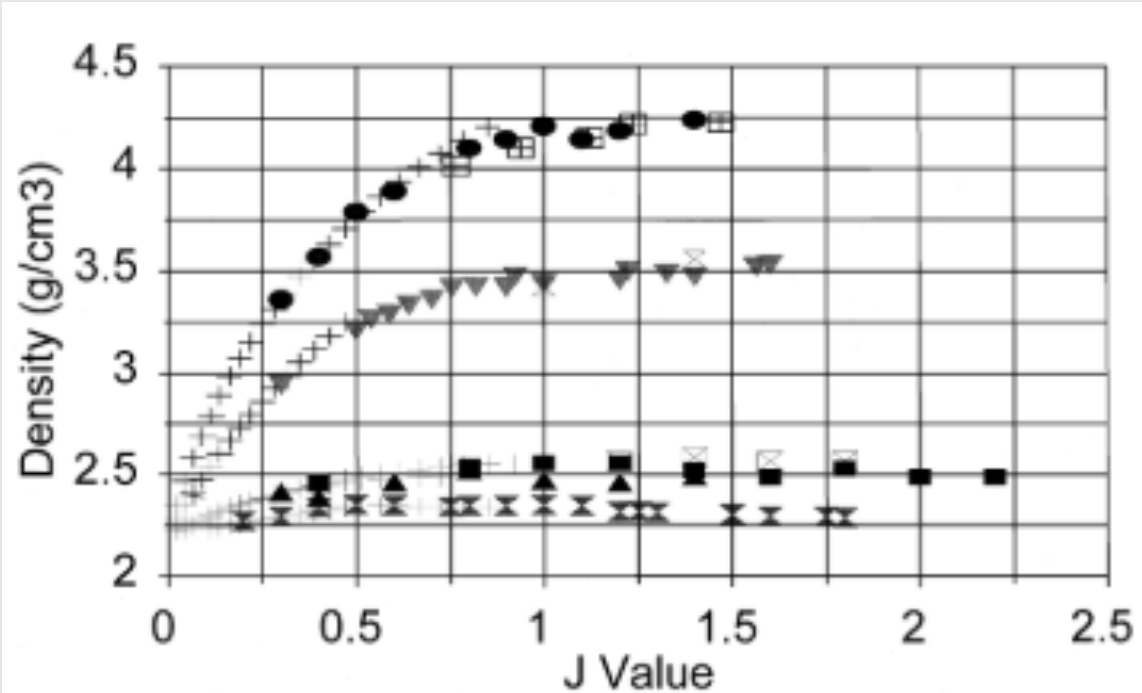# A New Structural Model for Alkali Germanate Glasses
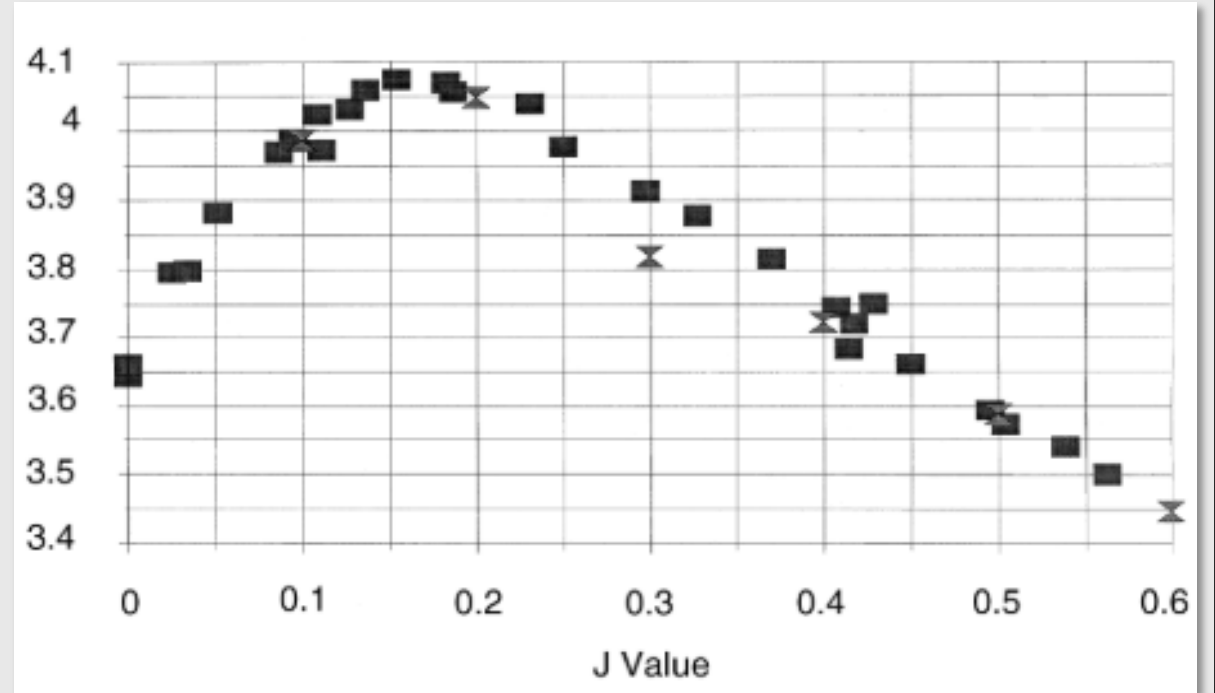
Rebecca Welch[1], Collin Wilkinson[2], Yueh-Ting Shih[3], Mikkel Bødker[4], Anthony DeCeanne[2], Morten Smedskjaer[4], Liping Huang[3], Mario Affatigato[1], Steve Feller[1], John Mauro[2]

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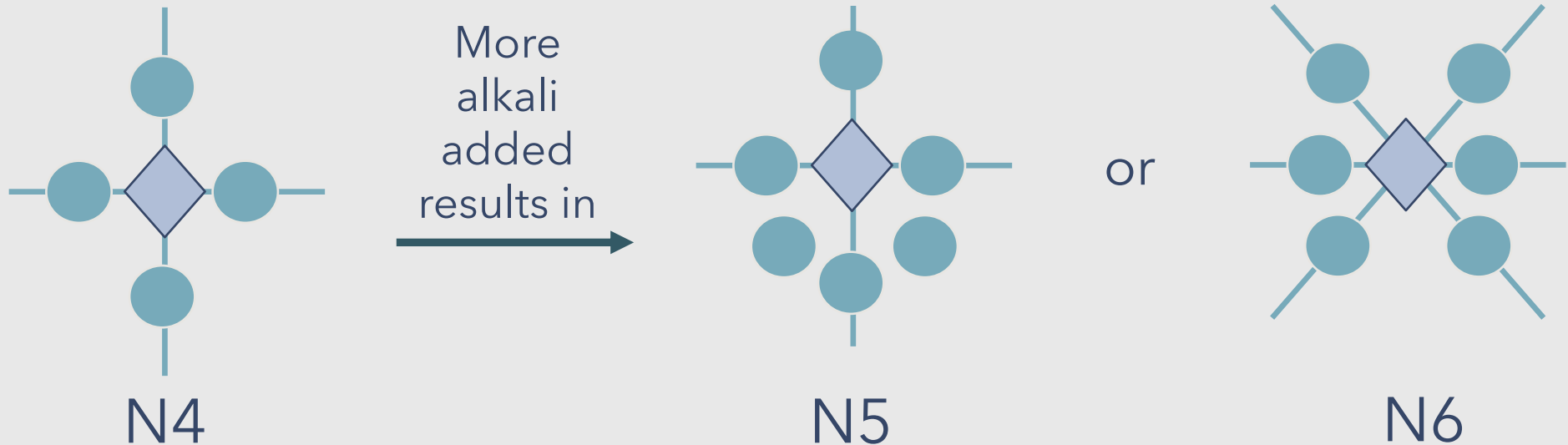
The Anomaly in Germanate Glasses

A) Monotonical trend observed in silicate glasses with added alkali.
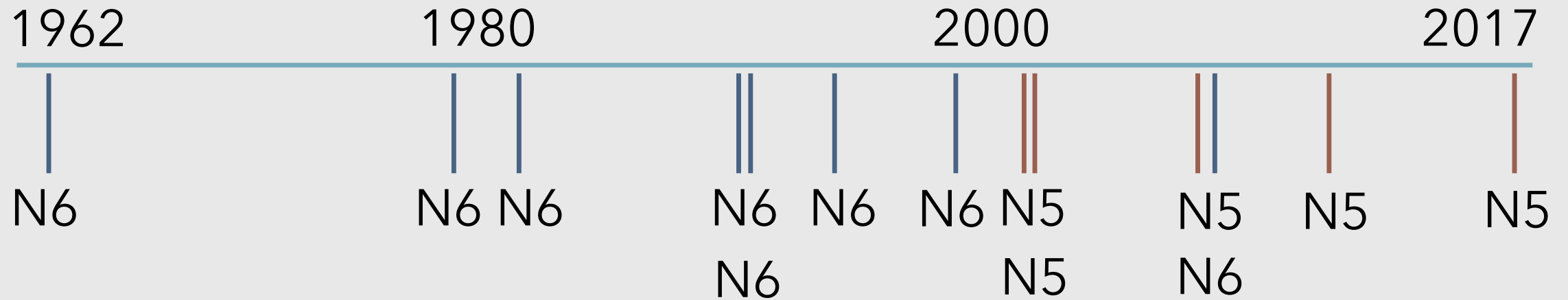
B) Anomalous trend observed in germanate glasses with added alkali.

The Anomaly in Germanate Glasses

❖ The anomaly is thought to be caused by the changes in the glass structure

❖ The germanium unit is four-fold coordinated, but changes with added alkali

❖ The new coordination is thought to be either five or six-fold coordinated

More alkali added results in

or

N4

N5

N6

Consensus on the Structure

1962   1980   2000   2017

N6   N6 N6   N6   N6   N6 N5   N5   N5   N5

N6   N5   N6

In the literature, many theories have suggested the existence of the N6 unit or the N5 unit. However, throughout the years, there has not been a solid agreement on which unit exists since experimental techniques are unable to detect either unit.

Proposed Method

Purpose

Try to understand what causes the the anomaly using Topological Constraint Theory.
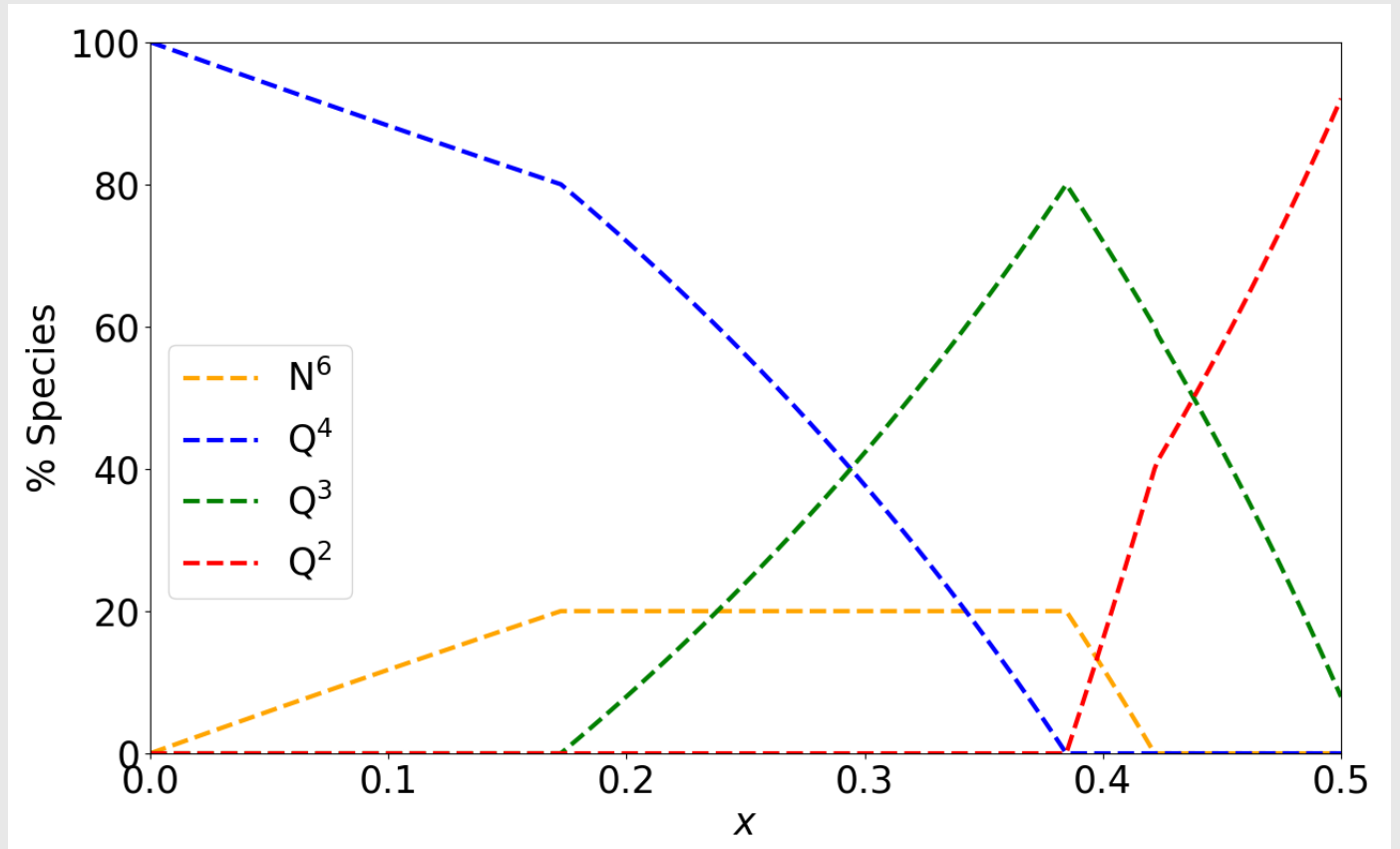
Method

1. Recreate the structure of alkali germanate glasses using statistical mechanics theory of glass formation.
2. Input the structure into Topological Constraint Theory
3. Recreate measurable glass properties such as the glass transition, elastic modulus, and fragility.

Statistical Mechanics

❖ Since experimental techniques are unable to capture the N5 or N6 unit, we must use modeling techniques such as statistical mechanics.

❖ Can be used to recreate the structure of a glass using physical parameters and probabilities.

Calculated Structure

The structure of a rubidium germanate glass created using statistical mechanics. We propose that the N6 unit exists in the glass, but topological constraint theory will determine if this is correct.
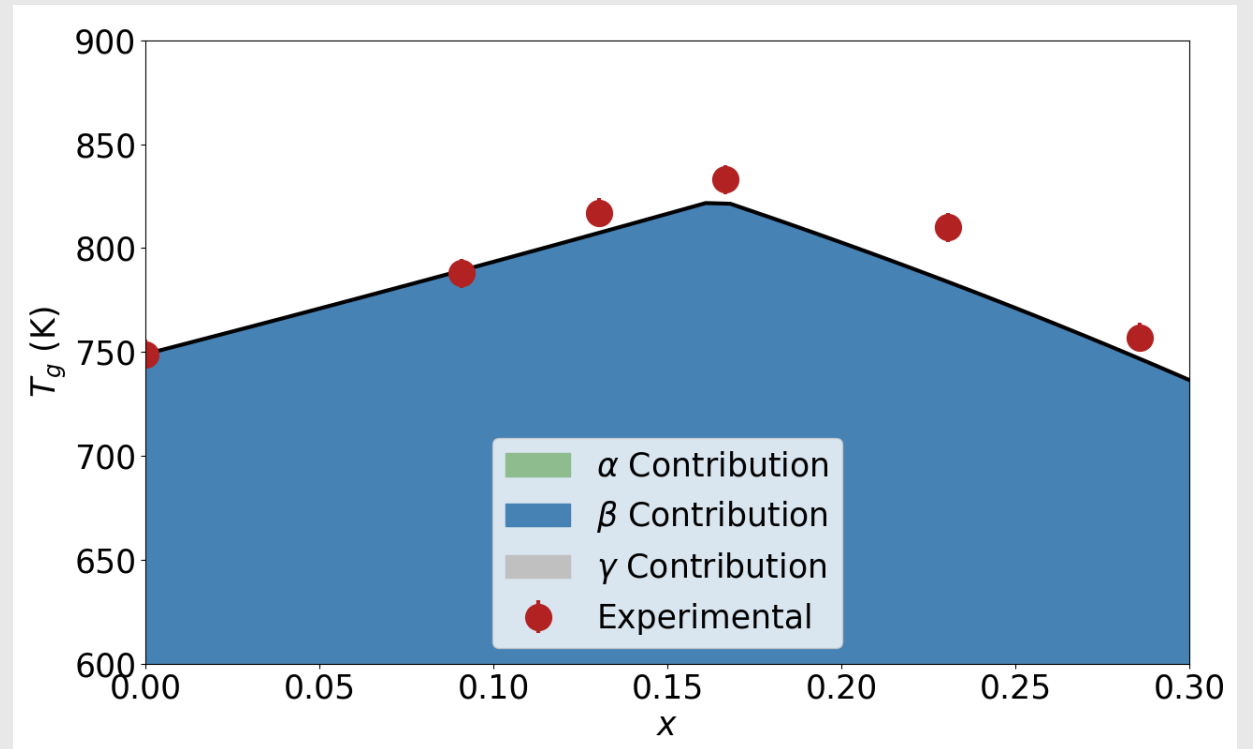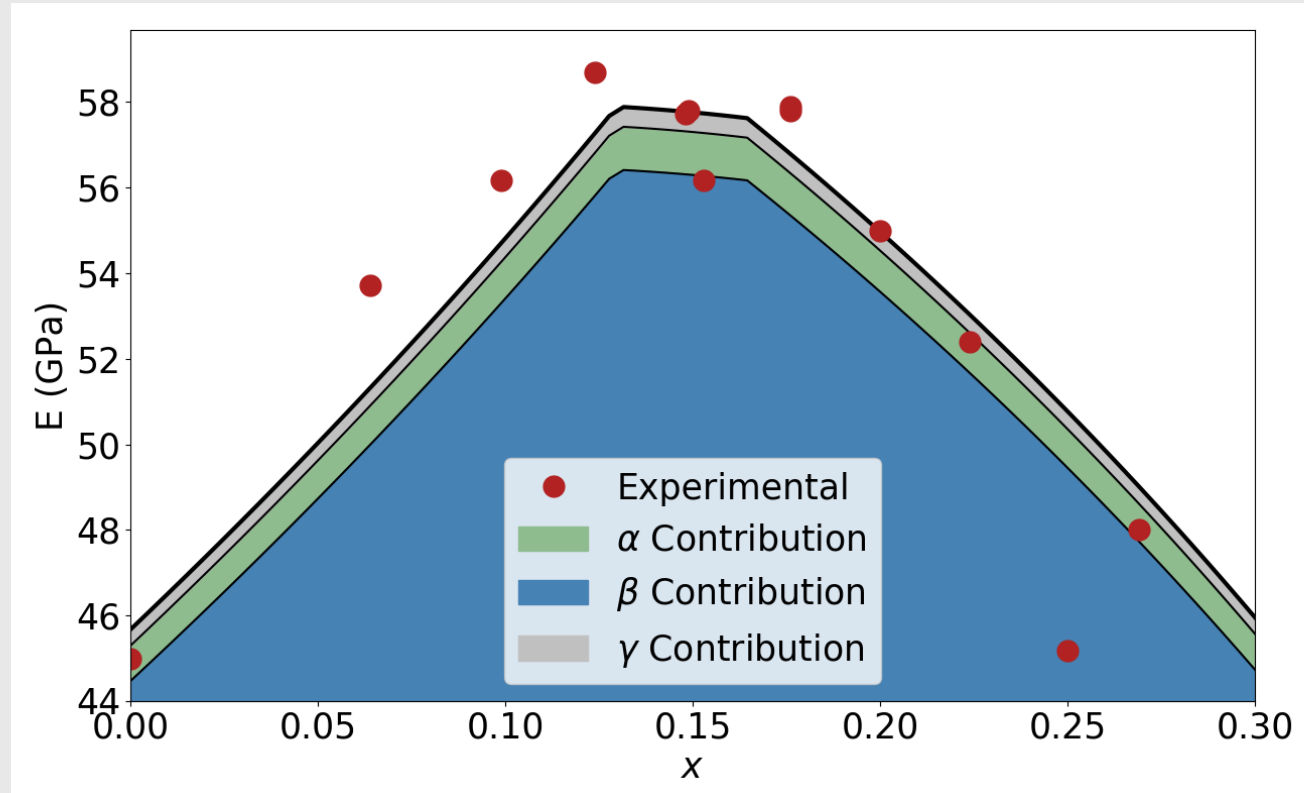
Topological Constraint Theory

❖ Looks at the bonds between atoms in each structural unit.

❖ Can be used to accurately predict mechanical and thermal glass properties.

❖ This will test whether our created structure is accurate.

T_g Results

Using the created structure from statistical mechanics, we predict the glass transition temperature with topological constraint theory and compare with experimental data.
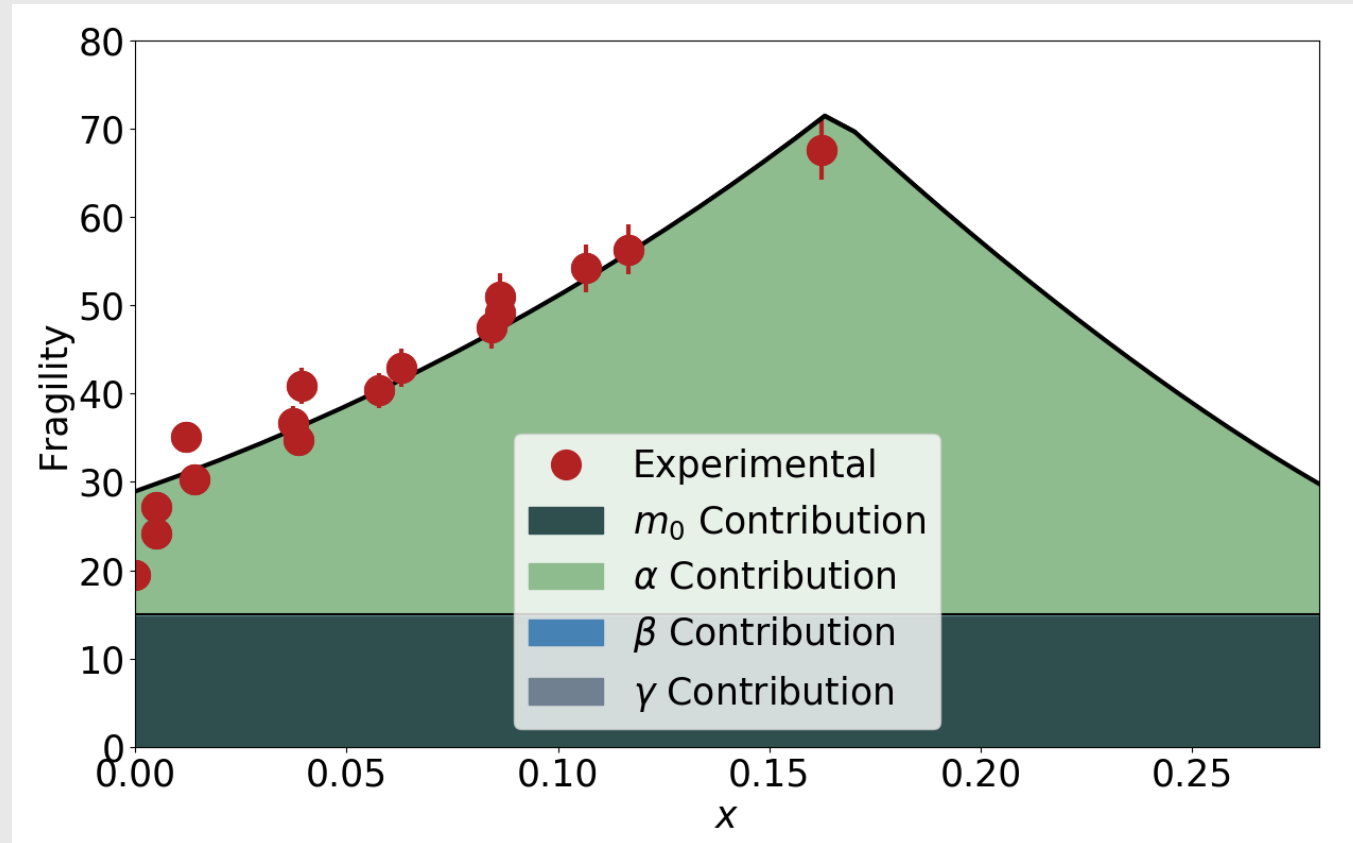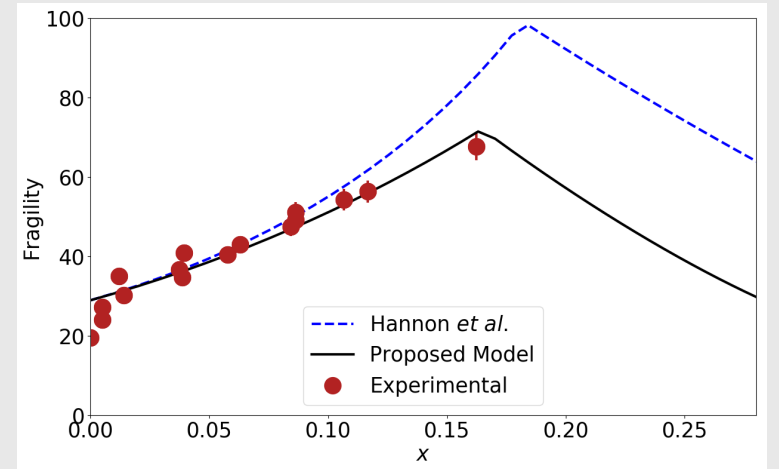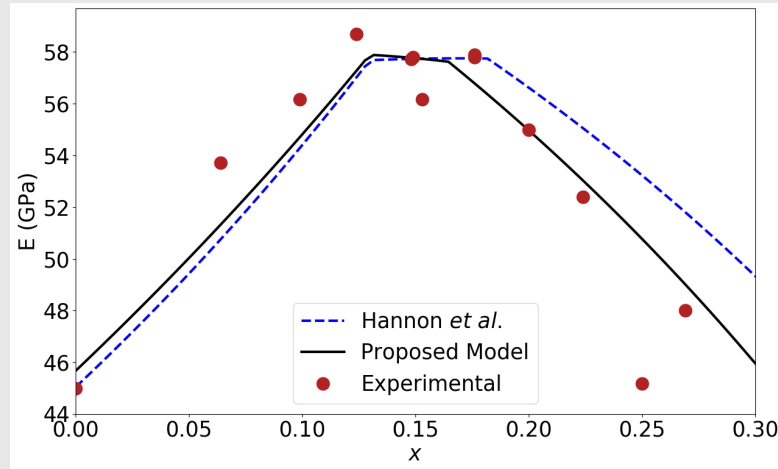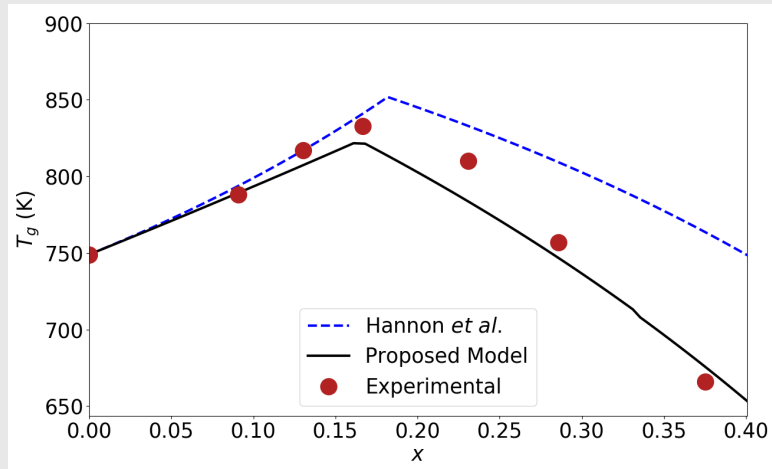
Elastic Modulus

The predicted elastic modulus using topological constraint theory and comparison to experimental data.

Fragility

The predicted glass fragility with comparison to experimental data.

Comparison to A Different Theory

Topological constraint theory was also used with an existing structural theory based on the existence of the N5 unit. This allows for a direct comparison between our model which assumes the N6 unit, with an existing one which assumes the N5 unit.

Conclusions

❖ From the excellent agreement in the predicted properties with the structure created from statistical mechanics, we support the existence of the N6 unit.

❖ When comparing with an existing theory that the N5 unit exists, we conclude that the N5 unit plays a lesser role in the germanate anomaly when compared to the N6 unit.