Analyzing the Onset of Yield in Thermoset Polymers: Angle Analysis

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Introduction

Thermoset polymers are an important component in the manufacturing of airplanes, such as the Boeing 787. However, not much is currently known about the failure mechanism in these materials. By better understanding how these materials begin to break, we can tailor them to have more desirable mechanical properties.

Understanding how and when the materials break is very difficult because of the complex structure of the crosslinked network (Fig. 1). It is hypothesized that as the material is strained, the long chains of molecules will rotate and begin to slide past each other. These rotations can be understood in terms of changes in torsion angles between monomers (Fig. 2), so by analyzing this angle data we may be able to better understand how damage accumulates over time and leads to catastrophic failure.

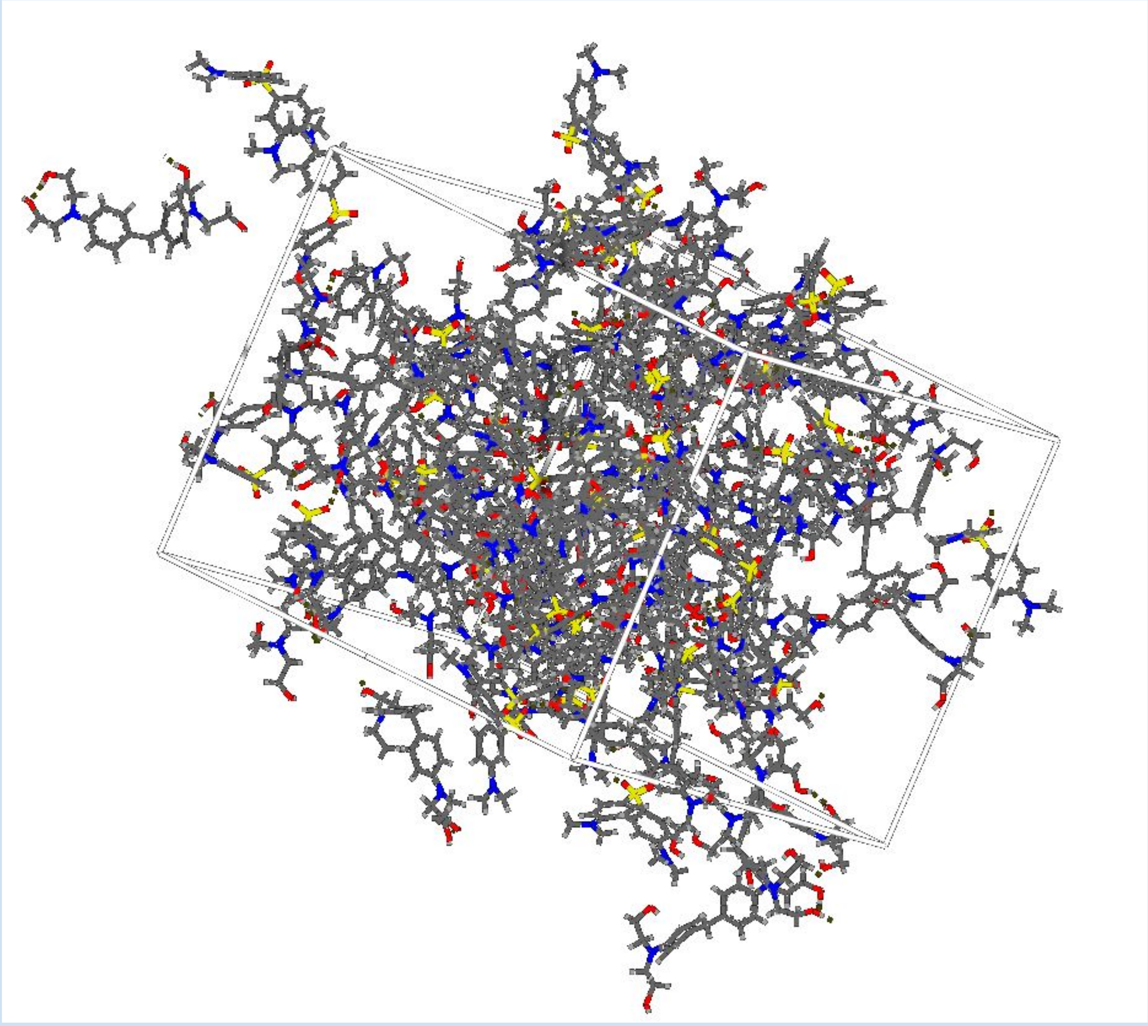

Fig. 1 (above): The crosslinked network being analyzed. Many of the long chains are intertwined, giving the polymer its strength.

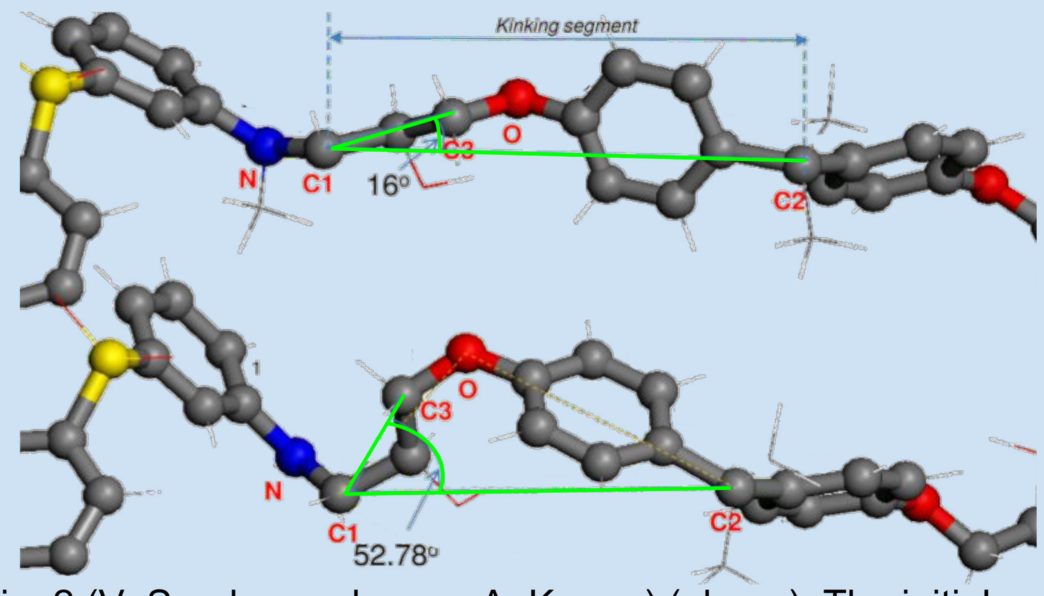

Fig. 2 (V. Sundararaghavan, A. Kumar) (above): The initial shape of a segment of a chain before kinking, and the final shape after the segment undergoes kinking. The angle we track for our analysis is shown in green.

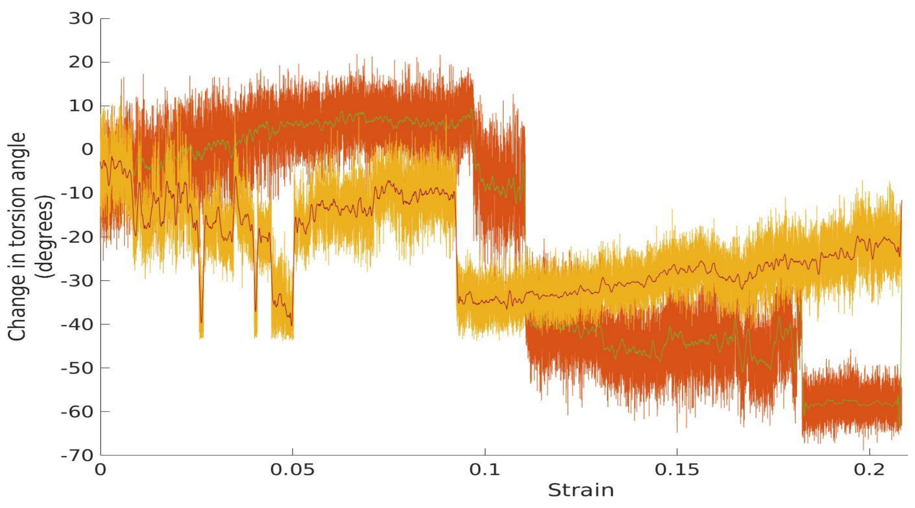

Fig. 3 (left): Here the smoothed angle data is superimposed on the raw, noisy data. This highlights the importance of noise reduction in data analysis.

Noise Reduction

Embedded within the angle data we collected is a large amount of high frequency noise (Fig. 3). This is almost entirely thermal noise, and it makes it difficult to see trends in the data. Technically it isn't truly random noise because the motion is deterministic, but because of the complexity of all of the intermolecular forces acting on each atom, it behaves practically like random noise. Therefore, we are justified in applying statistical noise reduction techniques to better show how the angles change over time. We used several methods, but settled on using a convolution that preserves higher order polynomial structure. This significantly reduced the noise, however it is a parameterized method, so we had to rely on our own judgement when deciding parameters.

Data Analysis

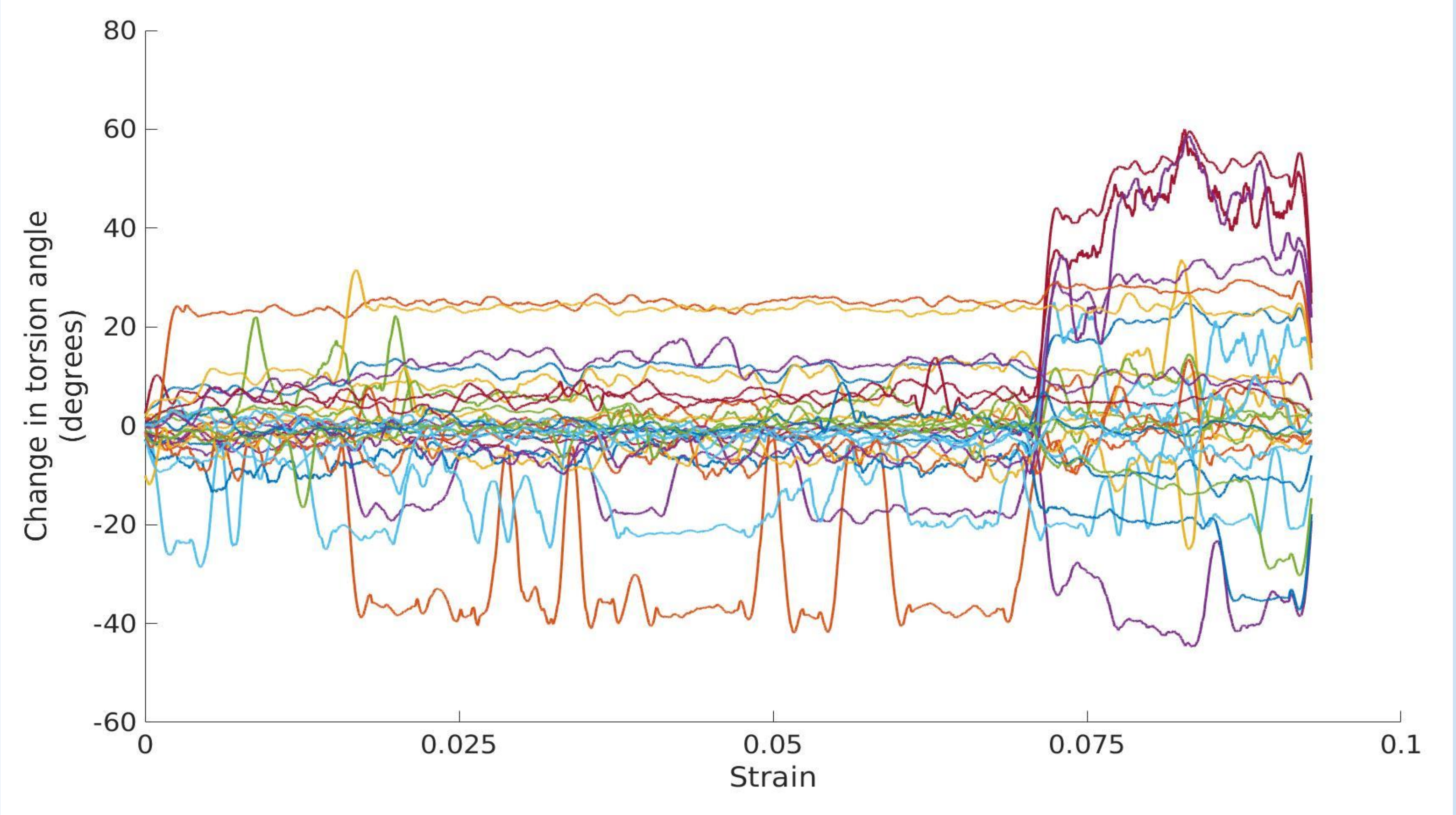

Fig. 4: Change in the angles relative to their initial positions as a function of the strain on the system. Each line represents a specific angle we are tracking. At .071 strain, the compressive force was reduced to zero and the system was allowed to relax. Interestingly, many angles do not return to their original shape.

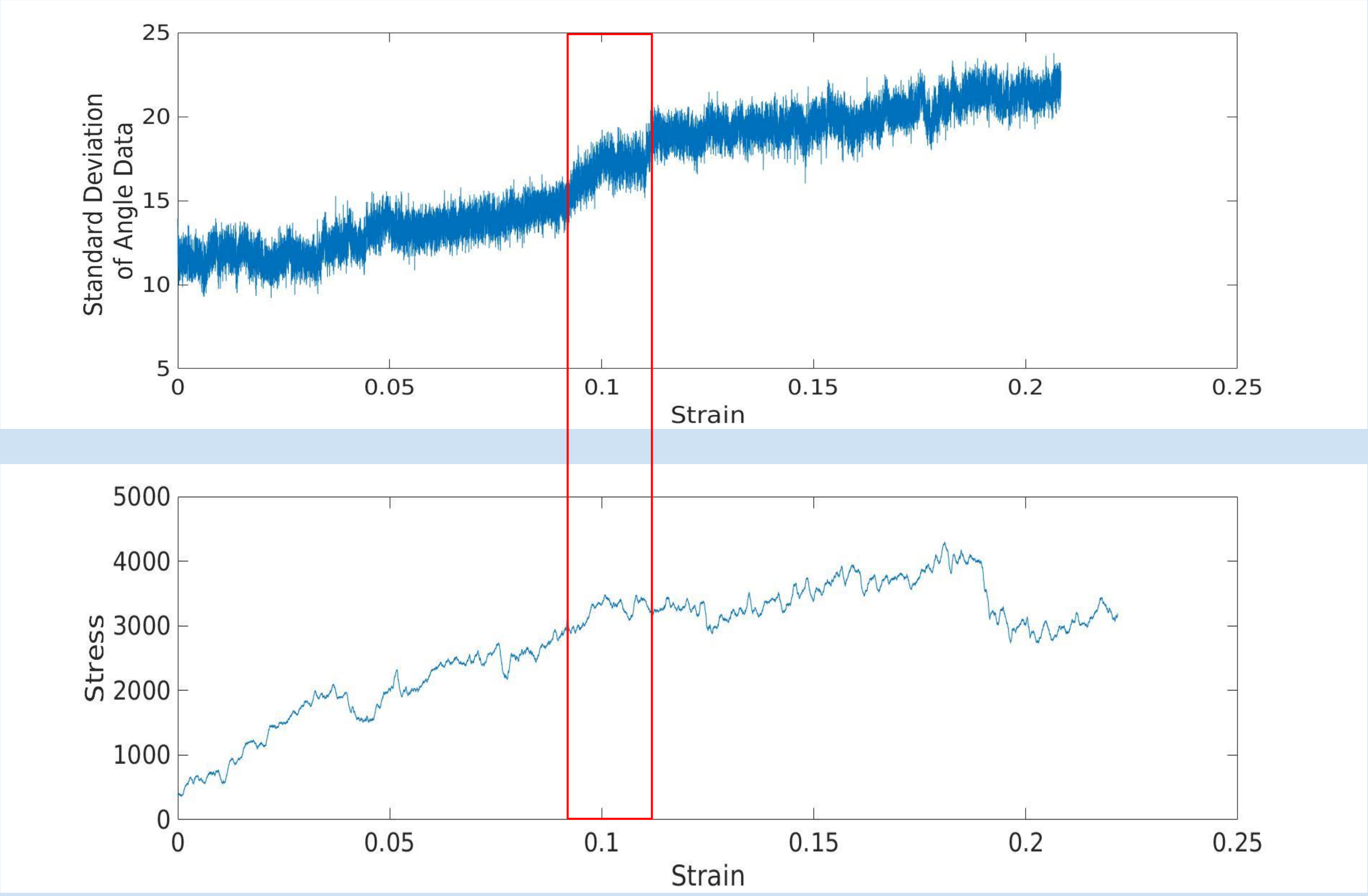

Fig. 5: Top: Standard deviation of our angle data as a function of the strain on the system. Bottom: stress-strain curve for the same simulation. The red window highlights where the standard deviation changes dramatically. This change aligns with the plateau of the stress-strain curve, which independent analysis indicates is the yield point.

The angle data used is created from an atomistic molecular dynamics simulation of a polymer system undergoing a compression test. We calculate each angle's value relative to that angle's initial value (Fig. 3, Fig. 4) to see how they change over time. We believe that significant changes in the structure will be associated with large changes in many torsion angles, so intuitively, a sharp increase in the standard deviation of the angle data (Fig. 5, top) will indicate that many angles have changed rapidly.

Key Findings

Fig. 4 indicates that permanent damage has already been done to the system, even before the system has yielded. This is important because it provides us with a mechanism for damage accumulation within the system, which has previously remained mostly unexplored. Other types of analysis, including stress-strain analysis (Fig. 5, bottom) and deformation-recovery analysis, provide an accurate indication of the yield point, but tell nothing about how the damage builds up before critical failure.

Fig. 5 shows the value of statistical analysis of angle data towards predicting the window in which the material has yielded.

Future Work

There could be an important difference between angles in the centers of polymer chains and angles at the ends of chains. We hypothesize that angles on free ends rotate more often because they have freedom to move as the material is strained. We believe that the angles in the centers of polymers slowly build up stress because they are more restricted in their movement. At a certain point, these internal stresses overcome the restrictive forces, and they suddenly "pop", or kink. We would also like to confirm our results from the residual angle analysis (Fig. 4).

Acknowledgements

We would like to thank our advisors, Dr. Paul Patrone and Dr. Judith Terrill for their guidance. We would also like to thank Terence Griffin for helping us with our (many) technical problems.