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PHASE-FIELD-BASED MODELING AND SIMULATION OF SOLIDIFICATION AND DEFORMATION BEHAVIOR OF TECHNOLOGICAL ALLOYS

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ABSTRACT

The purpose of this work is the formulation and application of a continuum field approach to the phenomenological modeling of the behavior of technological alloys undergoing solidification and attendant inelastic deformation. To describe the phase transition, a phase-field approach is utilized [e.g. 1,2,4]. This involves a Cahn-Allen relation for the order parameter, a Cahn-Hilliard relation for the concentration, and the temperature equation. Fig. 1 and Fig. 2 show intermediate states of the order parameter and of the temperature field in such a coupled simulation of a solidification process. All computations here have been carried out using the finite element package DEAL.II [e.g. 5].

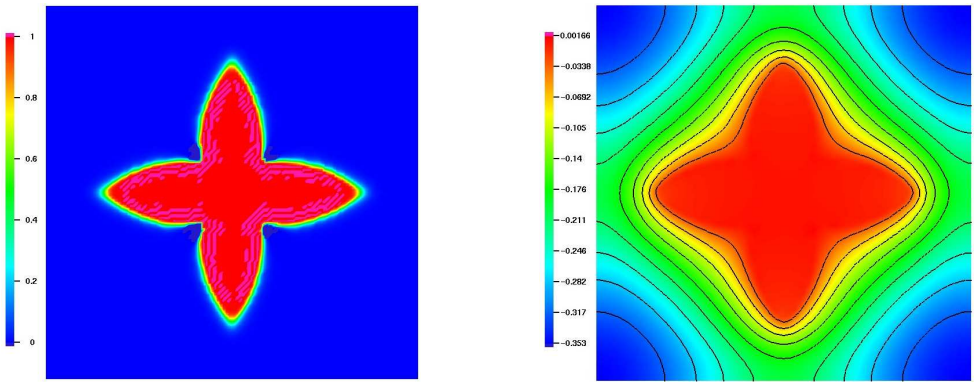

Figure 1: Solidification of an undercooled liquid. Anisotropy is modeled via a directionaly-dependent interface thickness. Left: Phase field variable. Right: Temperature field.

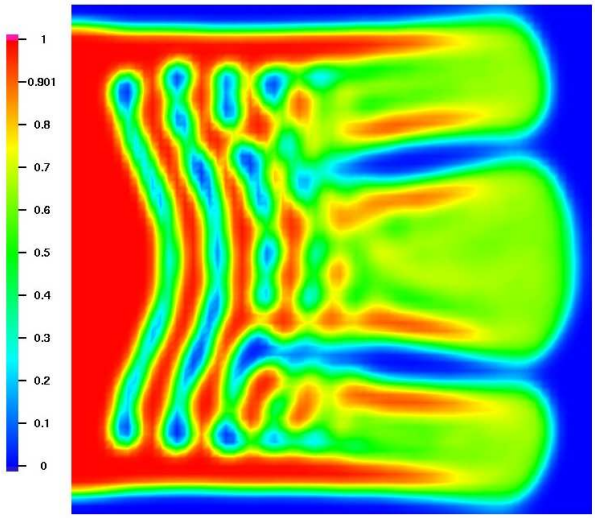

Figure 2: Phase field variable in the simulation of solidification of an undercooled liquid. The employed model is in accordance to [3]. Anisotropy is modeled via a directionaly-dependent thermodynamic potential.

The mechanical structure is considered in the framework of a thermodynamic, internal-variable-based formulation in which the deformation and temperature are in general coupled [eg. 7]. Coupling between the mechanical fields, the order parameter and the temperature field arises via the mechanical dissipation during the deformation process as well as by the spatial distribution of the areas of different phases being modeled by the order parameter.

For the fully coupled system, an algorithmic formulation is derived based on efficient finite element techniques. While first attemps to the finite element simulation of phase field models have been recently presented [eg. 6], their consideration in the context of a structural mechanical finite element simulation is a new issue. The presentation ends with a discussion of applications.

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