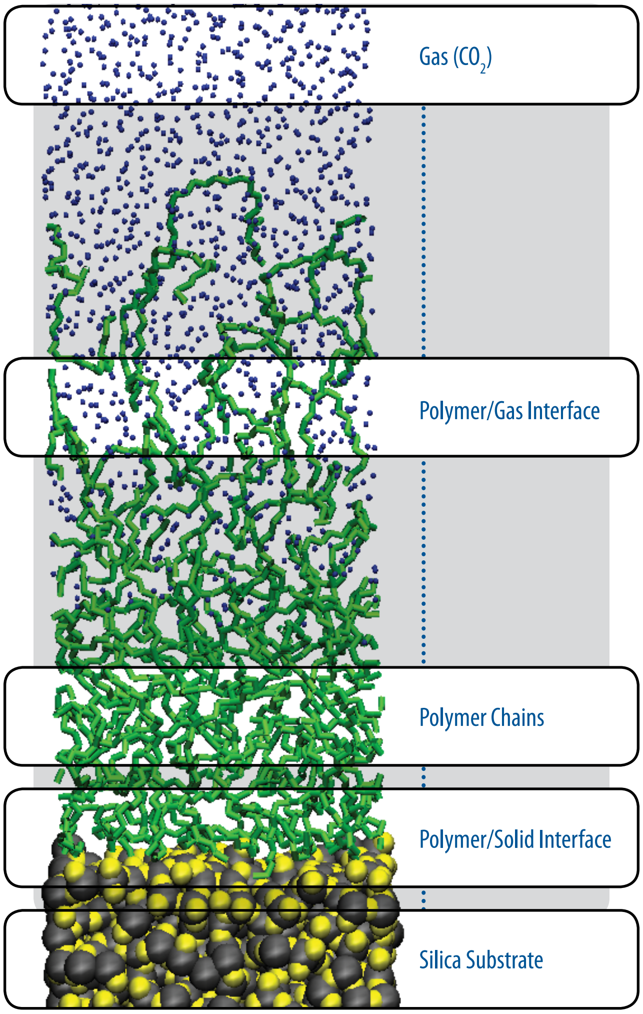
Understanding materials at the nanostructure level



above: Conducting research at the molecular level, OSU's Somnath Ghosh, Ph.D., uses the Ohio Supercomputer Center to create computer simulations such as this model of polystyrene-based polymer nanocomposite, with silica as a substrate. Carbon dioxide serves as a pressure-applying agent on polymer thin film. This modeling will help empower the design of nanosubstrates for use in biomedical devices.

Somnath Ghosh, Ph.D., a professor of mechanical engineering and materials science and engineering at The Ohio State University, believes that to develop new materials, it is paramount for researchers to understand material characteristics at the atomic level, especially when designing and fabricating nanostructures.

Recently, the Ohio Supercomputer Center awarded him 400,000 resource units to develop molecular dynamics based models that simulate polymer nanocomposites and polystyrene thin-films. Jim Giuliani, client and technology support manager at OSC, helped install and configure the project's required software.

"Because of the extremely small size of nanostructures — often smaller than one millionth of a millimeter — we can't conduct ordinary experimental observations," Dr. Ghosh said. "So to study and understand how the material behaves at these infinitesimally small scales, we must rely on molecular modeling simulations. The key to material modeling and design is to understand the structure, dynamical characteristics and response of the material under different external stimulus."

In particular, Dr. Ghosh and his team will use the modeling simulations to estimate how material of different dimensions behaves at different pressures and temperatures. Of particular interest is the glass transition temperature, the temperature at which a polymer changes from a liquid to a solid state.

"There is strong experimental evidence that properties of polymer thin-films are remarkably different from their respective bulk properties. One of our objectives is to capture this difference," Dr. Ghosh said.

Additionally, they will be investigating liquid carbon dioxide's effect on the thin-film's mechanical behavior, as the amount of carbon dioxide added to the polymer's manufacturing process affects the final product. They are developing a molecular model of a three-phase material (substrate-polymer-gas), which will help to analyze future products and applications, especially in drug delivery systems. They also will be devising strategies for faster models that can depict larger, more realistic systems.

"These models can be used as specific design tools to achieve desired properties in thin-film polymer nano-composites for nanodevices," said Dr. Ghosh. "But, universally, they also will enable the development of new or improved materials for a variety of commercial applications." ■

Project lead:
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