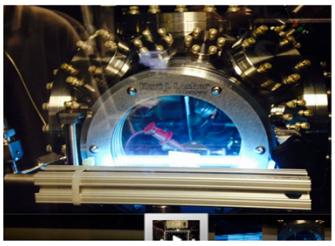
In-situ Environment Shines Light and Neutrons on Structure–Function Evolution of Polymers



ORNL's in situ multimodal test chamber tracks molecular dynamics in solutions as well as solids.

Herath et al., *Scientific Reports* 5, 13407 (2015) DOI:10.1038/srep13407, and Zhu et al., *Nanoscale* 7, 15134 (2015) DOI: 10.1039/C5NR02037a

Work was performed at the Center for Nanophase Materials Sciences and the Spallation Neutron Source, both at ORNL, and the Advanced Photon Source at Argonne National Laboratory.

Scientific Achievement

A unique environmental chamber enables a new level of manipulation of polymers in solution and in thin films, and used it to explore structure and function of materials while they were being made ("in situ").

Significance and Impact

The new capability aids understanding and prediction of structure, dynamics and function of soft matter from single molecules to mesoscale assemblies.

Research Details

- **Environment** allows control of temperature, pressure, humidity, light, compositions of vapors and solvents, and more.
- **Measurements** are made with several probing modes simultaneously (e.g., neutron, optical, electrical, magnetic) and direct feedback to data analytics and advanced simulations.
- **In situ analysis** led to high-impact papers about bottom-up and top-down manipulations of photovoltaic materials—assembly of a polymer in aqueous solution into functional structures and performance improvement of a solid via an additive, respectively.

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Researchers developed a sample environment where neutron and optical probes worked in concert to track molecular dynamics in solution[a] and in thin films[b]. They used their new capability—in situ multimodal interrogation of structures and functions—to make discoveries likely to improve photovoltaic materials, including assembling a polymer into functional structures in aqueous solution using a detergent-like molecule as a template and improving a solid's performance via an additive.

Once placed in the test chamber, a sample can be transported to different instruments for measurements. The chamber has a transparent face to allow entry of laser beams to probe materials. Probing modes include neutrons, X-rays, photons, electrical charge, magnetic spin, and calculations aided by high-performance computing; they can operate simultaneously to characterize matter under a broad range of conditions. The chamber can track molecules under changing temperature, pressure, humidity, light, solvent composition, etc. It extends the probing of materials from typical environments under resting conditions to operating environments that allow scientists to assess how working materials change over time and explore ways to improve their performance.

References

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[1] Center for Nanophase Materials Sciences, ORNL; [2] Biology and Soft Matter Division, ORNL; 3 Computer Science and Mathematics Division, ORNL; [4] Integrated Materials Design Centre, School of Chemical Engineering, UNSW Australia
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2. "Peculiarity of Two Thermodynamically-Stable Morphologies and Their Impact on the Efficiency of Small Molecule Bulk Heterojunction Solar Cells"
Nuradhika Herath,[1] Sanjib Das,[2] Jong Keum,[3] Jiahua Zhu,[3] Rajeev Kumar,[3,5] Ilia Ivanov,[3] Bobby Sumpter,[3,5] James Browning,[4] Kai Xiao,[3] Gong Gu,[2] Pooran Joshi,[6] Sean Smith,[7] Valeria Lauter[1]
[1] Quantum Condensed Matter Division, ORNL; 2 Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville; [3] Center for Nanophase Materials Sciences, ORNL; [4] Chemical and Engineering Materials Division, ORNL; [5] Computer Science and Mathematics Division, ORNL; [6] Materials Science and Technology Division, ORNL; [7] School of Chemical Engineering, UNSW Australia
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