Optimization of Compression Cell Geometry to Maximize Pressure Generation in Elastomers During Total Scattering Experiments via Finite Elements

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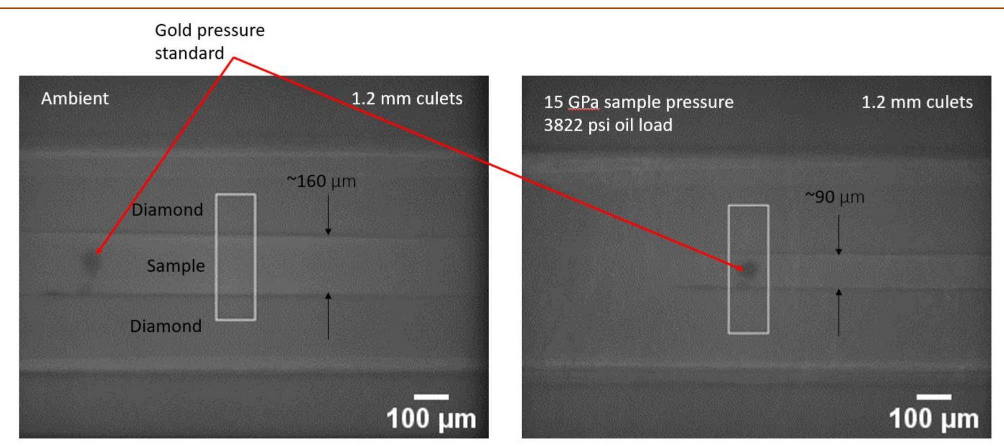
Background and Introduction

- Polyurea is an elastomer that has shown unique properties under large compressive stresses indicating that it could be a promising armor coating material
- Understanding the structure of polyurea under high pressure conditions is important to design effective polyurea coatings
- To do this, Professor Pedro Peralta's research team recently attempted to use X-ray diffraction experiments to characterize the atomic structure of polyurea under high stress



- Pressure generation for the sample was limited to 10 GPa (well below the desired pressure of 30 GPa) and the hypothesis is that this limitation is the result of the pressure cell's geometry
- The research question that this project seeks to address is: what are the optimal geometries for the aluminum gasket, diamond anvils, and polyurea sample?

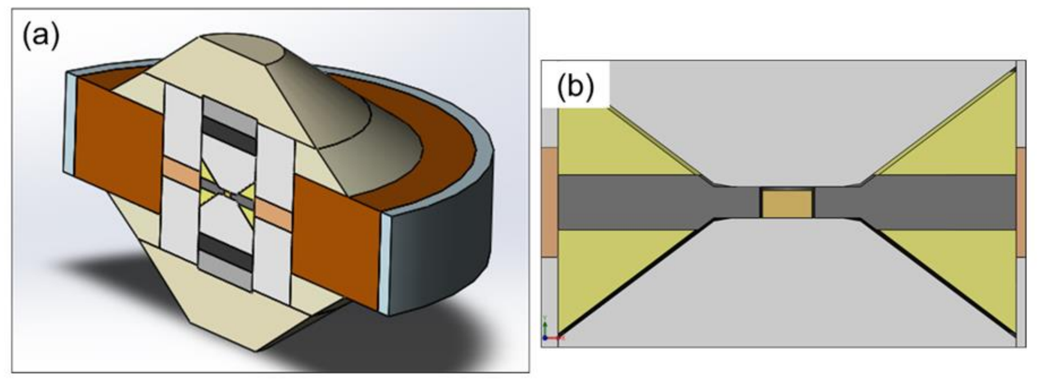
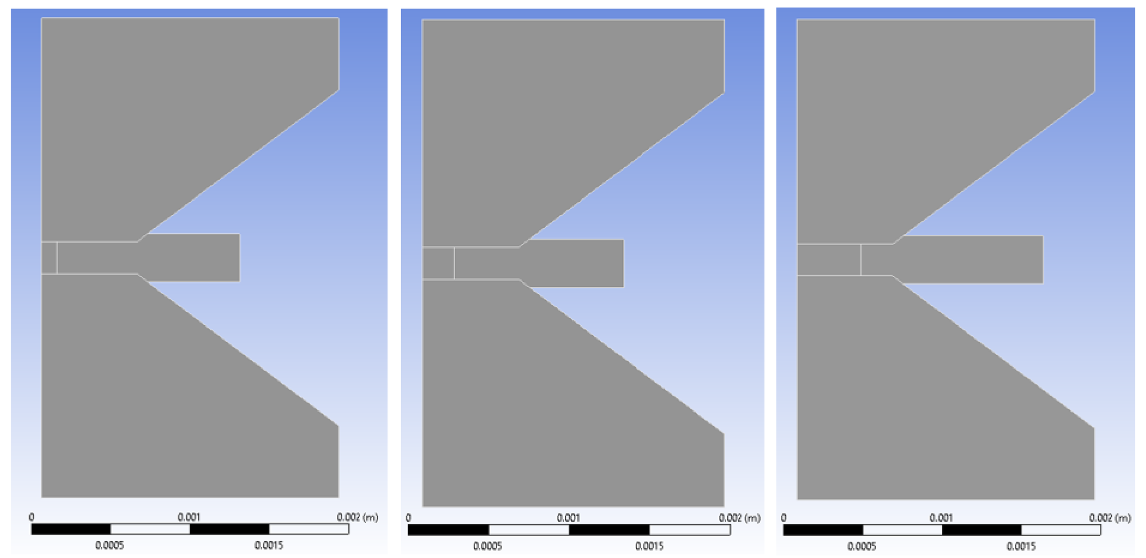


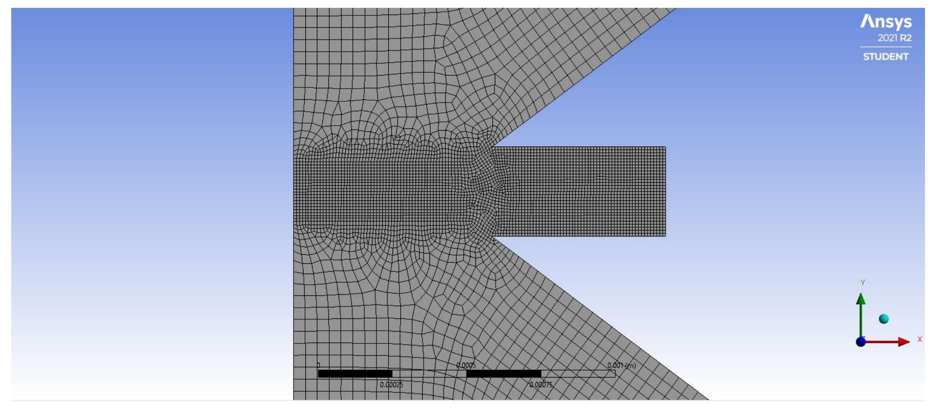
Figure 1: (a) Double-stage high pressure sample holder and (b) close up of the polyurea sample inside of the aluminum gasket between two diamond anvils.

Ansys Simulations of High-Pressure Cell

- In order to determine the optimal geometries for these components in the pressure cell, finite element analysis simulations were performed using Ansys software
- Because of the polar geometry of the High-Pressure Cell, axisymmetric analysis was performed on a 2-D cross section of these components in the cell

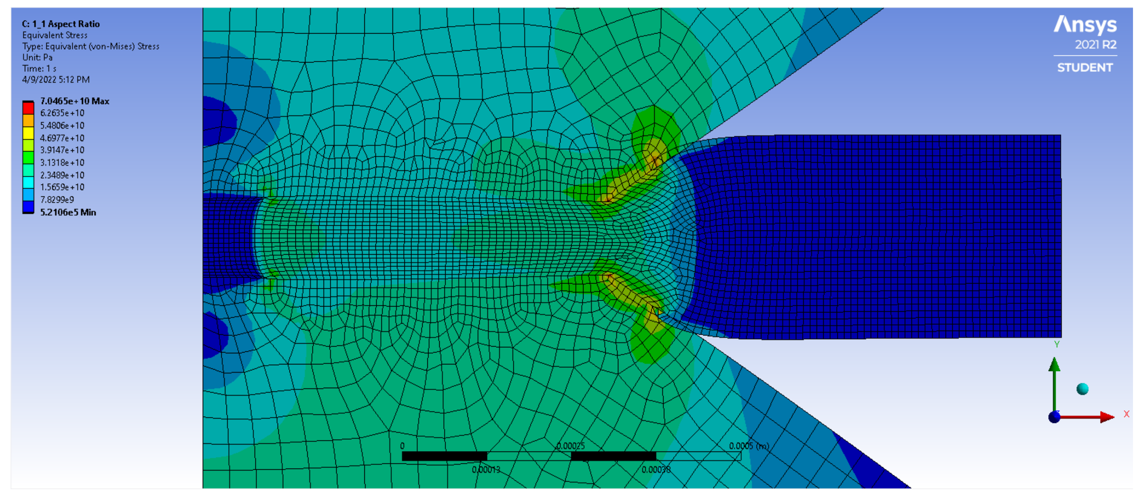


- Three different aspect ratios for the sample size in the pressure cell were simulated (1:1, 1:2, and 1:4 shown respectively above)
- These aspect ratios were based on sample height and sample diameter



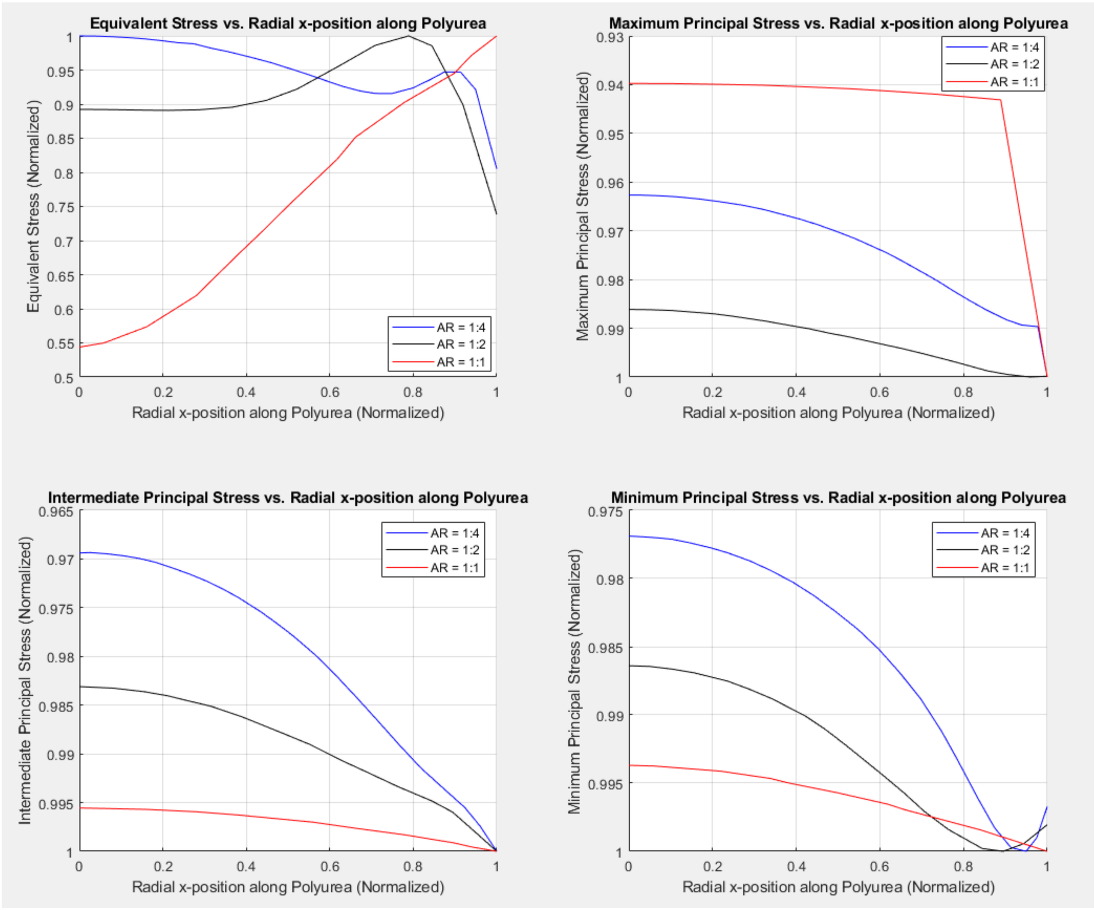
Simulation Results

- Ansys solutions calculated the deformation, equivalent von mises, max principal, intermediate principal, and min principal stress and strain contours



Data Analysis

- The stress as a function of radial x-position from the center to the outer edge of the polyurea is of interest for each of the aspect ratios



Conclusions

- The stress vs. position plots closely resemble some of the experimental results obtain from the 1:4 aspect ratio cells tested at the synchrotron
- Hydrostatic stress is preferable to avoid shearing in the sample during experiments
- An aspect ratio of 1:1 appears to avoid shearing the best out of all the aspect ratios based on the equivalent stress plot

Future Work

- Further experiments with an aspect ratio of 1:1 will hopefully be performed at the synchrotron
- Understanding how the polyurea molecules arrange themselves at high pressure will allow us to figure how to develop the armor coating in the future

Acknowledgements

I would like to thank Dr. Pedro Peralta for mentoring me and giving me the opportunity to help work on this research project. I would also like to thank Tyler Eastmond, a PhD student in Dr. Peralta's research team, for his support throughout the research process. I want thank the Fulton Undergraduate Research Initiative for their funding of the project and support throughout the semester.

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