SAND2012-1700P

Sandia National Laboratories

Project Accomplishment Summary

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Sandia National Laboratories

Operated for the U.S. Department of Energy by
Sandia Corporation
Albuquerque, New Mexico

PROJECT ACCOMPLISHMENTS SUMMARY

Cooperative Research and Development Agreement (#1640.11)

between **Sandia National Labs** and Goodyear Tire & Rubber Company

Note: This Project Accomplishments Summary will serve to meet the requirements for a final abstract and final report as specified in Article XI of the CRADA.

Title: Improved Rubber Nanofillers

Final Abstract:

During this task, Silane functionalized TiO2 and HK3Ti4O4(SiO4)3 were sent to Goodyear (GY) for testing. These materials were characterized based on their interaction with the model elastomer, squalene. The Van der Waals interactions and Hamaker Constants for ZnO particles in squalene and rubber materials were characterized and it was determined that a 10 – 20 nm spacing was necessary between primary filler particles to maintain a stable nanocomposite. Contact angle measurements on the ZnO and ZnO-silane materials indicated that the solvent should wet the particles, and solvophobic attractions should not be present. These studies showed that the surface modification with sulfosilane coupling agents was successful, and high levels of dispersion of the particles remained possible. Further, a novel surface charging phenomenon where negative surface charging is developed in the squalene environment was observed and corroborated by measurements of particle size and of the surface modified materials in squalene. This impacts the dispersion of the particles according to the traditional colloidal interpretation of electrostatic repulsive forces between particles.

Additionally, thin nanocomposite fibers were developed using electrospinning. The size and shape of the oxides did not change during the electrospinning process, although the shape of the fiber and the distribution of the particles, particularly for ZnO, was not ideal. There was an obvious increase in elastic modulus and hardness from the addition of the oxides, but differentiating the oxides, and particularly the surfactants, was difficult. The A-1289 lead to the greatest dispersion of the filler particles, while the A-1589 and the NXT produced clustered particle aggregates. This agrees with previous study of these materials in low molecular weight squalene solvent studies reported earlier. The behavior of the nanoparticle ZnO and the microparticle silica is different as well, with the ZnO being contained within the elastomer, and the SiO2 forming monolayers at the surface of the elastomer. The dynamic mechanical analysis did not show clear trends between the surface modification and the aggregate structure. In the silica particles, the NXT led to the least particle interaction, followed by the A-1289 and highest particle interaction found for the A-1589. For the nanosized ZnO, the best dispersion was found for the A-1589, with both the A-1289 and NXT exhibiting frequency dependent responses.

Background:

Samples of GY nanocomposites (natural rubber with CNT) were analyzed by Cryo-ultramicrotomy, which was evaluated as a technique to visualize and analyze the filler material. Frozen ultrathin sections are therefore the preferred method for this study. This sample was analyzed at Sandia using ADF STEM. The resulting images revealed a series of 'donuts and rods' throughout the matrix. The 'donuts' are believed to be the end of the CNTs (TEM data is 2D). The uniformity of distribution of the CNT fillers was not high.

Description:

Molecular dynamics (MD) simulations were conducted on coated nanoparticles in explicit solvents both in the bulk and at a liquid/vapor interface. These simulations were among the first ever atomistic simulations of chemically modified nanoparticles in a realistic environment. Both single nanoparticles and pairs of nanoparticles were evaluated to calculate the forces from solution and between nanoparticles. From these simulations the critical features that control the dispersion of nanoparticles in solution were determined. From measurements of both the velocity-independent (solvation) forces and velocity-dependent (lubrication) forces we are able to construct accurate and efficient coarse-grained potentials. Further, to successfully exploit the enhancement in the properties of nanocomposite materials, it was critical to understand how variations in the nanoparticle size and shape and their interaction with the matrix affect the properties of the resulting composite. It is readily apparent that the change in particle shape from spherical to jack has a dramatic effect on the shear viscosity of the suspension where the change from dot to jack affords an order of magnitude increase in the equilibrium viscosity.

Benefits to the Department of Energy:

This project started the development of an understanding of nanomaterials interactions with elastomers that can be immediately applied to solve existing SNL (i.e., NW seals, gaskets, parachutes, etc.) and future industrial problems. It will enhance SNL's existing nano synthesis/functionalization/modeling capabilities and other projects (i.e., CINT, DHS, BES) as well as involve students at all levels working on key novel problems. In addition, this program builds on existing nano-science based engineering efforts and provides future capabilities needed to support developing programs through innovative S&E solutions for sponsors of the SNL's lines of businesses and by creating or accelerating the development of the needed technical expertise for nanomaterials issues.

Economic Impact:

Polymeric nanocomposite materials promise to revolutionize the optical, electronic, catalytic, and mechanical properties of elastomeric. In particular we have focused on a multibillion dollar business, tire manufacturing whose principal business is the development, manufacture, distribution and sale of tires and related products and services worldwide. Goodyear manufactures and market numerous lines of rubber tires for: automobile, trucks, buses, aviation, motorcycles, earthmoving and mining equipment, industrial equipment, and various other applications. All improvements lend a massive impact not only in the tire industry but overall improve the efficiency of automobiles and other transportation methods.

Project Status:

The project has been completed. The results have been compiled into a more than 50 page SAND report.

ADDITIONAL INFORMATION

Laboratory/Department of Energy Facility Point of Contact for Information on Project

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Company Size and Points of Contact

Goodyear Tire & Rubber Company has approximately 70,000 employees.

Point of Contact:
Carl Pulford

CRADA Intellectual Property

The intellectual property is documented in the SAND report mentioned above.

Technology Commercialization

None

Project Examples

None

PROJECT ACCOMPLISHMENTS SUMMARY
Cooperative Research and Development Agreement (SC01/01640.11)
between **Sandia National Laboratories** and **Goodyear Tire & Rubber Company**

This summary has been approved for public release by Sandia and Goodyear Tire & Rubber Company

Sandia National Laboratories

By [signature] Date July 30, 2011
Timothy J. Boyle
Principal Investigator

Sandia National Laboratories

By [signature] Date 7/29/2011
Manager
WFO/CRADA Agreements

Goodyear Tire & Rubber Company

By [signature] Date 9/1/2011
Title:

In order to expedite the process, if we do not receive your signed reply by 09/07/2011 we will assume your concurrence for the release of this document to the public.