Lacks increasing fundamental **understanding of disordered systems**

Over time, the properties of polymer materials slowly change through a process known as aging. Aging can cause changes in volume, which may lead to cracks in a material, and alter mechanical properties, making it more brittle. Thus, aging can seriously impact the performance of polymer products used in a wide range of applications. While the effects of aging are often laboratory-tested in "accelerated-aging environments" (e.g., higher temperatures), extrapolation of results from accelerated aging environments to ordinary environments is not straightforward.

Daniel J. Lacks, Ph.D., a professor of chemical engineering at Case Western Reserve University, is employing Ohio Supercomputer Center systems to better understand the aging process at the molecular level. His research team is focusing on the interplay between aging and mechanical deformation: how aging alters mechanical deformation and, in turn, how mechanical deformation alters the aging process.

"We are using molecular simulations to elucidate unresolved theoretical issues associated with the mechanical response of disordered systems," Lacks said. *"The project is motivated by a set of recent experimental results that are not fully understood; the simulations address the same systems studied in the experimental investigations, and are being carried out with realistic potential functions to allow meaningful comparison with experimental results."*

The project will have three thrusts: the interplay of physical aging and mechanical deformation; the effects of nanoscale structure on the mechanical properties of disordered materials; and the impact of disorder on the mechanical properties of crystalline materials.

"We are conducting molecular dynamics (MD) simulations that impose a step change in strain on a polystyrene material and then monitor the time dependence of the relevant stress," Lacks explained. *"Additionally, we are conducting MD simulations of polystyrene to elucidate the interplay between aging and mechanical deformation."*

Lacks and Greg Chung, a Case doctoral student on Lacks' team, plan to leverage the findings to advance the understanding of disordered systems in general. The results for the specific materials will be used to enhance theoretical frameworks – the unusual and unexplained nature of the motivating experimental observations suggests that there are interesting theoretical underpinnings that are likely to have implications beyond these particular materials.

"The project has the potential to benefit society by enhancing the understanding of fundamental scientific phenomena, which can lead to improved technology," Lacks said. *"The findings might help facilitate the design of materials with superior aging properties, the development of applications for nanoporous materials and the use of these materials in novel applications."*

Project lead: Daniel J. Lacks, Case Western Reserve University

Research title: Molecular dynamics simulation of the aging and mechanical response of polymer materials

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Web site: www.case.edu/cse/eche/faculty_Lacks.html

left: In comparison to a new polymethylmethacrylate wine glass (left), a six-month-old wineglass (right) demonstrates volume contraction associated with physical aging (Kotlewski and Picken, unpublished). Case Western Reserve's Daniel Lacks is using Ohio Supercomputer Center systems to focus on the interplay between aging and mechanical deformation: how aging alters mechanical deformation, and, in turn, how mechanical deformation alters the aging process.