

Report from Prof. A.D. (Tony) Rollett,
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This report is short because we are still in the process of recruiting students to work on the project. This process will be completed next month (Oct.). The students will be co-advised by Prof. Greg Rohrer and myself.

The main thrust of the mesoscale modeling effort will be to implement Potts and Phase Field models that can simulate microstructural evolution in the presence of complexions at grain boundaries. In related work, we have added capability to an existing code set called MMSP (Mesoscale Microstructure Simulation Project) so that we can include descriptions of the anisotropic properties of grain boundaries in simulations of polycrystalline evolution (grain growth etc.). We are testing these simulations against experimental data for the (anisotropic) Grain Boundary Character Distributions (GBCD) in various materials. For the MURI project, we will add further capability to allow for transitions in the complexion state of any grain boundary in the system. The basis for such transitions will be local variations in composition, coupled with models that describe the transition nucleation.