Small Angle Scattering studies of nanoparticle packing into block copolymer micelles

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Micellar nanocomposites are finding increasing applications in medical nanotechnology because of their ability to encapsulate a variety of nanoparticles. In our work, we synthesize micelles composed of poly(styrene-b-ethyleneoxide) (PSPEO) co-encapsulating quantum dots (QDs) and superparamagnetic iron oxide nanoparticles (SPIONS) for in-*vitro* cancer cell detection and manipulation. We have extended this approach to introduce poly(lactic-co-glycolic acid) PLGA into PSPEO micelles either by solubilization or a mixed micelle formation mechanism. Successful application of these nanocomposites requires an understanding of how their morphology evolves with changing process conditions and the nature of polymer-encapsulant interactions. To understand the multifunctional properties of the micelles, it is also important to know the number of nanoparticles encapsulated within the micelle and their distribution inside the heterogeneous micellar micro-environment. Here, we evaluate nanoparticle packing as a function of number and shape, in PSPEO micelles using Small Angle X-ray Scattering.

Our multifunctional micelles are synthesized using the interfacial instability approach, which involves combining the polymer and nanoparticles initially present in a common solvent such as chloroform with a selective solvent such as water. Micelles form, trapping the hydrophobic nanoparticles. An emulsifier, poly vinyl alcohol (PVA) is used in this process. We investigated the micelle encapsulation behavior of differently shaped nanoparticles (spheres and cylinders) at different concentrations. At sufficiently high nanoparticle concentration, crystalline behavior is exhibited. Using small angle x-ray scattering (SAXS), we observed diffraction peaks in the scattering profiles at high nanoparticle loadings. The inter-nanoparticle spacings calculated for the QDs and the SPIONS are consistent with their size and geometry. Our future efforts are directed towards studying the onset of packing behavior within micelles for different classes of nanoparticles. Further, by changing the original polymer used to a longer polymer known to form cylindrical micelles, we observed nodular loading behavior of the nanoparticles inside the micelles. The dynamic behavior of the nodes within the cylindrical micelle was studied using fluorescence microscopy.

Nanoparticle loading was also compared to that of a hydrophobic polymer, PLGA. PLGA was found to exist in two phases, solubilized in micelles or as independent microspheres, based on initial conditions. We were able to observe the scattering behavior of each of these phases to determine PLGA distribution on a volumetric basis.

Nanostructure investigation using SAXS provides an in-*situ* exploration of the sample. Combined with other analytical tools such as Transmission Electron Microscopy (TEM) and fluorescence microscopy, scattering methods yield vital structural information about the sample probed. This forms the basis for successful implementation of these nanocomposites in a wide variety fields in nanotechnology and nanomedicine.