#### Polymer nanocomposites for functional applications

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While extensive research has been carried out in the field of structural polymer-based nanocomposites, much less investigations have been concerned with polymer nanocomposites for functional applications. Among the functional nanomaterials, nanocomposites consisting of metal nanoparticles dispersed in a dielectric matrix are of particular interest due to their novel functional properties offering hosts of new applications. Here, polymers are attractive as matrix, and several approaches have been reported to incorporate metal nanoparticles into polymers.

The present talk is concerned with the preparation of polymer-based nanocomposites by vapor phase co- and tandem deposition and the resulting functional properties. The techniques involve evaporation and sputtering, respectively, of metallic and organic components and inter alia allow the preparation of composites which contain alloy clusters of well defined composition. Emphasis will be placed on soft-magnetic high frequency materials with cut-off frequencies well above 1 GHz and high quality factors and on optical composites with tuned plasmon resonances suitable for ultra thin color filters, Bragg reflectors, and other devices. In addition, antibacterial coatings and selective sensors for organic vapors based on nanocomposites with filling factors close to the percolation threshold will be addressed. Moreover, a novel approach to produce magnetic nanorods for potential applications in high-density data storage and other fields will be presented.

**Keywords:** polymers, nanocomposites, coatings, nanoparticles, nanorods, evaporation, sputtering, magnetic, high frequency, antibacterial, optical

#### Polymer nanocomposites reinforced with polysaccharide nanocrystals

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There are numerous examples where animals or plants synthesize extracellular high-performance skeletal biocomposites consisting of a matrix reinforced by nanosize crystalline domains. Cellulose and chitin are classical examples of these reinforcing elements, which occur as whisker-like microfibrils that are biosynthesized and deposited in a continuous fashion. In many cases, this mode of biogenesis leads to crystalline microfibrils that are almost defect-free, with the consequence of axial physical properties approaching those of perfect crystals.

During the last decade we have attempted to mimic biocomposite by blending cellulose or chitin whiskers from different sources with polymer matrices. Aqueous suspensions of such nanocrystals can be prepared by acid hydrolysis of the substrate. The object of this treatment is to dissolve away regions of low lateral order so that the water-insoluble, highly crystalline residue may be converted into a stable suspensoid by subsequent vigorous mechanical shearing action. The resulting nanocrystals occur as rod-like particles or whiskers, which dimensions depend on the nature of the substrate. Starch can also be used as a source for the production of nanocrystals. The constitutive nanocrystals appear as platelet-like nanoparticles with a length ranging between 20 and 40 nm, a width ranging between 15 and 30 nm and a thickness ranging between 5 and 7 nm. Since the first announcement of using cellulose whiskers as a reinforcing phase, they were extensively used as model fillers in several kinds of polymeric matrices, including synthetic and natural ones.

Casting mixtures of polysaccharide nanocrystals and lattices led to composites with drastically enhanced mechanical properties, especially at T> Tg of the matrix, by virtue of the formation of a whiskers network, even when the whisker volume fraction was only a few percent. The formation of this rigid network, resulting from strong interactions between whiskers was assumed to be governed by a percolation mechanism. This hydrogen-bonded network induced a thermal stabilization of the composite up to 500 K, the temperature at which polysaccharides start to decompose.

In addition to some practical applications, the study of these nanocomposite materials can help to understand some physical properties as geometric and mechanical percolation effect.

**Key words:** nanocomposites, polysaccharide nanocrystals, cellulose whiskers, chitin whiskers, percolation

### Nanotechnology in rubber-myth or reality?

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Nanotechnology is fast becoming a key technology of the 21st century. Nanotechnology can be defined as, the purposeful engineering of matter at scales of less than 100 nanometers (nm) to achieve size-dependent properties and functions. Myths are being formed on the proverbial nanotechnology market, but the reality is nanotechnology is not a market but a value chain. The chain comprises of - nanomaterials (nanoparticles), nanointermediates (coatings, compounds, smart fabrics) and finally leading to nano-enabled products (cars, clothing, airplanes, robots).

Nowadays, polymeric materials are applied in almost all areas of our life and they have a stimulating function for the development of future technologies. In contrast to metallic and ceramic materials, polymers are relatively cheap, can easily be processed, as they need less energy for production and shaping, and have a variety of fields of application in textiles, electromagnetic shielding, coatings, automotive parts, electronic and household appliances etc.

Recently, elastomer-nanocomposites reinforced with low volume fraction of nanofillers have attracted great interest due to their fascinating properties. The incorporation of nanofillers such as layered silicate clays, carbon nanotubes, nanofibers, calcium carbonate, metal oxides or silica nanoparticles into elastomers improves significantly their mechanical, thermal, dynamic mechanical, barrier properties, flame retardancy etc. The very low particle size, the high aspect ratio and large interface area yield an extraordinary improvement of the properties in a wide variety of rubbery materials. The uniform dispersion of nanofillers in elastomer matrices is a general prerequisite for achieving desired mechanical and physical characteristics. In this presentation, current developments in the field of elastomer nanocomposites reinforced with layered silicates, silica, carbon nanotubes, nanofibers and various other nanoparticles will be highlighted. New theories and models promulgated to elucidate the role of polymernanofiller adhesion/interaction at the interface region in extracting high-performance from such nanocomposites even at low loadings will also be addressed.

Nanotechnology commercialization is approaching a broad-ranging transformation – a phase change. The scientific advances achieved through comprehension of the different fundamental principles are reflected in the increased government funding, startup development and corporate research interest. The ramifications of the technological advancements are the decisive improvements in existing products, creation of new products and production lines with superior process alternatives and obvious disruption of competitive dynamics and cost structures. Hence, nanotechnology in rubber is no more a myth, but a

reality. However, it is necessary to establish cooperation among research institutes, funding agencies and industries as soon as possible to achieve a rapid market growth.

**Key words:** nanotechnology, elastomer-nanocomposites, nanofillers, polymer-nanofiller adhesion/interaction

### Bis-GMA/TEGDMA/clay nanocomposites, hard materials for dental restorative materials and anti scratch coatings

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Photocurable acrylate based polymer/clay system of the title type has rarely been explored in the literature. The present work is a try to evaluate the said PLS system as hard materials for their applications as dental restorative materials and as anti scratch coatings for plastic sheets, PMMA. Therefore, mixture of Bis-GMA/TEGDMA (50/50 wt/wt) was used as the resin and then compounded with different clays (Cloisite93A, Cloisie30B, CloisiteNa<sup>+</sup>) at different loading levels and, appropriate photo-polymerization initiators. As dental restorative materials, characterization made on blue-light cured bulk materials including investigations by TEM, FTIR and XRD, polymerization volume shrinkage, double bond conversion and standard mechanical tests including flexural strength and flexural modulus measurements. The results showed superior mechanical properties over the pure resin for Bis-GMA/TEGDMA/clay nanocomposites at 3-5 wt% loading level of Cloisite30B. The major disadvantage of the clay in such application was detected to be slightly less double bond conversion compared to the pure resin.

For coating applications, the nanocomposite precursor was applied as a thin film over PMMA slabs and then photo-cured under UV radiation. Transparent coated samples were evaluated for their scratch properties and the results were interpreted using TEM, XRD and AFM. Viscoelastic deformation was obtained for all the coatings in scratch tests with different adhesion strength to the substrate. Different interphases involved in the systems (matrix/clay, matrix/substrate and clay substrate) were detected to be the controlling factors in the final properties of the coatings. On the other hand, the interphases themselves, found to be dependent to the relative exfoliation/intercalation state in the nanocomposite, which is primarily dependent to clay type and its content. The most improved scratch properties with excellent adhesion was obtained for the samples containing 1 wt% of Cloisite30B clay.

**Key words:** Photocurable acrylate based polymer/clay system, dental restorative materials, anti scratch coatings, TEM, XRD, AFM, FTIR

#### Polymer nanocomposites reinforced with polysaccharide nanocrystals

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During the last decade we have attempted to mimic biocomposite by blending cellulose or chitin whiskers from different sources with polymer matrices. Aqueous suspensions of such nanocrystals can be prepared by acid hydrolysis of the substrate. The object of this treatment is to dissolve away regions of low lateral order so that the water-insoluble, highly crystalline residue may be converted into a stable suspensoid by subsequent vigorous mechanical shearing action. The resulting nanocrystals occur as rod-like particles or whiskers, which dimensions depend on the nature of the substrate. Starch can also be used as a source for the production of nanocrystals. The constitutive nanocrystals appear as platelet-like nanoparticles with a length ranging between 20 and 40 nm, a width ranging between 15 and 30 nm and a thickness ranging between 5 and 7 nm. Since the first announcement of using cellulose whiskers as a reinforcing phase, they were extensively used as model fillers in several kinds of polymeric matrices, including synthetic and natural ones.

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# Preparation polyamide-12 composites powders for SLS and its sintering characteristics

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Polyamide-based composites have been proven to have great potential for the RP industry to fabricate functional parts; however, it is difficult to disperse the reinforcements such as whiskers and nano-fillers to the powder uniformly by mechanically mixing, more importantly, the SLS process limits the particle diameter to smaller than 100 µm and near sphericity. This paper reports a new method for preparing polyamide-12 composite powders for applications in selective laser sintering (SLS) by using a dissolution-precipitation process. The potassium titanium whiskers (PTW), nano silica, montmorillonite and glass bead polyamide composites powders were obtained. The characteristics of the composites powders would be evaluated. The sintering characteristics and mechanical properties were also compared to pure polyamide-12 and glass filled polyamide-12.

#### Keywords

Selective laser sintering (SLS), Polyamide-12, Composites dissolution-precipitation, powder

#### Preparation and properties of thermoplastic polyurethane nanocomposites by melt blending: effect of organoclay on mechanical, thermal, morphological and dynamic mechanical properties

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Polymer nanocomposites based on medical grade thermoplastic polyurethane (TPU) and organically modified montmorillonite (OMMT) has been prepared by melt intercalation technique using a Haake batch mixer at 185°C with a rotor speed of 100 rpm and mixing time of 6 minutes. Varying amount of organically modified nanoclays (1, 3, 5, 7, & 9 wt %) was added to the TPU matrix in order to examine the influence of the organoclay on nanophase morphology and materials properties. The interactions between TPU matrix and nano filler were evidenced by FTIR spectra of the TPU/OMMT nanocomposites. XRD, TEM & SEM analysis showed that melt mixing by a batch mixer was effective in dispersing OMMT through the TPU matrix. The X-ray analysis revealed that exfoliation occurred for low montmorillonite content, whereas for higher contents the intercalated clays get rearranged to a minor extent. It is evident from the TEM images that the nanoclay stacks were smaller and more evenly distributed in the composites prepared by melt intercalation. The aggregated clay morphology was characterized with SEM. Because of the difference in scattering density between the clay and PU, large clay aggregates can be easily imaged in SEM. Nanoparticle dispersion was the best at 5-wt % of OMMT. Nanocomposites exhibit higher mechanical, dynamic mechanical and thermal properties than that of pristine TPU matrix, which increases with the increase in OMMT content. The mechanical properties showed an improvement of the elastic modulus, tensile strength and elongation at break but a decrease in the stress and strain values at breaking point on increasing the clay content. TGA data revealed that 5-wt % incorporation of organoclay enhances the thermal stability of nanocomposites significantly. Melting point and glass transition temperature of soft segments were found to shift towards higher temperature with the inclusion of organoclays. DSC data revealed Tg, crystallization and melting temperature of polyurethane matrix are shifting towards the higher temperature with inclusion of nanoclays. Rheological behavior of TPU nanocomposites were characterized by rubber process analyzer. DMA result indicates that below the  $T_{\rm g}$ , addition of OMMT has strongly influenced the elastic (corresponding to E') and plastic (corresponding to E'') properties of the TPU matrix. Significant enhancement of E' and E'' can be seen for the TPU/OMMT. This is due to the mechanical reinforcement resulting from strong interaction between OMMT and the TPU matrix for the enhancement of E', and the improvement of E'' indicates that plastic response to the deformation is prominent in the presence of the OMMT.

Key words: medical grade TPU, organoclay melt processing, DMA, TGA, RPA

## Electrical and dielectrical properties of the epoxy-hematite nanocomposites

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 $\alpha$ -Hematite nanorods were used as filler for the epoxy resin. Electrical and dielectrical properties of the obtained nanocomposite were investigated. DC-conductivity measurements showed a significant influence of Fe<sub>2</sub>O<sub>3</sub>-nanorods on the DC-electrical properties of the epoxy matrix. However, the observed effects of the filler below and above the glass transition are different. Because of their high specific surfaces, nanorods affected segmental mobility of epoxy molecules to a large extent, which resulted in an increase in the glass transition temperature ( $T_g$ ) and a decrease in the real part of dielectric permittivity in high frequency/low temperature region.

Key words: nanocomposites, epoxy matrix,  $\alpha$ -Hematite nanorods, glass transition temperature, dielectric permittivity

#### **Polymers for space applications**

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A number of exotic materials having a wide range of properties are required for accomplishing various space missions. These requirements are met to a large extend by the use of high performance polymers. The most important polymeric system used in satellite launch vehicle is the polymeric fuel binder for composite solid propellants. The present day binders have a polybutadiene backbone. Hydroxyl terminated polybutadiene (HTPB) is the sate of the art binder which has been developed and produced inhouse. Polymer based insulations and inhibitors are used to protect the rocket motor case and to give the desired burning pattern to the propellant grain.

Thermal protection systems are another class of polymeric systems used in rockets and satellites and silicone resins are widely used as coatings in this regard. Preceramic polymers, which give ceramic residue on pyrolysis at 1500°C, find applications as oxidation resistant coatings. Phenolic resins continue as the material of choice for making ablative liners of rocket nozzles and re-entry vehicles that encounter very high heat flux. The high thermal stability of polyimides makes them ideal candidates as thermal control barrier in satellites.

Polymer matrix composites have many applications in aerospace industry. Epoxides, cyanate esters, bismaleimides, polyether ketones etc are the matrices of choice, while polyaramid fiber and polyacrylonitrile co-polymer based carbon fibers are the most widely used reinforcements. Since aerospace structures consist of dissimilar materials, different adhesives are used for joining them. The use of cryogenic fluids as propellants poses the challenge for developing compatible thermal insulations.

Reusability of the launch vehicles is a major step towards the reduction of launch cost. This calls for the development of polymers capable of withstanding higher heat fluxes and oxidizing environments, for which carbon-carbon and ceramic matrix composites are developed. Interplanetary missions of the future need materials of high specific strength which are able to withstand hard vacuum and hostile environment of very low and high temperature, cosmic radiation etc. Intelligent materials are needed for long duration and far off missions. Such challenging future demands of the space industry give enormous opportunities for developing new high performance polymers and tailoring the existing ones for specific missions.

Key words: high performance polymers, polymeric fuel binder, preceramic polymers, thermal insulations

#### Nonlinear elongational flow behavior of complex thermoplastic melts

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The control of strain hardening under elongational flow for polymer melts is discussed. Control of the strain hardening is strongly associated with a change of the relaxation time and relaxation time distribution. A few examples are given here. First one is polypropylene (PP). PP is a well-balanced material in terms of the physical properties such as the stiffness and heat resistance, and the cost. PP is, however, one of the linear polymers exhibit low melt strength and weak strain hardening. We focused on an introduction of a small amount of high molecular chain in order to enhance the strain hardening under elongational flow. This polymer system is very complex comparing with conventional PP. Another is poly(vinyl chloride) (PVC)/plasticizer systems. PVC forms physical gels in various solvents, and the physical properties and structure have been extensively studied mainly for low polymer concentration system. We studied the dynamic and elongational viscosity of PVC/plasticizer systems from the view point of critical gelation phenomena.

Key words: elongational flow, strain hardening, polypropylene, poly(vinyl chloride)

### Morphology Control and Enhancement of Mechanical Properties of Polypropylene Blends

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The impact of miscibility on mechanical properties and final morphology in a set of binary blends of isotactic polypropylene (PP) and rubbery olefin copolymers are studied. It is found that the ethylene– $\alpha$ -olefin copolymers having more than 50 mol% of  $\alpha$ -olefin are miscible with iPP where the copolymers are completely incorporated into the amorphous region of PP. The miscible blends show significantly high drawability with pseudo affine deformation of spherulites. On the other hands, the immiscible blends showing phase-separated morphology exhibit more brittle behavior accompanied by void formation inside the rubber domains.

Key words: morphology, isotactic polypropylene, ethylene– $\alpha$ -olefin copolymers, miscibility, mechanical properties

#### Composition effects on proton conductivity of hybrid polysiloxane membranes

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Burning carbon based fuels has been for centuries the most common technology how to produce energy. Nowadays, the growing demand for energy has caused the steep increasing of  $CO_2$ concentration in the atmosphere for last several years. This development could cause serious climate changes and the flooding of areas close to seashore. The solution how to reverse this trend is switching from carbon fuels to carbon-free, namely hydrogen. To economically produce electric energy from hydrogen we need effective H<sub>2</sub>/O<sub>2</sub> fuel cells equipped with high proton conducting membranes. In our laboratory we have developed fast proton conducting hybrid membranes that can be applied in the H<sub>2</sub>/O<sub>2</sub> fuel cells operating in dry conditions at room and elevated temperatures. The main constituent of the membrane is the polydimethylsiloxane polymer with phosphorous heteroatoms. As the most important property of the membrane is its high proton conductivity, we developed the synthesis procedure that guarantee the high concentration of stable hydroxyl groups promoting the fast proton migration. To enhance the conductivity, we fill the polymer with  $SiO_2$  nanoparticles and achieve the conductivities about 0.02 S/cm at 130°C in dry atmosphere. The conductivity is precisely determined by using impedance spectroscopy. The membrane is placed into the electrochemical cell with Pt electrodes and its impedance is measured in the frequency range from 0.01 Hz to 1 MHz at temperatures from 25 to 180°C. The recorded impedance data are analyzed in the Nyquist complex plane diagram using the equivalent circuit approach. In our paper we discuss the effects of membrane's components and the influence of the preparation procedure on the membrane's proton conductivity and its performance in the laboratory  $H_2/O_2$  fuel cell.

**Key words:** fuel cells, proton conductivity, polydimethylsiloxane, SiO<sub>2</sub> nanoparticles, impedance spectroscopy

#### A reactive nanoparticle route to prepare hybrid nanocomposites

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Hybrid nanocomposites having nanoscale inorganic domains dispersed within an organic polymer can afford materials with a synergistic combination of properties that are characteristic of the inorganic and organic components of which they are comprised. The ability to obtain materials with select properties from the organic and inorganic components allows these materials to find uses in optical, electrical, biomedical, and other specialty areas. The inorganic phase can be pre-made and blended into a polymer melt or solution, which allows precise control of composition, but blending is energy-intensive, and often the dispersed phase does not interact effectively with the matrix, so properties might not be optimized, and the dispersed phase may not be stable. Alternatively, a reactive pre-cursor to the inorganic species may be blended into the polymer melt or solution and reacted to produce the inorganic phase in situ in a sol-gel reactive. This often allows better dispersal of the inorganic phase and better interaction between the two phases, but offers less control over composition, and many reactive precursors are so highly reactive that they phase separate into macroscale, rather than nanoscale domains, and so choice of both reactive precursor and organic matrix is often limited. Here we describe a reactive nanoparticle route that allows hybrid nanocomposites to be prepared with comparatively few limitations on composition by incorporating the reactive precursor into a nanoparticle and converting it to the inorganic component in situ before the final film formation. Effects of synthetic variables are described on the reaction process and film properties.

Key words: nanocomposites, inorganic phase, reactive precursor

## Studies on the crystalline transitions in syndiotactic polystyrene – solvent complexes

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Amorphous syndiotactic polystyrene (sPS) was crystallized at room temperature in norbornadiene (bicyclo[2,2,1]-hepta-2,5-diene), mesitylene (1,3,5-Trimethylbenzene), 3carene (3,7,7-trimethyl bicyclo[4,1,0]hept-3-ene) and DMN (1,4-dimethylnaphthalene) to form the sPS-solvent complex ( $\delta$  form) with respective solvent molecules. In situ HTFTIR studies showed that the  $\delta$  form to  $\gamma$  form transformation temperature occurs well below the glass transition temperature of sPS, which is depressed due to the presence of solvent in the amorphous phase; higher the solvent content in the complex, lower the transition temperature. Glass transition temperatures determined by modulated differential scanning calorimetry (MDSC) coincide with the transition temperatures, indicating that the  $\delta$  form transforms into  $\gamma$  form at the glass transition temperature for these complexes. Such a behavior is very different from the behaviour of the sPS- solvent complexes formed by dichloromethane, chloroform, toluene, o-dichlorobenzene, decalin (cis-trans) etc. and for these complexes the transition occur well above the Tg.

Key words: syndiotactic polystyrene, HTFTIR, modulated differential scanning calorimetry

## Mechanical behavior, processing and characterization of biocomposites

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Natural fibers are increasingly used as reinforcement in commercial thermoplastics due to their low cost, high specific properties and their renewable nature, as well as the environmental concerns and a shortage of petroleum resources. In this study, the mechanical behavior of biocomposites based on biodegradable polymer matrix (PLA) was investigated. Two different kind of natural fibers using pineapple leaf and rice stem fiber as reinforcements were prepared, respectively. The natural fiber and PLA pellet were mixed and biocomposites were fabricated using a compression molding method. Regarding the chemical treatment, maleic anhydride (MA) was used as a compatibilizer between fiber and matrix. Alkali treatment can remove the lignin, oil and other impurity on the surface of the fiber. The mechanical behavior of present biocomposite is estimated to be better than that of pure PLA.

Key words: biocomposites, natural fiber, mechanical behavior, processing

#### Rubber in underwater sensor technology

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Rubber is extensively used in the underwater acoustic sensor scenerio. The applications include transducer encapsulants, sound absorbers, acoustic window materials, acoustic baffles, shock and vibration isolators, seals, 'O' rings etc. Underwater transducers operate over large ranges of frequency, temperature and pressure. The marine environment in which the transducers are deployed represents one of the most variable and a harsh environment with its corrosive saline water, salt laden above–water atmosphere, wind, waves, tides etc. The service life normally expected for underwater transducer is 15-20 years. It is important that rubber used for the protection of sensors, in addition to being able to sustain the mechanical rigours of the marine environment, must be able to withstand severe stresses imposed by temperature extremes, ozone attack, and the chemical attack of seawater, pollutants, and physical abuse. A number of physical, chemical, electrical, mechanical and acoustic characteristics have been identified as critical for efficient and reliable system behaviour. The technology involved in tailoring the basic rubber materials, acoustic baffles etc., has been evolved and matured. The talk will address the major issues involved in the development of rubbers for underwater sensors applications.

Conventional engineering of rubbers does not suffice to meet with the exact, often stringent performance specifications envisaged for passive acoustic rubbers. The material should satisfy a set of complex and demanding end-use situations imposed by the marine environment, material limitations, and application specific requirements. The major parameters include (1) water absorption & permeation (2) electrical resistivity (3) dynamic mechanical properties (4) acoustic impedance (5) bondability to metal (6) ease of processing (7) permanence of properties etc. Performance of the rubber in terms of both short and long-term properties is understood as a function of composition, cures condition and environmental parameters. Each parameter is to be optimized through judicious compound development and characterization. An optimised formulation is thus designed and its quality –control techniques developed to guarantee the reproducibility of intended performance.

The rubber vulcanisate during their service absorb substantial amount of water. The absorbed water may significantly alter the performance characteristics leading often to product

failures or de-rated performance. Problem has been successfully addressed in the case of neoprene rubber with the development of a patented curing process.

Underwater transducers are basically high voltage electrical devices and hence their electrical insulation should be high and stable. Use of carbon black is imperative for optimum mechanical properties, whereas inclusion of carbon black in large quantities is detrimental for electrical insulation, particularly for Neoprene. The amount and type carbon black for optimal behaviour has been developed. Transducers are also dynamic devices operating in a wide frequency band and temperature range. Rubbers are visco-elastic materials characterized by wide variation of stiffness and damping with of frequency and temperature. Dynamic mechanical properties determine the acoustic behaviour of elastomers; thus, it is imperative that rubbers used for encapsulation be optimised for specific dynamic mechanical behaviour within the operating frequency band.

In the construction of a transducer, encapsulation material comes in the acoustic path between transducer and seawater. The intervening medium should not adversely affect acoustic wave propagation across it to the water medium. The product of density and sound velocity, the acoustic impedance, in the material decides the propagation losses. For reflection free transmission the acoustic impedance of mediums should match. This has been achieved by tailoring dynamic complex modulus and density of the rubber. Also, dynamic loss factor, tan delta, has been optimised to minimize sound attenuation. Material developed in NPOL serves as a perfect acoustic window with near zero echo reduction. The rubber compositions have been optimized for compound viscosity; scorch safety, cure characteristics, bonding to metals, and permanence of properties and ease of fabrication.

Conventional heat aging method of estimation of safe service life of rubber products has been substantiated by mathematical equation correlating elongation at break properties with Arrhenius model and curve fitting methods. However, they seldom reflect the effect of aging on functional properties of the transducers.

Estimation of service life of underwater elastomers is important from the point of fleet readiness and reliability. The controlling parameters selected are, water diffusivity and permeability, electrical resistivity, dynamic and static mechanical properties. Estimation of diffusion coefficient at accelerated environment allows prediction of the depth of penetration and hence the life. Permeation of water across the encapsulation rubber is another aspect that has been studied. The rate of permeation follows Arrhenius type temperature dependence. Continued permeation of water vapour through the barrier material can lead to high build up of moisture into the transducer, which can be modelled for reliable life prediction.

Some of the important parameters as out lined above will be discussed in the talk.

**Key words:** underwater acoustic sensor, encapsulation material, dynamic mechanical properties, acoustic impedance, life prediction

#### Monte Carlo simulation of reactions in bilayer polymer blends

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Simulations provide a powerful tool for visualizing the processes that take place at the interphase boundaries of molten polymers. In this work, an off-lattice Monte Carlo simulation of the reaction and interdiffusion in a bilayer A/B polymer blend is carried out using the coarse-grained bead-spring model with Morse potentials. Two types of macromolecular reactions are studied: (i) polymeranalogous autocatalytic units transformation  $A \rightarrow B$  (B-units accelerate the reaction) and (ii) interchain exchange.

(i) The evolution of the number density of A-units and units initially belonging to polymer A chains is studied for a compatible system. Local average characteristics of the composition distribution of reacting chains and length distribution of A and B blocks are calculated. It is demonstrated that these distributions are much broader than those for a Bernoullian copolymer of the corresponding mean composition. Such effect is due to the diffusive intermixing of reacting chains as predicted earlier for the theoretical model that describes large-scale interdiffusion in reacting polymer blends.

(ii) The evolution of the local molecular mass and block length distributions in close vicinity to a phase boundary is studied for an initially incompatible system. It is found that at the early stage the reaction takes place within a narrow interfacial layer until rather short copolymer AB blocks are formed, which then penetrate the bulk phases. In the simulation box of a finite size, a stationary state is finally formed, in which short homopolymers and copolymer blocks are distributed uniformly over the system whereas long blocks are located in the corresponding phases. At higher temperatures, this state is more homogeneous while the time of its establishment depends mainly on the interchange reaction rate.

Key words: Monte Carlo simulation, interphase boundaries, diffusive intermixing