



# POLYMER TECHNOLOGY CENTER

Spring 2009 Edition



## PTC Newsletter

|                                |        |
|--------------------------------|--------|
| PTC Short Course               | Page 1 |
| PTC Faculty Research Highlight | Page 2 |
| PTC Announcements              | Page 3 |
| PTC/SPE Announcements          | Page 4 |

## Polymer Specialty Certificate Program

TAMU students can apply for this program. Please visit:

<http://essap.tamu.edu/polymer.htm>

## MARK YOUR CALENDAR FOR PTC's NEXT CONFERENCES!

**October 8th - SCRATCH**

@ Detroit, MI

**October 29th-30th - PTIC**

@ Texas A & M University

## Polymer Technology Center

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Isabel Cantu

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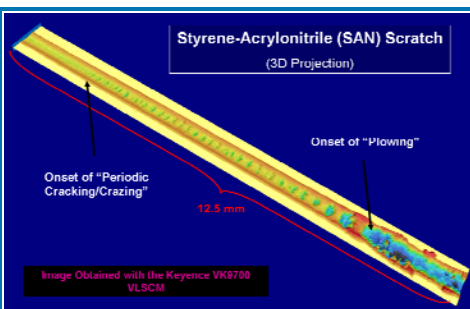
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Website: <http://ptc.tamu.edu>

Dr. Anastasia Muliana is awarded Air Force grant, Dr. Jaime Grunlan is awarded NIST grant: read more on page 3.

Dr. Donald E. Witenhafer of SPE-South Texas Section is elected into the Plastics Hall of Fame: more on page 4.



## PTC Short Course: Scratch and Wear of Polymers and Composites October 28-29, 2009 Texas A&M University

This short course offers a unique opportunity to learn about fundamentals and applications of polymer and composite wear from presenters respected in the field. This short course, held at Texas A&M University, will expose attendees to cutting-edge research and practices involving polymers and composites. Additionally, it

may fulfill your professional development requirements.

The course will cover a number of topics relevant to anyone working with polymers with an interest in surface issues. "Such fields include final-form polymer manufacturing, solid lubrication, coatings, composite structures, polymer formulation, filler and reinforcement suppliers, product designers, and new product development." The course will present key theories behind scratch and wear, as well as illustrative examples. To learn more about this short course, visit: <http://ptc.tamu.edu>

## INSTRUCTORS

### Klaus Friedrich

Dr. Friedrich received his Ph.D. Degree from Ruhr University in Bochum, Germany in 1978. After gaining industrial experience in the construction of machine elements, he held a position at the Center for Composite Materials at the University of Delaware. He later served as Research Director for Materials Science at the Institute for Composite Materials (IVW) at the University of Kaiserslautern, and as a Professor of Polymers and Composites at the Technical University Hamburg-Harburg. He acts as a Scientific Board Member for various international journals in the fields of material science, composites, and tribology. Dr. Friedrich is the editor of five books based on polymer and composite tribology. After retiring from the position of director at IVW in March 2006, Dr. Friedrich now acts as a research consultant to various institutes and industrial companies.

### H.-J. Sue

Dr. Sue has been a Full Professor in the Department of Mechanical Engineering at Texas A&M University since 1995. He obtained his Ph.D. from the University of Michigan. Before joining TAMU, Dr. Sue was employed by Dow Chemical for about seven years. He focuses most of his research work on the fundamental understanding of structure-property relationships of polymeric materials. His recent research interests include micro- and nano-scratch behavior of polymers and preparation of polymer nanocomposites for nanotechnology applications. Dr. Sue is currently the Director of the Polymer Technology Center at TAMU.

### Cris Schwartz

Dr. Schwartz received his Ph.D from Iowa State University in 2006. He is an Assistant Professor in the Department of Mechanical Engineering at Texas A&M University. His research focuses primarily on polymer tribology and engineering design. He heads the INNOMAT research group at TAMU that investigates phenomena related to the tribological behavior of the human body including artificial joint devices and polymer haptics. Prior to his position at TAMU, Dr. Schwartz served as a senior research engineer at Southwest Research Institute® as a project manager, technical investigator, and systems designer. He is also a licensed professional engineer and faculty member of the Polymer Technology Center.



**Dr. K.R. Rajagopal**  
**Department of Mechanical Engineering**  
**Crystallization of polymer melts and its application**  
**to fiber spinning and film blowing**

Professor Rajagopal is currently a University Distinguished Professor and Regents Professor and holds the Forsyth Chair in Mechanical Engineering. He also has joint appointments in Mathematics, Biomedical, Chemical and Civil Engineering Departments and is a Senior Research Scientist at the Texas Transportation Institute.

His primary interest is in the area of continuum mechanics and also researches various aspects of fluid and solid mechanics, continuum thermodynamics, mixtures, biomedicine, and traffic flow modeling. He has worked in modeling the response of both polymeric solids and fluids as well as the transition from polymeric melts to semi-crystalline polymeric solids. Dr. Rajagopal's research into the crystallization of polymers has been supported by the National Science Foundation and the Polymer Technology Center.

Dr. Rajagopal and his former student, Dr. I. J. Rao, developed a theory for the crystallization of polymeric melts within a very general thermodynamic framework which is able to capture the transition from the fluid-like behavior of the polymeric melt to the solid-like response of the semi-crystalline body. The anisotropy of the crystalline phase that is dependent of the deformation of the melt is built into the framework. This framework was used by Dr. Rajagopal and his former students, Dr's. Krishna Kannan and I. J. Rao, to model important industrial processes such as the film blowing and fiber spinning problem of polyethylene terephthalate, and the simulation of fiber spinning, including flow induced crystallization, for various nylons. The model also included a detailed study of the effect of the mass flow rate, the quench air speed, capillary diameter, molecular weight, type of polymer, and additives. The model is able to predict much of the available industrial spinline data exceptionally well (see Figs 1-3), and has been shown to perform better than existing models. The thermodynamic framework developed by Dr. Rao and Dr. Rajagopal also forms the basis of recent work by them concerning the modeling of shape memory alloys.

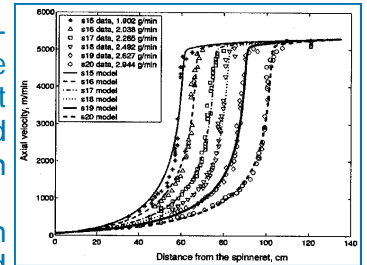


Figure 1

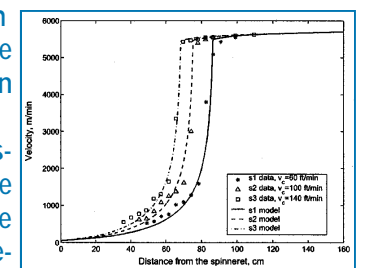


Figure 2

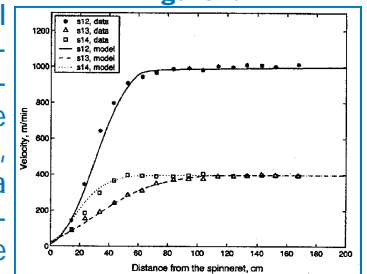
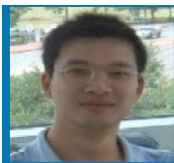


Figure 3



Dr. Han Jiang

Han Jiang is currently a PhD student in Mechanical Engineering. His dissertation work is "Experimental and numerical study of polymer scratch behavior", with an emphasis on the fundamental knowledge of damage mechanisms during the scratch process.

Mr. Jiang will officially graduate in Summer 2009 and plans to conduct his post-doc research at Texas A&M University. His research interests include structure-property relationship of polymers/composites, damage & failure analysis, tribology, finite element modeling, constitutive relationships. He is willing to be contacted for R&D related job opportunities at (979) 739-8603 or [jianghantamu@gmail.com](mailto:jianghantamu@gmail.com).

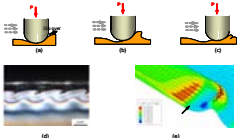


Figure 1. Fish-scale formation: (a) slipping, (b) drawing, and (c) substrate compression; (d) longitudinal-section of the fish-scale along the scratch path for TPO; (e) maximum principal stress of polymer scratch

### Three PTC students receive their Ph.D



Dr. Jia (Daniel) Liu

Dr. Jia (Daniel) Liu will officially receive his Ph.D. degree in Material Science and Engineering in May 2009. His dissertation topic is "Toughening of Epoxies Based on Self-Assembly of Nano-Sized Amphiphilic Block Copolymer Micelles." Dr. Liu is conducting his research at the Polymer Technology Center (PTC) under the supervision of Prof. Hung-Jue Sue. His research interests include polymers, composites/nanocomposites, structure-property relationship, mechanical and fracture behaviors, and polymer toughening and strengthening. Before joining PTC, Dr. Liu obtained his B.S. in Polymer Materials and Engineering from Fudan University (Shanghai, China) in 2002, and M.Phil. in Mechanical Engineering from Hong Kong University of Science and Technology (Kowloon, Hong Kong) in 2004. Dr. Liu will start working in industry in late May. His permanent email address is [danieljliu@gmail.com](mailto:danieljliu@gmail.com).



Dr. Dazhi (Peter) Sun

Howdy, my name is Dazhi Sun. I came to PTC in Fall 2005 for my Ph.D. degree. Before I joined TAMU, I received my Bachelor and Master degrees in Chemical Engineering from Tsinghua University in Beijing, China. My research here has been under the supervision of Prof. Hung-Jue Sue, and has been focused on various materials of interest in nanotechnology, including quantum dots, carbon nanotubes, and nanoplatelets. I really have enjoyed working with these fantastic materials, which are very promising in the many areas. I passed my defense in March 2009 with the dissertation topic of "Colloidal Manipulation of Nanostructures: Stable Dispersion and Self-assembly." After graduation, I will continue to pursue my research interest in colloidal nanoparticles at Brookhaven National Lab as a research associate, and I plan to work in academia for my future career. Finally, I would like to thank my advisor and PTC faculty and staff for their help throughout my Ph.D. study. They really made my time at TAMU a great experience and I am going to miss it!

**Congratulations to these students and best wishes in their future endeavors!!!**



### Multi-scale Framework for Multi-field Analyses of Smart Composites

Anastasia Muliana (Texas A&M University)  
Sponsor: Air Force Office of Scientific Research (AFOSR)

The development of smart composites offers a great potential for advancing structural health monitoring techniques, stealth and morphing aircrafts, high-speed vehicles, and many other fields. Each of the above applications could subject the composite to simultaneous mechanical loading, extreme environments, and electric fields leading to nonlinear behavior and strong coupling between various physical properties within the composite systems. Heat generation and shape changes at different rates during high-speed flight, where dynamic effect such as vibration are pronounced, cause complex multi-field responses at multiple time scales. Heterogeneities in the composites at multiple length scales, i.e., laminate, ply, and constituent phases, present discontinuities in stress, strain, temperature gradient, etc., at the interphases due to mismatches between the properties of the constituents. Current understanding of load transfer mechanisms between the active and non-active constituents and their effects on the overall responses of smart composite structures are far from satisfactory. In addition, long-term response and life prediction of smart composites under multi-field effect have not been fully explored.

This study investigates the effects of the coupled thermal, electrical, and mechanical responses, including the loading rate effect at the constituent levels, on the multi-field performance of smart composites, and develops interphase models between the active and non-active constituents that minimize stress discontinuities. Laminated composites, having flexible piezocomposite transducers with applications to multifunctional morphing structures, are studied. The flexible PZT fiber/epoxy is conformable to curved structures resulting in better morphing performances. The objectives are to build a multi-scale framework that integrates nonlinear coupled multi-field responses of the constituents to the overall behaviors of the smart composite structures and to effectively model and characterize the nonlinear properties of the constituents. Figure 1 shows the multi-scale framework. The upper level presents finite element (FE) models of structural components, i.e., morphing components. The macro-scale material determines effective properties, e.g., strength, moduli, thermal conductivity, piezoelectric constant, etc., of the smart composite systems. At the meso-scale, micromechanical models for smart fiber-reinforced composites are formulated. The micro-scale evaluates constitutive models that include mechanical, thermal, and electrical coupling effects and time-effect for the fiber and polymer matrix constituents.

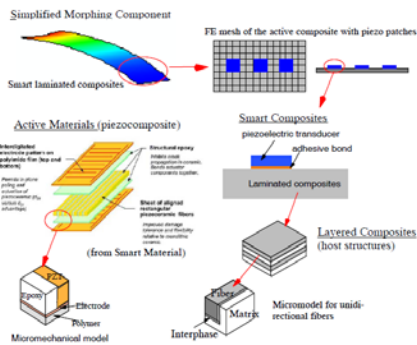


Fig. 1 A multi-scale framework of smart composite structures.

### Polymer Specialty Certificate Program Update

Since the approval of the Polymer Specialty Certificate Program in fall of 2006 and students began taking advantage of the program in spring of 2007, PTC is pleased to announce the following:

- Six students have received the Polymer Specialty Certificate to date
- Three students will be receiving a certificate in May '09
- Three new students have just enrolled

PTC is working hard in keeping students aware of the Polymer Specialty Certificate Program.

### Grunlan receives grant for flame-resistant coating



Dr. Jaime Grunlan, assistant professor in the Department of Mechanical Engineering, has received a grant worth more than \$250,000 over three years from the National Institute of Standards and Technology (NIST) Building and Fire Research Lab for flame-resistant coatings.

Grunlan, director of the Polymer Nanocomposites Lab, developed a thin film composite coating (of polymer and clay) that three-dimensionally lines the walls of a foam object and renders it flame resistant. In fabric, each thread can be individually coated with a flame retardant clay-filled thin film and still remain soft and flexible.

The proposed research, carried out by Ph.D student Yu-Chin Li and undergraduate student Jessica Schulz, seeks to understand the mechanism by which these thin nanocomposite coatings are able to render foams and fabrics flame retardant. Understanding exactly how the coating work and the variables that influence the performance of the coatings will allow for more effective protection for foams and fabrics.

"Many buildings use polyurethane foam insulation, which has been attributed to numerous fires that have cost the lives of civilians and firefighters over the years," Grunlan said. "Anti-flammable clothing, especially in children's wear, is also a challenging problem that we may have the answer to."

The researchers will also investigate combining the benefits of these unique coatings with those of other flame-retardant additives (such as metal hydroxides or boric acid) to further enhance flame suppression.



### Shinji Iio PTC's Visiting Scholar from Japan

I spent 21 months in PTC since I came from Japan to do research on nylon nanocomposites as a visiting scholar in August 2007. Although I didn't know

anything about Texas before I came, I have learned a great deal, learned new technology, honed my English skills, and have made many great friends. It was a tremendous opportunity and experience for me. I really appreciate the advice from Dr. Sue, the support from Isabel san, and the assistance of the PTC members during my research. I also want to thank my company, Tokai Rubber Industries Ltd., for sending me to PTC. I am going to continue to work on developing new materials based on the experience I have gained at PTC for both my company and myself once I return to Japan. Finally, I wish PTC continued outstanding success.

**Farewell Iio san & Best Wishes!!!**

# PTC Faculty

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## Faculty Awards

- **Dr. K.R. Rajagopal, Forsyth Chair Professor, named Regents Professor**
- **Dr. Cris Schwartz, Assistant Professor, received the Peggy L. & Charles L. Brittan '65 Teaching Award for Outstanding Undergraduate Teaching and SLATE Award for Teaching**

**Congratulations to these Professors!!!**



Dr. Donald E. Witenhafer of SPE-South Texas Section is elected into the Plastics Hall of Fame



Dr. Donald E. Witenhafer of SPE-South Texas Section has been elected to the Plastics Hall Of Fame in recognition of his pioneering technical achievements that saved the polyvinyl chloride (PVC) industry. The PVC industry was threatened when it was discovered that the vinyl chloride monomer used in making PVC is a human carcinogen and is dangerous when humans are exposed to it. Environmental groups urged the immediate ban of PVC.

At the time of the discovery, Witenhafer was a polymer scientist working for the B. F. Goodrich Company of Akron, OH, the world's largest producer of PVC resins. His research resulted in three key patented breakthroughs that were used to save the industry and protect the public. He invented steam stripping columns, which remove the dangerous residual, un-reacted, vinyl chloride monomer from the manufactured PVC resins. He also invented the first water based, absorbing, clean reactor wall coating that made it possible to run successive polymerization batches without opening the polymerization vessel. Workers no longer needed to enter the vessels to scrape polymer buildup off the walls, limiting their exposure to the dangerous monomer. He also invented a steam pressure process to apply these coating to the reactor walls.

Worldwide, almost all PVC plants today use a water based, absorbable clean reactor coating similar to that invented by Witenhafer, applied with steam pressure. In the well designed Goodrich 16,500 gallon reactors, over 700 batches are normally polymerized before the vessel is opened for cleaning. Throughout the world, steam stripping columns are used in the vast majority of PVC plants to remove the residual monomer to below one part per million. No new cases of liver cancer associated with vinyl chloride have been reported in the last 25 years. The volume of PVC resin produced in the world has tripled to about 75 billion pounds per year.

Dr Witenhafer will be installed in the Plastics Hall of Fame at the NPE 2009 meeting in Chicago on June 22, 2009.

## SPE Scholarships for 2009-2010

PTC is pleased to announce the TAMU recipients of the SPE scholarships for 2009-2010.

### SPE Henry Kahn Scholarship

- Johannes Guenther, Chemistry, research in: *"Immobilized Tridendate Phosphine Ligands on SiO<sub>2</sub>: Synthesis, Characterization and Applications in Polymerization Reactions"*

### SPE Dale Walker Memorial Scholarship

- Kevin White, Industrial Engineering, research in: *"Improvement in the Mechanical Strength and Fracture Toughness of B-Staged Epoxy/SWCNT Nanocomposite Thin Films for VARTM Application"*

### SPE Scholarships

- Geetha Pravallika Chimata, Mechanical Engineering Dept., research in: *"Injectable Biodegradable Polymer Carriers for Bone Morphogenic Proteins"*
- Jennifer A. Carvajal Diaz, Chemical Engineering, research in: *"Molecular Modeling of Polypeptide Based Materials for Biomedical and Biotechnological Applications"*
- Guanqun Wang, Material Science and Engineering, research in: *"A New Drug Delivery System of pH Sensitive Polymer with Ion-Exchanger"*



Left to right: Johannes Guenther, Chemistry Dept.; Kevin White, Industrial Eng. Dept.; Geetha Pravallika Chimata, Mechanical Engineering Dept.; Jennifer A. Carvajal Diaz, Chemical Engineering Dept.; and Guanqun Wang, Materials Science and Engineering.

**Congratulations to these students!!!**

**PTC Newsletter prepared by: Isabel Cantu  
Edited by: Adrienne O'Reilly and Kevin White**