Role of Finite Size Effects on Dispersion and Glass Transition of Polymer Nanocomposite Films

Dispersion of nanoparticles in polymer matrix plays the most important role in determining the properties of polymer nanocomposites. We have shown [1] how confinement affects the dispersion of nanoparticles in polymer nanocomposite films using X-ray reflectivity, scanning electron microscopy and atomic force microscopy. Our particles are grafted with polystyrene with gold core and dispersed in polystyrene matrix of various molecular weights. A systematic variation in the dispersion of nanoparticles with confinement for various compositions and matrix polymer chain dimensions has been observed.

While the grafted molecular weight is much smaller than that of matrix, a thicker film shows segregation of particles on the surface and film-substrate interface of the film. But a reduction in film thickness (comparable to the radius of gyration of the matrix chains) leads to a clear homogenization of the particle density into the film which has been quantified from the electron density profile, along the film thickness, extracted from XR profile. On the other hand if the ratio between grafted polymer molecular weight and matrix polymer molecular weight, represented by f=M_g/M_m, increases, the film even with higher thickness becomes almost homogeneously dispersed.

We have summarized these results in terms of the dispersibility parameter, D=(φ^blk/φ^seg), where φ^blk is the volume fraction of the particle in the interior(bulk) of the film and φ^seg is that of the particles segregated on the surface and interface. A phase diagram is shown in the figure

Increasing D indicates higher dispersion and D > 1 denotes complete dispersion. The D value for 20 nm films for all volume fractions of nanoparticles are higher than the values for 65 nm films, thus clearly indicating the enhancement in the dispersion with confinement. We have also shown how glass transition temperature, T_g, is affected by dispersion in nanocomposite films [2-3]. We have also shown recently [1] that confinement induced re-dispersion of nanoparticles in ultra-thin polymer nanocomposite films leads to further reductions in T_g.

Reference:

