

TOPOLOGY AS A SURFACE-ACTIVE AGENT FOR NANO-STRUCTURED POLYMERS AT THE INTERFACE

G Pellicane¹, F M Gaitho¹, G T Mola¹ and M Tsige²

¹UKZN-School of Chemistry and Physics King Edward Avenue, South Africa

²University of Akron-Goodyear Polymer Center, USA

Physical techniques for surface modification of plastics use surface-active agents, which are allowed to self-assemble at the surface. Many techniques, which are important in modern technologies, use polymer blends, and there is considerable interest to understand the extent the composition of the surface layer differs from that in the bulk for molten polymer mixtures. Dynamical and structural properties of polymers in the melt state are strongly influenced by molecular architecture and blending polymers with different molecular topologies could be potentially exploited to control interfacial segregation of the polymer film, and to achieve optimal mechanical properties of the plastic material. However, a deep understanding of the role of chain architecture and molecular mass in determining which species preferentially adsorb at a given interface is lacking. Experiments to resolve the matter are typically conducted by mixing polymers possessing the same repeat chemistry, but different molecular architecture. Here, we show the results obtained in large-scale molecular dynamics simulations of linear-cyclic polymer films, and we find clear evidence of enhancement of linear polymers at the interface, in agreement with recent experimental results. The behavior predicted by the self-consistent field theory (SCF), i.e., enhancement of cyclic polymers at the interface, emerges for relatively long chains. In our presentation, we provide a picture of the microscopic mechanisms through which the chain length arbitrates the competition between the different packing constraints imposed by the loop and linear geometry of the two polymers. We also discuss the role of enthalpic and entropic factors of the interfacial free energy of the system in determining which species in the blend preferentially adsorbs at the interface.

Biography

G Pellicane is an Associate Professor in the School of Chemistry and Physics, at the University of Kwazulu-Natal (South Africa). He took his PhD in Physics at the University of Messina (Italy) in 2001. He is the Author of more than 50 peer-reviewed articles indexed in the web of Science-core collection database. His field of expertise is the theory and computer simulation of simple/complex fluids. He has acted as a Reviewer for several international journals, including Journal of Smart and Nano Materials (Taylor & Francis), Journal of Physical Chemistry C (American Chemical Society), Chemical Physics Letters (Elsevier), Journal of the Royal Society Interface (Royal Society Publishing), Journal of Physics A (Institute of Physics), Physica Scripta (Elsevier), Molecular Physics (Taylor & Francis), Physica A (Elsevier), Physical Review Letters (American Physical Society), Soft Matter (Royal Society of Chemistry), Physical Chemistry Chemical Physics (Royal Society of Chemistry), Journal of Physical Chemistry B (American Chemical Society), Journal of Chemical Physics (American Institute of Physics), Physical Review E (American Physical Society), Journal of Physics: Condensed Matter (Institute of Physics), European Journal of Physics (Institute of Physics), New Journal of Chemistry (Royal Society of Chemistry).

pellicane@ukzn.ac.za