Evolving microstructures in energy-based Allen-Cahn- and Cahn-Hilliard-type phase field theories

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ABSTRACT

Phase field theory is a promising technique for understanding complex material phenomena. For instance, grain boundary motion or recrystallization processes can be captured by phase field theory. The main advantage of this theory compared to many other techniques is that the interface motion is described by a suitable evolution equation and therefore, an explicit tracking is not necessary. Due to different elastic properties in the phases, interfacial energies, crystallographic eigen strains and chemical diffusion processes, the constitutive modeling is indeed very challenging within a phase field framework. Typically, phase transformations such as those characterizing twinning are captured by an Allan-Cahn-type approach, while a Cahn-Hilliard-type formulation is used, if the respective interface motion is driven by the concentration of the species [1]. Although the Allen-Cahn and the Cahn-Hilliard formulation are indeed different, they do share some similarities. To be more precise, a Cahn-Hilliard model is obtained by enforcing balance of mass in the Allen-Cahn approach. Within an energy-based formulation [2], this can be implemented by adding additional energy terms to the underlying Allen-Cahn energy. Such a universal energy-based framework is elaborated in this presentation. Furthermore, implementation aspects concerning the enforcement of natural constraints are also discussed within this work.

REFERENCES

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