New technology analyzes rubber materials

By Masato Naito
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Executive summary

In order to develop the high performance tire rubber materials that will become increasingly essential in the near future, we must first return to square one and consider how rubber performance traits are manifested. Thus, it will be necessary for us to elucidate and understand the internal structures and mechanisms of rubber at the micrometer and even the nanometer scale. Sumitomo Rubber Industries Ltd. has developed our New Materials Development Technology: "Advance 4D nano design."

It makes use of the advanced technologies of the K computer and other cutting-edge equipment such as SPring-8, J-PARC in Japan, enabling the analysis of rubber chemicals at a molecular level. In this paper, some cases of development of rubber, including the development of high strength rubber to improve wear resistance using large scale simulation, will be described.

The author

Naito

Masato Naito has been involved in tire simulation and rubber material simulation research for Sumitomo Rubber Industries Inc. for more than 15 years. He is working in Research Department I as manager of the material simulation team.

Naito received his master's degree in engineering from Kobe University, Graduate School of Science and Technology in 2002 and joined Sumitomo in Kobe, Japan, in 2002. He received his doctorate in mechanical engineering from Kobe in 2008.

Naito is responsible for material simulation research to create innovative rubber materials by developing renewable polymers, new nanofillers and new additives.

Tires are extremely important automotive parts that play an essential role in the most basic functions of an automobile: supporting a vehicle's weight, in addition to driving, turning and stopping.

At the same time, as is the case with any other automotive part, there is a growing demand for tires that respond to environmental issues such as climate change and the depletion of fossil fuel resources.

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Consequently, the rapid development of high-performance rubber materials has become increasingly essential for the development of high-performance, high-quality tires that combine vehicle safety with environmental friendliness.

Thus, in 2011, Sumitomo Rubber Industries completed the development of 4D nano design (**Fig. 1**), a proprietary new materials development technology that enables us to predict accurately, and thereby freely control, the structures and properties of rubber materials so that we may design the materials needed for high-performance tires with high precision at the nanometer scale.

Since the inception of 4D nano design, we actively have been utilizing this advanced technology in the development of rubber materials for high-performance, fuel efficient tires for Falken and our other brands.

However, our automative society is changing at a rapid pace, while the performance requirements of tires continue to rise ever higher, meaning that even further advancements in rubber materials development technology now have become necessary.

In particular, there is a growing need for new technologies for the development of high-performance tire rubber materials that feature superior wear resistance in order to achieve further reductions in tire weight, thereby contributing to the global environment through improving vehicle fuel efficiency and saving rubber resources.

In response to this need, Sumitomo Rubber Industries has completed the development of advanced 4D nano design, a breakthrough new materials development technology that enables us to realize significant, simultaneous improvements in the inherently contradictory three key tire performance traits: fuel efficiency, grip performance and wear resistance.

Advanced 4D nano design accomplishes this through the coordinated utilization of the SPring-8 Large-Scale Synchrotron Radiation Facility, the J-PARC Proton Accelerator and Experimental facility and the powerful K computer in order to precisely and realistically simulate the structures and behavior of rubber at the molecular level. For reference:

- SPring-8 is the world's most powerful synchrotron radiation facility. (Location: Sayo, Hyogo, Japan)
- J-PARC is a proton accelerator and experimental facility that is used for cutting-edge research. (Location: Tokai, Ibaraki, Japan.)
- K Computer is one of the world's most powerful supercomputers in terms of processing capabilities. (Location: Kobe, Hyogo, Japan.)

Advanced 4D nano design

As indicated in **Fig. 2,** tire rubber contains many different materials in addition to its polymer framework, including reinforcing agents such as silica and carbon, additives such as oil and resin as well as sulfur crosslinking agents that link the polymer chains together.

These various materials have close, interlocking relationships that manifest themselves in the overall performance traits of a tire.

Thus, in order to develop higher performance tires, it is essential we gain a more detailed understanding of the complex relationships between rubber mate-

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Fig. 1. 4D nano design: Multi-scale simulation.

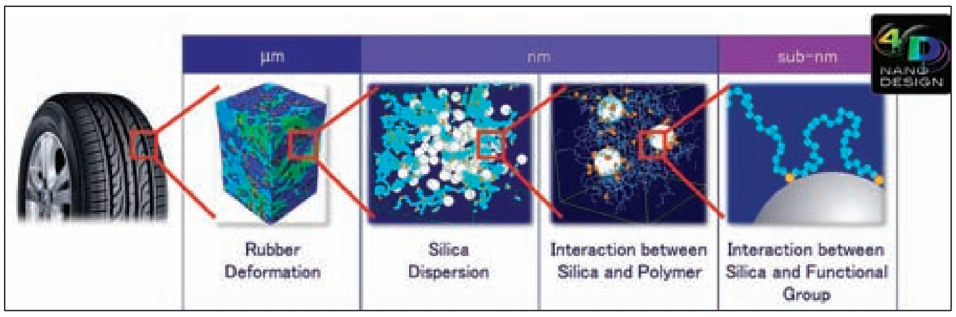
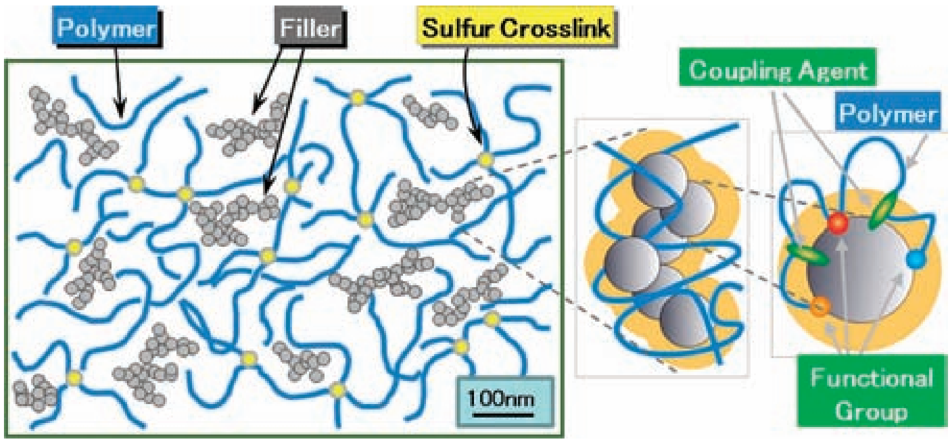


Fig. 2. Tire rubber materials.



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rials and tire performance so we may apply this knowledge for the purpose of exploiting the full performance potential of rubber materials.

While the complex interrelationships between the structures and properties of various raw materials within rubber at the nanoscale give rise to the overall performance traits of the rubber at the macro scale, breakdown phenomena in rubber are believed to originate with rupturing that occurs at the molecular level, leading to the formation of cracks that expand and eventually permeate throughout the rubber before ultimately resulting in rubber failure.

However, until now, it has been extremely difficult to conduct experimental observations of these phenomena, as they occur across a wide range of scales of magnitude.

And so we have recently developed large-scale molecular simulation technology capable of precisely analyzing molecular phenomena across multiple scales (nm~µm) while maintaining consistently high resolution, a feat made possible by the world-class computational power of the K Computer, a supercomputer operated by Riken, public research institute in Japan.

Applying this analysis technique to the observation of rubber failure has enabled us to observe, for the first time, the entire breakdown process from its origin in the formation of voids at the molecular level to the development of these voids into cracks.

We believe that the new information that we obtain on rubber wear phenomena at the molecular level using these simulations will translate into design guidelines for the development of new rubber materials that feature superior wear resistance.

One of the major challenges we faced in realizing this simulation technology was the creation of realistic simulation models that could recreate accurately everything from the behavior and interactions of the molecules surrounding the filler materials at the sub-nanometer scale to the polarization and heterogeneous structures of silica within rubber at the sub-micron scale.

Thus, we have utilized the SPring-8 Large-Scale Synchrotron Radiation facility to analyze the structures within rubber and the world class J-PARC Proton Accelerator Research Complex to analyze the behavior of rubber molecules.

By combining the capabilities of these two cutting-edge experimental facilities, we are now able to observe the internal structures and molecular behavior of rubber in greater detail than ever before and, by incorporating the analysis data obtained from these two advanced experimental facilities, we now have succeeded in creating highly realistic molecular simulation models (**Fig. 3**).

Fig. 4 is an example of one of the large scale molecular simulations we have performed. The white dots represent silica and the blue mass that makes up the remainder of the model represents polymer.

The image on the left indicates the internal state of the model on the right when it is stretched.

This simulation demonstrates that, when the rubber is stretched in a deformation mode consistent with tire wear, molecular-level breakdown occurs in the areas surrounding the filler material, leading to the formation of voids within in the polymer.

Fig. 5 includes an observational image, produced using our newly developed X-ray CT scanning technology, of the internal state of a block of actual rubber that has been stretched in the same deformation mode as tire rubber during wear, as well as the results of a large-scale molecular simulation conducted using the model described above, presented at three progressive levels of magnification and with the voids colored black for ease of recognition.

Conventional X-ray CT imagery is only able to observe the three dimensional structures of objects that are at rest.

However, utilizing the high intensity X-rays produced by SPring-8, we have developed a new technique, called 4-dimensional X-Ray CT (4D-CT), that enables us to perform three dimensional observation of rubber as it is being deformed.

In experiments conducted using 4D-CT, we observed the formation of voids within actual rubber during wear, which occurred in a manner consistent with the results of our simulations.

Furthermore, detailed analysis of the results of our large-scale molecular simulations revealed that these voids form due to the detachment of the polymer at the molecular interface between the polymer and silica.

We believe that these simulation results represent the first ever successful

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Fig. 3. Development of high resolution simulation models.

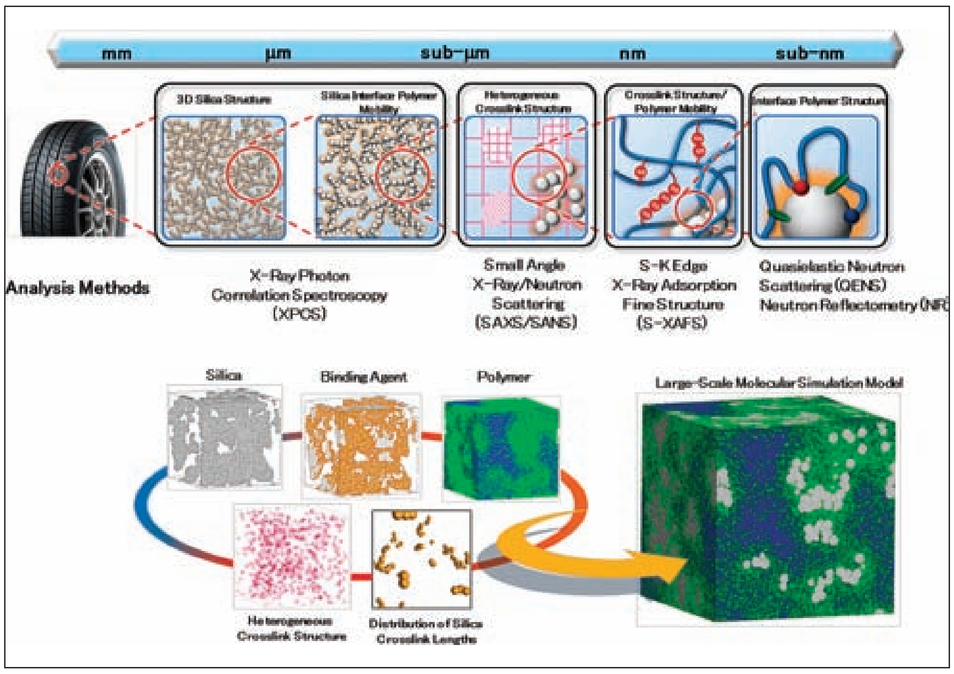
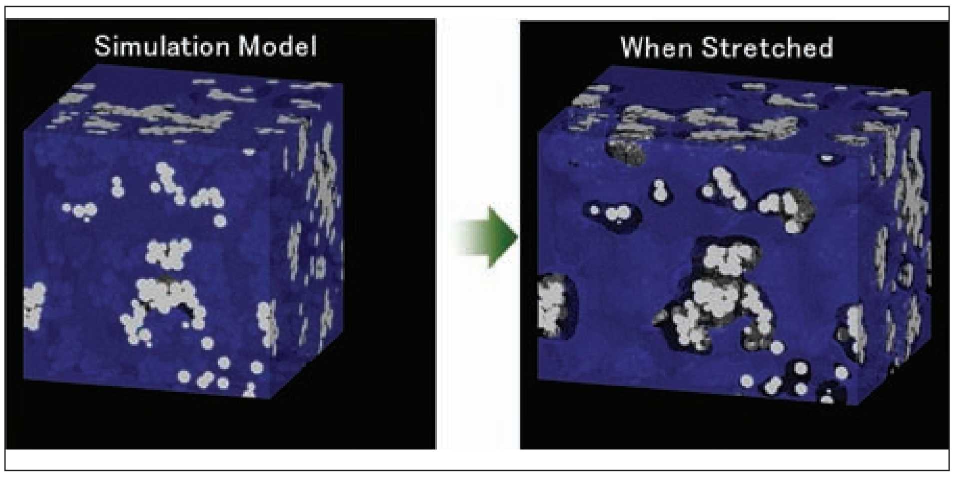


Fig. 4. Large-scale molecular simulation.



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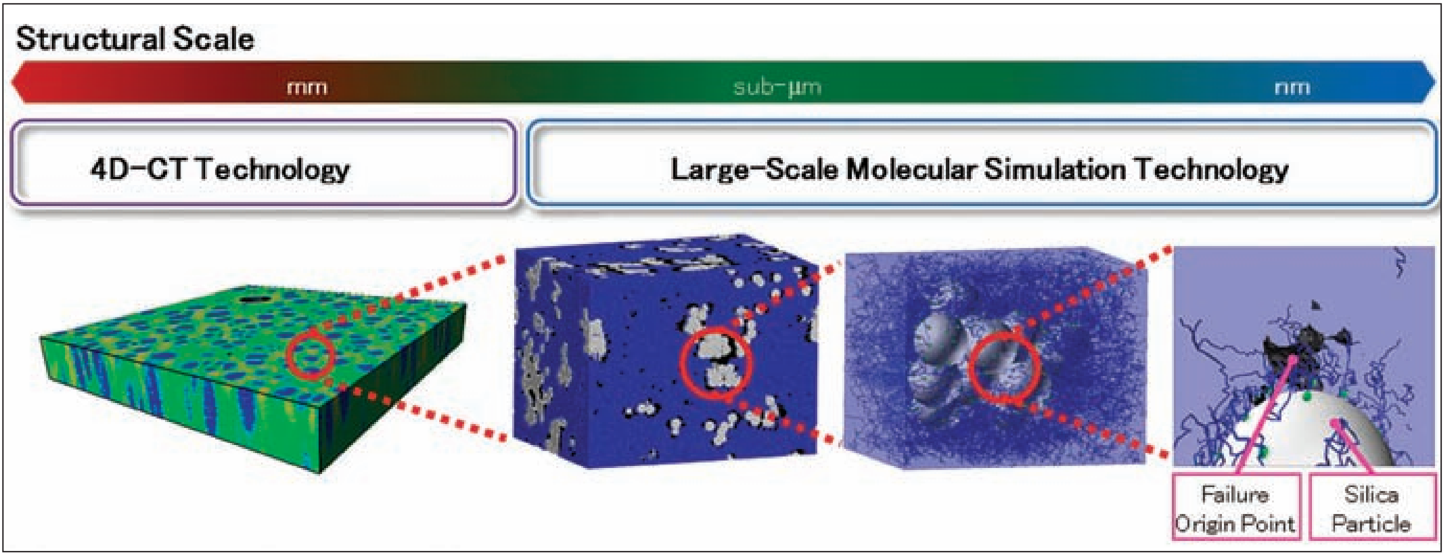
attempt at visualizing rubber failure phenomena at the molecular level, which is the elementary process behind the wear phenomena that cause a tire to wear away at the macro level.

In the future, we believe further use of the techniques described above will enable us to design, for example, new types of synthetic rubber or additives that impede and reduce the formation of voids at the interface between polymer and silica, thereby allowing us to achieve significant improvements in tire wear resistance.

Fig. 5 Visualization of breakdown occuring within rubber.



Conclusion

With the aim of responding to the increasingly high and diverse performance requirements of modern tires by developing higher performance rubber materials, we have developed advanced 4D nano design, an innovative new materials development technology that combines advanced experimental facilities with cutting-edge simulation techniques to simulate and analyze rubber precisely at the molecular level.

It thus enables us to achieve significant, simultaneous improvements in all three of the inherently contradictory key performance traits of tires: fuel efficiency, grip performance and wear resistance.

This advanced technology already is bearing fruit in terms of new rubber materials development: Sumitomo Rubber Industries already has succeeded in the development of tire tread rubber that achieves 200 percent wear resistance compared to the tread rubber used in our company's tires in 2011.

We unveiled a prototype tire featuring this new and improved tread rubber at the 2015 Tokyo Motor Show.

In the future, we plan to adopt the new materials we have developed using advanced 4D nano design in mass-produced products while also continuing to utilize this technology in the development of various new materials for high performance tires.

Collaborating organizations

Large-Scale Synchrotron Radiation Facility SPring-8.

Proton Accelerator & Experimental Facility J-PARC.

Riken Advanced Institute for Computational Science (K Computer).

High Energy Accelerator Research Organization Institute of Materials Structure Science.

Frontier Soft-Material Beamline (FSBL) Consortium.

University of Hyogo Institute for Research Promotion and Collaboration, Synchrotron Radiation Research Center.

JSOL Corp.

Joint R&D collaborators

Professor Yoshiyuki Amemiya and Assistant Professor Yuya Shinohara, Tokyo University Graduate School of Frontier Sciences.

Professor Yuichi Masubuchi, Nagoya University National Composite Center.

Associate Professor Tadanori Koga, Stony Brook University.

Participating/collaborating projects

Photon and Quantum Basic Research Coordinated Development Program.

West Pharmaceutical executive gets award

EXTON, Pa.—Karen Flynn, West Pharmaceutical Services Inc. senior vice president and chief commercial officer, has won a Stevie Award.

Flynn heads the global Commercial Team and works to drive growth across three major markets: Biologics, Generics and Pharma. She was announced as the Silver Stevie Award in New York recently. She received the honor in the Female Executive of the Year—Business Products—More than 2,500 employees category.

"I am honored and humbled to be in the company of such dynamic female executives," Flynn said in a statement. "It has been my fortune to work for West, a company that shares my commitment to championing the accomplishments of women within the organization and ensuring they are in a position to succeed. The end result is a more richly talented company that is better positioned to improve health care for patients around the world."

Flynn is active in the community, serving on the Board of the Directors for the Chester County Economic Development Council and the Advisory Board for Downingtown STEM Academy, a Pennsylvania school for students pursuing science- and technology-focused education.

The Stevie Awards for Women in Business are recognized as one of the top honors for female entrepreneurs, executives and employees. Nominations are submitted by individuals and organizations worldwide.

The 2016 awards submissions included entries from 31 nations and territories.

The Exton-headquartered West Pharmaceutical is a manufacturer of packaging components and delivery systems for injectable drugs and health care products. West recorded sales of $1.4 billion in 2015, the company said in a news release, adding that 110 million of its components and devices were used by patients around the world that year.