Flow-induced coalescence of block-copolymers and polymer coated nanoparticles stabilized drops

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Polymer-coated Janus gold nanoparticles (PJGNPs) are amphiphilic, highly surface active and have been proposed as new compatibilizers in immiscible polymer blends as an alternative to block-copolymers (BCs) to increase the optical, magnetic and mechanical properties of the resulting composite material. However, the gold cores in PJGNPs also increase the magnitude of the disjoining pressure (Π^{part}), i.e. the van der Waals interactions per unit area, in the thin film between the drops, favoring coalescence. In this talk I will show quantitatively the effect on the drainage time (the time it takes for the thin film between the drops to drain) of PJGNP stabilized drops by using parametric boundary integral simulations of two drops stabilized by PJGNPs undergoing a flow-induced head-on collision in extensional flow. The PJGNPs are treated as surfactants and an ad hoc expression for Π^{part} is used that takes into account the nanoparticle concentration and size. The PJGNP interfacial diffusivity (D_s), via the surface Peclet number (Pe_s), and the surface elasticity, via the Marangoni number (*Ma*), were also varied. Flow-induced coalescence was found very sensitive to all these three parameters. The gold cores in PJGNP stabilized blends reduce dramatically the drainage time when the interparticle distance is small (up to 60% for 3nm core diameter and touching cores, significant for drop sizes <5mμ) with respect to the same system stabilized by BCs. However, the soft coronas diminish this effect considerably. Thus, we can design the nanoparticle ligand to hinder enhanced VDW interactions, but at the same time to retain the nanoparticle appealing properties. Our simulations, used to interpret recent drainage time head-on coalescence experiments, suggests that, besides the enhanced Π^{part}, other causes, like a D_s higher than the one estimated via the Stokes-Einstein relation and the presence of entropic attraction between the drop interfaces stabilized by PJGNPs, have to be simultaneously present to explain the dramatic drainage time reduction reported in the PJGNP stabilized system compared to the BC stabilized one.

A second topic considered in this talk is the flow-induced stabilization of drops by BCs. Again, boundary integral simulations are used to show the importance in immiscible polymer blends of the entropic attraction between two interfaces with grafted dry polymer brushes. Our computational study shows that the entropic attraction between block-copolymers stabilized drops is an important cause in determining the drainage time. In fact, a strong additional attractive force, other than the computed van der Waals interactions, was necessary to match our full-drop boundary integral simulations with the experimental data obtained in a computer controlled four-roll mill.