Structural Evolution of Polyurea under Hydrostatic Pressure in a DAC

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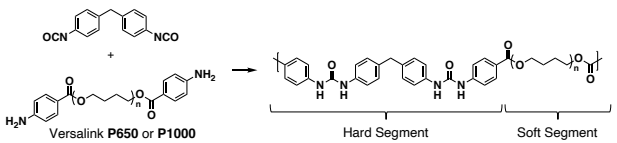
FOCUSING ON THE FUTURE

Polyurea (PU): Strong, Tough, and Healable

Structure, Applications, and Challenges

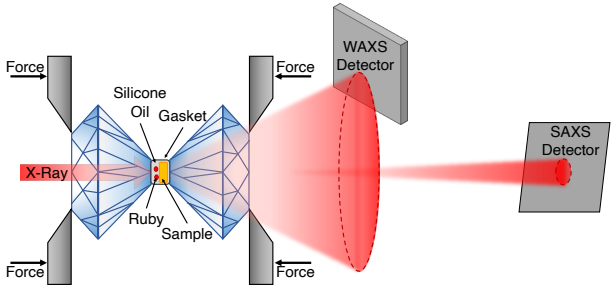


- Greatly enhance blast and ballistic response
- Design is largely trial and error

Grand Challenge: *Elucidate the structure of PU under hydrostatic pressure and determine the role of the soft segment length*

Experimental Setup

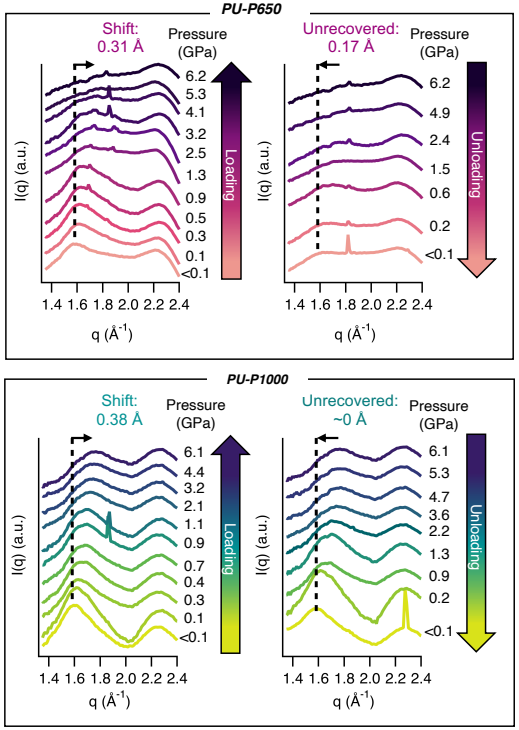
High-Pressure SAXS/WAXS of PU



- Pressure in DAC monitored using ruby fluorimetry
- Two PU samples:
- PU-P650 & PU-P1000

Influence of Soft Segment Length

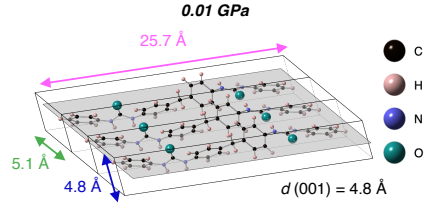
Deformation and Recovery of the Crystalline Structure



- Primary WAXS peak (q*) shifts toward higher q with loading and at least partially recovers to its original position with unloading
- Persistence and recovery of q* peak differ between PU-P650 & PU-P1000

Molecular Dynamics Simulations

Justification for the Shift in the Primary WAXS Peak



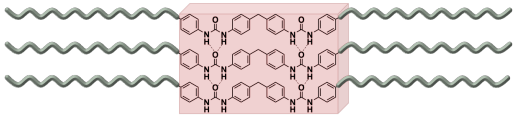
Pressure ↑

d (001) ↓

Pressure (GPa)	*d* (001) (Å)
0.5	4.74
1.0	4.72
1.5	4.69
2.0	4.66
2.5	4.63
3.0	4.60

- Unit cell contracts as pressure increases

Conclusions



- Soft segment length influences structural evolution
- Deformation is at least partially reversible
- MD simulations support experimental findings

Acknowledgements

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References: Barsoum, R. G. Elastomeric Polymers with High Rate Sensitivity: Applications in Blast, Shockwave, and Penetration Mechanics; William Andrew: Waltham, Ma, **2015**; *Macromolecules* **2008**, *41*, 7543; *Polymer* **2014**, *55*, 1883; *Polymer* **2013**, *54*, 901.