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Efficient variational constitutive updates for Allen-Cahn-type phase field theory coupled to continuum mechanics

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Abstract

This paper deals with efficient variational constitutive updates for Allen-Cahn-type phase field theory coupled to a geometrically exact description of continuum mechanics. The starting point of the implementation is a unified variational principle: A time-continuous potential is introduced, the minimizers of which describe naturally every aspect of the aforementioned coupled model – including the homogenization assumptions defining the mechanical response of the bulk material in the diffuse interface region. With regard to these assumptions, classic models such as the one by Voigt/Taylor or the one by Reuss/Sachs are included. Additionally, more sound homogenization approaches falling into the range of rank-1 convexification are also included in the unified framework. Based on a direct discretization of this time-continuous potential in time and space, an efficient numerical finite element implementation is proposed. In order to guarantee admissible order parameters of the phase field, the unconstrained optimization problem is supplemented by respective constraints. They are implemented by means of Lagrange parameters combined with the Fischer-Burmeister NCP functions. This results in an exact fulfillment of the aforementioned constraints without considering any inequality. Several numerical examples show the predictive capabilities as well as the robustness and efficiency of the final algorithmic formulation. Furthermore, the influence of the homogenization assumption is analyzed in detail. It is shown that the choice of the homogenization assumption does influence the predicted microstructure in general. However, all models converge to the same solution in the limiting case.

Keywords: Phase field; Continuum mechanics; Homogenization; Variational principles; Constraint optimization; Rank-1 homogenization

1. Introduction

Over the last years both phase field theory and phase field modeling have attained a crucial importance in solid mechanics. Nowadays, phase field modeling can be found in many classical fields like fracture mechanics Francfort and Marigo (1998); Bourdin et al. (2000), topology optimization Bourdin and Chambolle (2003) and in material science Steinbach (2013). Particularly, in metallurgy, e.g. alloys, many phenomena like precipitation and phase transformation are analyzed and studied via phase field theories. In such cases the driving force governing phase transformations is strongly

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