

**M.Sc. Defense**  
**Russell Spencer**  
**DATE: Thursday September 9<sup>th</sup>, 2010**  
**TIME: 1:00p.m.**  
**PLACE: MacNaughton 222**  
**University of Guelph**

**THESIS TITLE:**

Simulation of nucleation dynamics at the lamellar-cylinder transition in diblock copolymer melts

**ABSTRACT:**

We simulate the time-dependent Landau-Brazovskii equation in three dimensions, focusing on the kinetics of the nucleation mechanism of the lamellar-cylinder transition in a diblock copolymer melt. The underlying microstructure leads to a complicated droplet interface structure, an orientation-dependent interfacial velocity and non-spherical nuclei. In part, our motivation is to show that our simulation method is a viable way of studying nucleation. We compare our phase diagram with predictions by Wickham et al. J. Chem. Phys (2003), finding good agreement, supporting the use of a single mode approximation for the density field at weak segregation. We find critical droplets which compare well with the theory near coexistence but the theory breaks down for small droplets. Our growing droplets adopt a lens-shape with a major axis normal to lamella. The aspect ratio is better described by a ratio of growth velocities than equilibrium theory. We go beyond the static theory to find orientation-dependent interfacial velocities which are constant for large droplets and depend linearly on quench depth in the nucleation regime.

**EXAMINING COMMITTEE:**

**Chair: Dr. John Dutcher**

**Advisor: Dr. Robert Wickham**

**Advisory Committee Member(s): Dr. An-Chang Shi (McMaster University), Dr. Russell Thompson (University of Waterloo)**