to be solved. A currently active research subject is the interaction of plasticity and material interfaces. To be more precise, it is not clear how a dislocation is affected by a phase boundary. For instance, a dislocation could simply be pushed away by a phase boundary such that the transformed domain would initially be dislocation free. The other limiting case would be that a dislocation can easily pass through phase boundaries and thus, the transformed phase inherits the dislocations of the original phase. Problems of this type are considered in Bartel et al. (2011), Mosler and Homayonifar (2012), Spatschek and Eidel (2013). Unfortunately, only little experimental information on this account seems to be available, cf. Kim et al. (2009). For this reason, the predictive capabilities of the models cannot currently be checked.

While the aforementioned problem, i.e., the interaction between plasticity and phase boundaries, is already relatively complex, a significantly simpler, yet unanswered and probably more fundamental problem is considered in this paper. It is related to the averaging of the bulk's energy within domains where more than one phase exists. That is, this paper deals with the underlying homogenization assumptions in phase field theory. According to the authors' knowledge, the only published paper dealing with this subject is Ammar et al. (2009). Within the cited work, the authors analyzed three different homogenization assumptions within a geometrically linearized setting: (a) Voigt/Taylor model, (b) Reuss/Sachs model and (c) Khachaturyan model, cf. Khachaturyan (1983). They show that the Khachaturyan model, although frequently applied in the phase field community, is strictly speaking not a homogenization method, since the bulk's average energy is not the average of the energies of the involved phases. Furthermore, the energies of the involved phases are not well-defined in the diffusive interface region where the phases co-exist. However, this localization property is indeed important, since the difference in energy between phases represents a driving force that moves the interface. With respect to the classical Voigt/Taylor and Reuss/Sachs model, the authors of the paper (Ammar et al., 2009) demonstrated that the Reuss/Sachs model underestimates the influence of mechanics on diffusion. By way of contrast, the Voigt/Taylor model was found to provide a more realistic prediction on the coupled response, similarly to the non-classical homogenization approach by Khachaturyan (1983).

As implicitly mentioned in the previous paragraph, phase field models can be subdivided into two different classes with respect to the underlying homogenization assumptions. Within the first of those classes, an effective bulk's energy is a priori postulated, cf. Khachaturyan (1983). This effective energy depends on the concentration and/or on the order parameters. By way of contrast, an individual constitutive model is separately defined for each phase within the second class and, subsequently, the average bulk's energy is computed by homogenization theory. Models falling within this range can be found in Ammar et al. (2009) and references cited therein. Clearly, these two classes are not disjunctive. However, they are not equivalent either. To be more precise, every model belonging to the second class (models based on homogenization theory) also falls into the first class (since an average energy can be derived). However, the opposite is not true, i.e., the localization condition is not always fulfilled. Another disadvantage of models within the first class is that the definition of an effective energy is not always obvious – particularly if the involved phases show completely different material behavior. The focus of the present paper therefore relies on the second group of phase field models.

The classical homogenization assumptions considered so far in phase field theory are the Voigt/Taylor model and the Reuss/Sachs model, cf. Ammar et al. (2009). However, as shown in several classical textbooks on homogenization theory (see, e.g. Nemat-Nasser and Hori, 1993; Fish, 2009) both of them are known to represent limiting cases, i.e., by adopting a variational setting based on (incremental) energy minimization the Voigt/Taylor model leads to an upper bound whereas the Reuss/Sachs model leads to a lower bound. In this paper, a more realistic homogenization assumption is elaborated. It is closely related to the framework of rank-one convexification, cf. Ortiz and Repetto (1999), Miehe and Lambrecht (2003), Carstensen et al. (2002), Aubry et al. (2003), and Mosler and Homayonifar (2012). This framework has already been successfully applied to the analysis of evolving microstructures at the macroscale. The averaged energy predicted by this