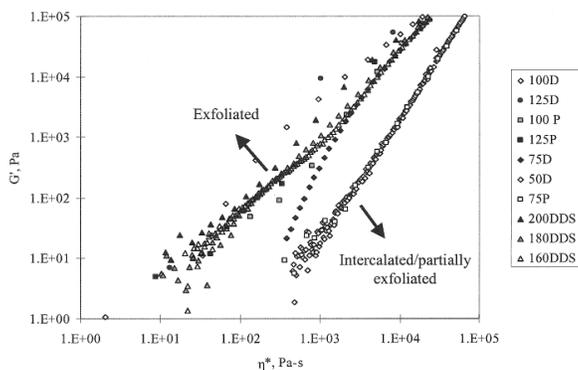


Novel polymer nanocomposite materials

We develop new materials for structural, electronic, electrical, and shape memory applications by combining nanoscopic metallic, semi-conducting, and non-metallic inorganic particles with high performance engineering thermoplastics, thermoplastic elastomers, and thermosetting polymers. The focus of this research is to develop fundamental understanding on nanofiller dispersion in thermosets (epoxies and PMR polyimides), polyolefins, thermoplastic polyurethane elastomers and foams, shape memory polymers, and polymer blends.

Our study revealed that low molecular weight thermosetting resins can be used as dispersing agents of nanoparticulate fillers, such as fumed silica and layered silicates in thermoplastic polymers, such as polyethersulphone, polyphenyleneether, polyphenylene sulphide, etc.

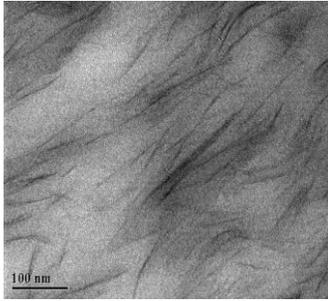
- (a) **Epoxies:** We also found that in epoxy-nanoclay systems, the ratio $G'/|\eta^*|$ plays an important role in determining whether exfoliation, partial exfoliation, and intercalation occurs;



G' is the storage modulus of intra-gallery epoxy and $|\eta^*|$ is the complex viscosity of extra-gallery epoxy at an instant of time. Complete exfoliation is obtained for values of $G'/|\eta^*|$ greater than ~ 4 1/s. Similar observations were made in the case of thermoset polyimides. A list of peer-reviewed publications is

presented at the end of this document.

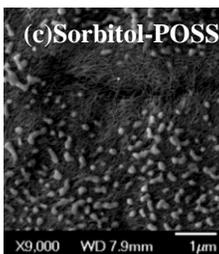
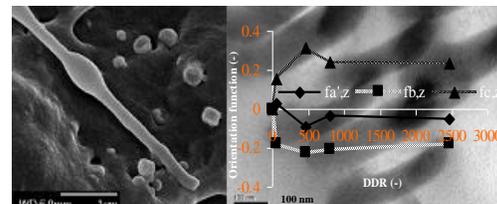
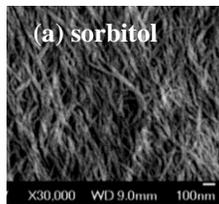
- (b) **PMR resins:** We developed a novel method of nanoclay exfoliation in synthesis of nanocomposites of PMR-type thermoset resins. The method involves nanoclay intercalation by lower molecular weight PMR monomer prior to dispersion in primary, higher molecular weight PMR resin and resin curing to obtain the final composites. It was found that sonication of clay at the time of intercalation by lower molecular weight PMR resin helps achieve higher degree of exfoliation. In addition, clays obtained from ion exchange with a 50:50 mixture of N-[4(4-aminobenzyl)phenyl]-5 norborene-2,3-dicarboximide (APND), and dodecylamine (C12) showed better exfoliation than Cloisite® 30B clay and resultant nanocomposites show higher thermal stability and higher tensile modulus. A list of peer-reviewed publications is presented at the end of this document.
- (c) **TPU:** Our group has developed a bulk polymerization method for efficient exfoliation of reactive layered silicate nanoparticles in thermoplastic polyurethane



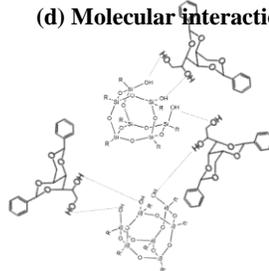
nanocomposites. The resultant materials with 3 wt% clay content offer more than 100% increase in tensile modulus and strength and almost no decrease in tensile elongation. Only micro-composites are produced in the case of non-reactive clays. It was also found that a balance between shear and extent of chemical reactions must be maintained to obtain best results – excessive clay-polymer reactions and low shear stress in polymerization results in micro-

composites. A list of peer-reviewed publications is presented at the end of this document.

- (d) **Polyolefins:** We investigated the nature of interactions between the molecules of polyhedral oligomeric silsesquioxane (POSS) containing silanol functionalities (silanol-POSS) and di(benzylidene)sorbitol (DBS) encountered in the development of nanocomposite fibers from the compounds of POSS, DBS, and isotactic polypropylene (iPP). The synergistic interactions were investigated using Fourier transform infra-red (FTIR) spectroscopy, differential scanning calorimetry (DSC), wide angle X-ray diffraction (WAXD), nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry, and oscillatory shear rheology. Mass and NMR spectrometry revealed that the molecules of silanol-POSS and DBS formed several amorphous non-covalent molecular complexes promoted by hydrogen bonding. More abundant complex formation was observed with silanol-POSS molecules carrying four silanol groups and phenyl substitutions. Such complex formation deterred fibrillation of DBS when the compounds of iPP, DBS, and silanol-POSS were cooled from the homogeneous melt states. It was also revealed that POSS-DBS complexes were of much lower viscosity than iPP, which resulted in significant reduction of viscosity of compounds of iPP, DBS, and silanol-POSS. A list of peer-reviewed publications is presented at the end of this document.



(d) Molecular interactions



Publications:

1. Roy, S., Lee, B.J., Kakish, Z.M., Jana, S.C. 2012 Exploiting sorbitol-POSS interactions: Issues of reinforcement of isotactic polypropylene spun fibers. *Macromolecules*, 45(5), 2420-2433.
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14. Jimenez, G., Jana, S.C., 2007 Polymer composites of oxidized carbon nanofibers prepared by chaotic mixing. *Carbon* 45(10), 2079-2091.
15. Jimenez, G., Jana, S.C., 2007 Electrically conductive polymer nanocomposites of polymethylmethacrylate and carbon nanofibers prepared by chaotic mixing. *Composites Part A: Appl. Sci. Manu.*, 38, 983-993.
16. Cao, F., Jana, S.C., 2007 Nanoclay-tethered shape memory polyurethane nanocomposites. *Polymer*, 48(13), 3790-3800.

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22. Pattanayak, A., Jana, S.C., 2005 Synthesis of thermoplastic polyurethane nanocomposites of reactive clay by bulk polymerization methods. *Polymer*, 46(10), 3275-3288.
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24. Park, J.H., Jana, S.C. 2003 A case study on the effects of plasticization of epoxy networks by organic treatment on exfoliation of nanoclay. *Macromolecules*, **36**, 8391-8397.
25. Park, J.H., Jana, S.C., 2003 Mechanism of exfoliation of nanoclay particles in epoxy-clay nanocomposites. *Macromolecules*, **36**(8), 2758-2768.
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