Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)

Intellectual Merit of the Center: The Center for Macromolecular Topology (CMT) will address the need in the polymer industry to characterize, synthetically control, model, and simulate complex macromolecular architectures to manipulate mechanical and rheological properties. This topic has broad industrial and academic interest making it ideal for an I/UCRC Center. Control and quantification of complex macromolecular architectures is of pivotal importance in the polyolefin industry where the addition of one long chain branch per ten thousand carbon atoms in polyethylene can increase the viscosity by a factor of 35. Often the source of trace amounts of long chain branching is difficult to determine and characterization is challenging. Similarly, control of branching in gels, networks and elastomers remains a synthetic and characterization challenge of broad importance to industry. Complex macromolecular topologies are also of importance to model polymeric systems that are targeted for new technologies such as molecular machines. Some of these synthetic systems serve as simple representatives of molecular characteristics displayed by biological molecules. The two PI's offer complementary skill sets of interest to industry focusing on characterization and rheology. The two universities can also offer expertise in synthesis, modeling and simulation. Interactions with other universities and international centers, particularly the Polymer IRC at the University of Leeds, are planned. The Leeds center differs from CMT in that it focuses on simulation and modeling of complex topologies while the CMT will focus on characterization and rheology. Ron Larson, already has strong interactions with the Leeds Center.

One initial focus of the center will be on control of molecular topology in polyethylene. Both the Michigan and Cincinnati groups have active research programs in this area that have significant industrial interaction. Currently, work in understanding structure/property relationships in branched polyolefins is duplicated at a number of industrial research labs. CMT can serve as a hub for pooling of non-proprietary information and to set standards for the description of complex molecular topologies especially in polydisperse systems of industrial importance. Manufacturers of polyolefins such as Dow, LondellBasell and ExxonMobil have expressed a strong interest in the proposed center. The topic of molecular topology is also of interest to industries involved in gels, elastomers and hyperbranched structures such as P&G, Goodyear and DSM. National laboratory participation in the center will involve characterization techniques involving neutron scattering (ORNL) and interest in utilization of these materials in weapons systems and other high technology areas (Sandia NL, AFRL).

Broader Impact of the Center: The CMT will develop human capacity in the chemical industry. The center will significantly enhance the nation's research infrastructure base, which is losing ground to European, Asian and Middle Eastern competition in the polyolefin and other industries targeted by the center. The center will coordinate internet based video courses on rheology, scattering, synthesis and modeling of complex macromolecular systems that will be available to industrial as well as academic participants and the general public on arrangement with the Universities. CMT will actively recruit women and minority graduate students.

The center has as a main goal enhancement of the intellectual capacity of the engineering workforce and capabilities in controlling molecular topology. Improvement in our control of molecular topology will lead directly to improvements in a wide range of consumer and industrial products from gels to tires; from plastic packaging to viscosity enhancement in oils.