Abstract: We consider a space-time adaptive splitting scheme for the numerical simulation of the formation of spherulites in polycrystallization processes described by a two-field phase field model. The phase field model consists of a coupled system of evolutionary processes for the local degree of crystallinity $\phi$ and the orientation angle $\Theta$ one of them being of first order total variation flow type. The splitting scheme is based on an implicit discretization in time which allows a decoupling of the system in the sense that at each time step minimization problems in $\phi$ and $\Theta$ have to be solved successively. The discretization in space is taken care of by a standard finite element approximation for the problem in $\phi$ and $\Theta$ an Interior Penalty Discontinuous Galerkin (IPDG) approximation for the one in $\Theta$. The adaptivity in space relies on equilibrated a posteriori error estimator for the discretization errors in $\phi$ and $\Theta$ in terms of primal and dual energy functionals associated with the respective minimization problems. The adaptive time stepping is dictated by the convergence of a semismooth Newton method for the numerical solution of the nonlinear problem in $\Theta$. Numerical results illustrate the performance of the adaptive space-time splitting scheme for two representative polycrystallization processes.

* The results are based on joint work with Basanta Pahari and James Winkle.

* The support by the NSF and the chemical company BASF is acknowledged.