Enforcing inequality constraints in phase-field method using Uzawa algorithm

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KEYWORDS: *Microstructure evolution, Constrained Optimization, Augmented Lagrangian Method, Uzawa Algorithm*

Multiphase-field models are essential for investigating materials systems where secondary precipitates emerge within a primary matrix. A prominent example is the titanium-molybdenum system, where the parent β phase and distinct ω phase variants coexist. These variants differ based on the crystallographic orientation with respect to the β phase [1]. In this study, a phase field framework [2] is applied to model the β→ω transformation. Each phase is defined by an order parameter that is bounded between zero and one and satisfies a sum-to-unity constraint. The microstructural evolution is driven by the minimization of a global rate-potential [3], where interfacial contributions are modeled via a double-obstacle potential [2]. In this system, the energy associated with ω–ω interfaces is significantly higher than that of the ω–β interfaces [4]. So, the potential must be penalized to favor the formation of the β phase between ω variants. Enforcing these sharp energy gradients via the standard penalty method requires excessively high penalty parameters, which drastically increases the condition number of the system matrix. This induced ill-conditioning prevents the efficient application of iterative linear solvers that are needed in the case of large-scale simulations, particularly in 3D.

To overcome these limitations, an augmented Lagrangian framework is employed to transform the constrained minimization into a well-conditioned saddle-point system. This system is solved using the Uzawa algorithm, which iteratively computes the primal variables while holding the dual variables (Lagrange multipliers) constant, followed by an iterative update of the dual variables to approach the saddle-point solution. The results demonstrate that this reformulated optimization approach provides a numerically efficient and robust method for simulating complex transformations in metallic alloys, bypassing the convergence issues typical of high-penalty regimes.

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