415a Measuring and Modeling of Flow-Induced Nanostructure of Nanoclay/Polymer and Nanofiber/Polymer Melt Composites

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Polymer nanocomposites incorporating nanoclays or carbon nanotubes/nanofibers have gained tremendous research interest in recent years. Results to date have shown that these nanocomposites exhibit desirable mechanical, thermal, and electrical properties. These properties largely depend on the orientation of the fillers. For thermoplastic polymer composites the filler orientation is introduced during processing. Thus, it is desirable to be able to model and predict the evolution of particle orientation induced by processing flow.

In this study, we prepared nanoclay/polystyrene and carbon nanofiber/polystyrene composites using different methods, namely melt blending and solvent casting. Disk-shaped specimens for shear rheology measurements were made by injection molding. Steady and transient shear rheological measurements were performed. The samples were sheared at controlled shear rates until steady state was reached. Particle orientation in the un-sheared and sheared samples was measured at strategic locations within the sample disks on two mutually orthogonal planes using TEM.

A 3-dimensional nanostructually-based model based on rigid particles suspended in a viscoelastic matrix has been constructed. The model is centered on tracking the particle orientation tensor induced by the flow. The particle orientation tensor combines the contributes of a collection of particles to dictate the mesoscale properties of nanocomposites. The evolution of the orientation tensor is described by Jeffrey's model with the particle-interaction term proposed by Folgar and Tucker 1. The stress contribution from the polymer is calculated using a modified Giesekus model where the polymer/particle interactions are also included. The stress generated by the addition of particles is computed following the method proposed by Tucker's equation2. The model is able to accurately predict the measured rheology and orientation of the melt phase composites, and the effect of the polymer/matrix interaction (ƒã) and particle-particle interaction (CI) is discussed. Our results show that both effects have significant impact on the predictions of the model. Varying CI as a function of shear rate can give more accurate predictions of steady state viscosity and particle orientation.

Reference:

1. Folgar, F.; Tucker, C. L. Journal of Reinforced Plastics and Composites 1984, 3, 98-119. 2. Tucker, C. L., III. Journal of Non-Newtonian fluid mechanics 1991, 39, 239-268.