MOLECULAR-DYNAMICS STUDY OF EPOXY/CLAY NANOCOMPOSITES: RHEOLOGY AND LONGEST ROUSE RELAXATION TIME

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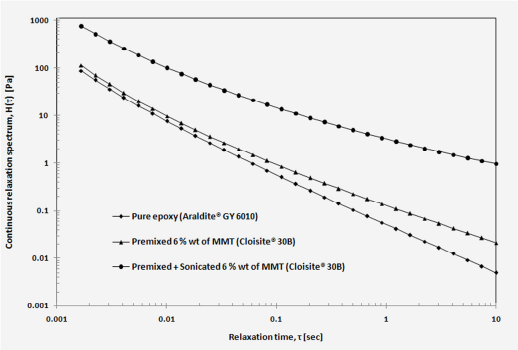
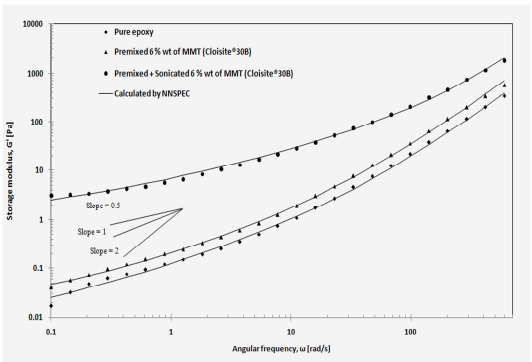
Very similar to the concept of entanglement which has an important role in polymer rheology, intercalation/exfoliation of nanoparticles can strongly affect the linear rheological responses especially both frequency depended moduli and relaxation process. For instance, polymers which filled with nanoparticles (depends on degree of dispersion) last more to relax from imposed deformation regarded to unfiled systems. On the other hand, these unusal behaviors can be confirmed perfectly with molecular dynamics study. Since the rouse model is suitable for polymers with low molecular weight, longest rouse relaxation time has been determined for epoxy model nanocomposites. Here the value of zero shear viscosity which calculated during generation of continuous relaxation spectrum, employed to join rheological observations to molecular dynamic view point. Among the different parameters consisting of statistical segment length, degree of polymerization, molecular weight and temperature which influence the longest rouse time, it is concluded that friction coefficient between diffused chains, governed the increase of about 80 orders of magnitude of longest rouse time for filled epoxy regarded to unfilled one.

Sample ID	Mixing method	Δd_{001} (Å)	$G' \sim \omega^m$	$\eta^* \sim \omega^n$	η_0 (Pa.s)	τ_R (s)
1	Pure epoxy	-	1.51	0.00	14.17	2.14
2	Premixed	8.05	0.81	-0.02	24.33	3.67
3	Premixed+sonicated	21.01	0.19	-0.42	1146.85	173.13





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