

Mechanical Engineering Doctoral Defense

Investigation of the High Pressure Atomic-Level Response of Aromatic Polymers via In Situ Energy Dispersive X-ray Diffraction Experiments

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Abstract

Aromatic polymers, with benzene-like rings in their main chains, include materials such as polyurea, an amorphous elastomer capable of dissipating large amounts of energy under dynamic loading, which makes it a promising coating for defensive systems. Although computational research exists that investigates the atomic-level response of polyurea and other amorphous aromatic polymers to extreme conditions, there is little experimental work to validate these models 1) at the atomic-scale and 2) under high pressures characteristic of extreme dynamic loading. Understanding structure-property relationships at the atomic-level is important for polymers, considering many of them undergo pressure and temperature-induced structural transformations, which must be understood to formulate accurate predictive models.

This work aims to gain a deeper understanding of the high-pressure structural response of aromatic polymers at the atomic-level, with emphasis into the mechanisms associated with high-pressure transformations. Hence, atomic-level structural data at high pressures was obtained in situ via multiangle energy dispersive X-ray diffraction (EDXD) experiments at the Advanced Photon Source (APS) for polyurea and another amorphous aromatic polymer, polysulfone, chosen as a reference due to its relatively simple structure. Pressures up to 6 GPa were applied using a Paris Edinburg (PE) hydraulic press at room temperature. Select polyurea samples were also heated to 277 °C at 6 GPa. The resulting structure factors and pair distribution functions, along with molecular dynamics simulations of polyurea provided by collaborators, suggest that the structures of both polymers are stable up to 6 GPa, aside from reductions in free-volume between polymer backbones.

As higher pressures ($\lesssim 30$ GPa) were applied using diamond anvils in combination with the PE press, indications of structural transformations were observed in both polymers that appear similar in nature to the sp^2 - sp^3 hybridization in compressed carbon. The transformation occurs gradually up to at least ~ 26 GPa in PSF, while it does not progress past ~ 15 GPa in polyurea. The changes are largely reversible, especially in polysulfone, consistent with pressure-driven, reversible graphite-diamond transformations in the absence of applied temperature. These results constitute some of the first in situ observations of the mechanisms that drive pressure-induced structural transformations in aromatic polymers.

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Zoom Link: <https://asu.zoom.us/j/85063862999>