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Homogenization of viscoplastic constitutive laws within a phase field approach

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ABSTRACT

The present work provides an original consistent framework for combining different constitutive laws, possibly nonlinear, within diffuse interface models (phase field) by homogenization rather than by mixing the material parameters, such as to offer a greater flexibility. The framework relies on the choice of relevant thermodynamic potentials such that the homogenization schemes are natural choices in the thermodynamic formulation. Thus, it justifies previously proposed classic schemes (Ammar et al., 2009b) and gives clues to explore new schemes (Durga et al., 2013; Mosler et al., 2014) by defining relevant potentials. The proposed framework is illustrated by addressing two issues. First, Reuss and Voigt homogenization schemes are shown to deliver the same kinetics of diffusion-controlled transformations in the pure elastic case in the limit of vanishing diffuse interface width. Second, using the Voigt homogenization scheme, we demonstrate that the influence of viscoplasticity, either isotropic or crystalline, on diffusion-controlled transformations is non-trivial and cannot be inferred from simple qualitative arguments. Depending on the competition between the time scales of diffusion and viscoplasticity, the growth kinetics may exhibit intermediate behaviors between purely chemical and elastic cases. Moreover, it is shown how viscoplasticity can change the morphological stability of growing circular precipitates.

1. Introduction

The phase field approach has become a ubiquitous tool to simulate microstructure evolutions in materials undergoing phase transformations (Steinbach, 2009; Finel et al., 2010). Phases are described by continuous fields where each one is endowed with a transport equation, or phase field equation. Such fields vary rapidly inside the phase boundaries over a given width, which is also called the interface thickness. The interface is then said to be diffuse, which can have a physical justification when the thickness comes close to a few inter-atomic distances. The transport equations associated to the phase field variables allow us to predict the evolving morphology of new phases, and naturally embed the phase transformation kinetics. For many diffusion-controlled phase transformations, stresses can play a significant role in both the transformation kinetics and the morphology evolution of the growing phases. The transport equations for phase fields were firstly coupled to Cauchy's first law of motion restricted to the elastic behavior of the phases in Wang et al. (1993) and Dreyer and Müller

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(2000). More recently, the attention was focused on the extension to plasticity and viscoplasticity, as done by Guo et al. (2005), Ubachs et al. (2005), Uehara et al. (2007), Gaubert et al. (2008, 2010), Yamanaka et al. (2008), Ammar et al. (2009b), and Schmitt et al. (2014).

Two main approaches have been proposed to determine the effective behavior of the interface. They are namely the interpolation and homogenization approaches according to the terminology by Ammar et al. (2009b, 2011, 2014). These methods are closely related to the "coarse-graining" and the "two-phase" approaches mentioned in Plapp (2011), respectively. In the latter reference, and in the "two-phase" approach, the diffuse interface is "*seen as a mixture of two phases that each retain their macroscopic properties*", and for which standard homogenization methods coming for instance from the mechanics of heterogeneous materials (Sanchez-Palencia and Zaoui, 1987; Zaoui, 2002; Qu and Cherkaoui, 2006; François et al., 2012), can be used to derive the effective response. In this case, the phase field parameter then plays a role akin to the volume fraction of one phase within the diffuse interface. In contrast, a single constitutive behavior is used for both phases in the interpolation approach for which the corresponding material parameters are interpolated between the bounding values reached in each phase.

The choice of an homogenization relation for the interface effective behavior originates from the work of Tiaden et al. (1998) who introduced two concentration fields on the basis of the mixture theory. Kim et al. (1999) have then recognized that such a solute partitioning, combined with a Reuss like assumption called quasi-equilibrium condition, could remove a spurious contribution to the interfacial energy scaling with the interface thickness. Later on, by analogy to the work of Kim et al. (1999) and Steinbach and Apel (2006) have used the Reuss assumption to describe the elastic behavior within diffuse interfaces. Ammar et al. (2009b, 2011, 2014) also applied the Voigt homogenization scheme that relies on identical strain values taken by both phases at each material point. Very recently, mixed schemes as they arise in laminate microstructures have been proposed by Durga et al. (2013) and Mosler et al. (2014) in order to reduce spurious stress concentration within the interface. Nevertheless, the popularity of the interpolation method, known as Katchaturyan's approach, was such that the first attempts to introduce nonlinear material behavior of phases relied on the interpolation method, see for instance Guo et al. (2005), Gaubert et al. (2008, 2010) and Cottura et al. (2012).

The choice of a suitable homogenization scheme generally depends on the morphology of the mixture of phases within the diffuse interface. As such a mixture very often does not correspond to a physical reality of actual interfaces. This is why various schemes have been applied without reference to the real structure of the interface. But the homogenization and interpolation schemes can be of practical importance with respect to the convergence of the diffuse interface problem on the sharp interface problem. It is now admitted that the Reuss-like assumption done in Kim et al. (1999) improves such a convergence. Finally, Ammar et al. (2014) highlighted the paradigm of the interpolation and homogenization method though the concept of inheritance. The interpolation method embeds inheritance of the internal variables during the phase transformation. On the contrary, the homogenization method makes the internal variables of each phase independent from each other. Nevertheless, inheritance can be added or discarded by the use of suitable evolutionary laws for the internal variables.

Although there have been significant recent advances along this line, in particular in Durga et al. (2013) and in Mosler et al. (2014) for purely elastic and elasto-plastic behaviors respectively, the present study addresses two novel aspects that have not been dealt with so far:

(i) we settle the thermodynamic foundations for the formulation of homogenization based phase field models;
(ii) we perform a systematic computational analysis of the response of the proposed models in the presence of crystal viscoplasticity.

Hence, we first present in Sections 2–4 the constitutive setting based on an original thermodynamic framework extending the continuum thermodynamic framework used in nonlinear mechanics of materials to the phase field approach (Germain et al., 1983; Maugin, 1992, 1999). Second, based on the implementation of Ammar et al. (2009a), this framework is applied in Section 5 to investigate the diffusion controlled growth of precipitates associated with eigenstrains responsible for the activation of plasticity during transformation. Finally, the major achievements are summarized in the conclusion together with a few remaining issues to address.

2. Phase field modeling within the homogenization approach

In the present work, the role of thermodynamics is emphasized, and especially the second law or entropy principle, in selecting suitable homogenization schemes in the phase field models. The constitutive setting is presented based on an original thermodynamic framework extending the continuum thermodynamic framework used in nonlinear mechanics of materials to the phase field approach (Germain et al., 1983; Maugin, 1992, 1999). It heavily relies on the exploitation of the second principle of thermodynamics in order to formulate constitutive assumptions systematically ensuring the positivity of the dissipation rate at each time and at each material point. This represents an alternative to the use of variational derivatives of the free energy function as done classically in phase field approaches since the pioneering work by Cahn and Hilliard (1958). It has the advantage that the theory can be readily applied to finite bodies with specific and unambiguous boundary conditions, in contrast to usual periodic or infinite microstructures and corresponding vanishing boundary

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