Phase field modelling of the chemo-mechanical responses of solid solutions far from equilibrium

Complex physical and chemical processes rule the evolution of solid solutions as the system moves towards its steady state. When considering a deformable medium, chemical reactions may affect the solid strength and its mechanical properties. Analogously, high mechanical strength may suppress either the volumetric shrinkage or swelling associated with the local volume changes caused by the chemical processes. Moreover, the nucleation and growth of new phases as a result of chemical reactions induce heterogeneous stresses. On the other hand, the phases that compose the solid have an interface of non-zero thickness where the physical and chemical properties vary from one phase to another. Therefore, the theoretical and computational modelling of solid solutions enduring chemo-mechanical processes together with interfacial interactions require to capture the stress-assisted volume changes mechanism as the phases diffuse and react. In this effort, phase field models emerge as promising tool to simulate coupled interfacial phenomena. These models rely on a diffuse order parameter to monitor the interfaces implicitly. Thus, we propose a thermodynamically-consistent phase field framework to describe the dynamics of solid solutions undergoing mass transport and chemical reactions, deformation, and interfacial interactions. We use isogeometric analysis to discretize in space the system of partial differential equations. We solve the system using the PetIGA isogeometric analysis framework in their primal version. Simulation results provide insights into the phenomenon and verify the interleaving between these chemo-mechanical processes.