Effects of Chain-Branching on Stress Relaxation in Polyurea

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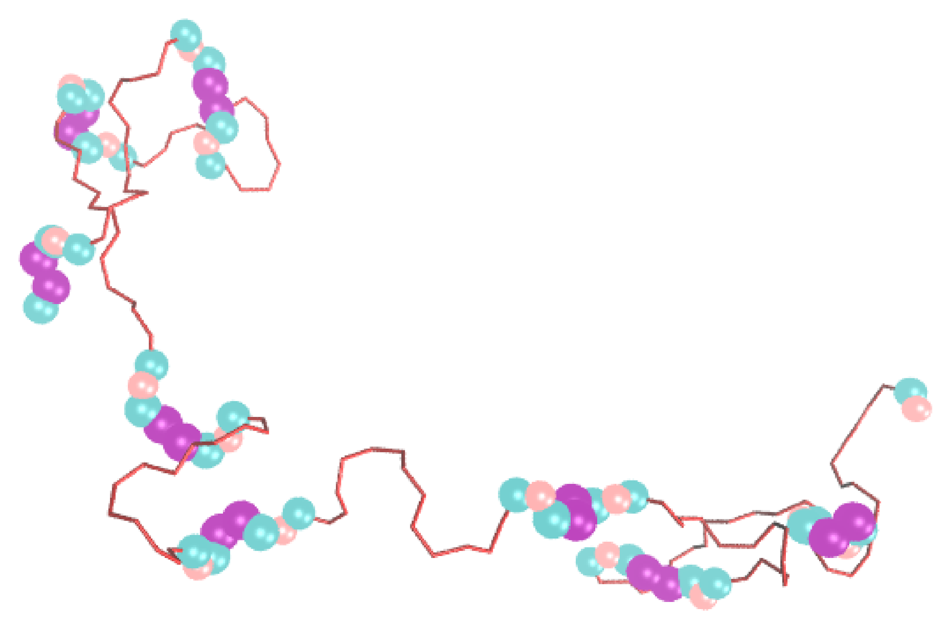
What is the effect of chain branching on stress relaxation in polyurea as a function of the percentage of branches to linear segments?

Objective:

Understand effect of chain branching in alternating block co-polymers on mechanical properties related to viscoelasticity.

Branched co-polymer



Linear co-polymer

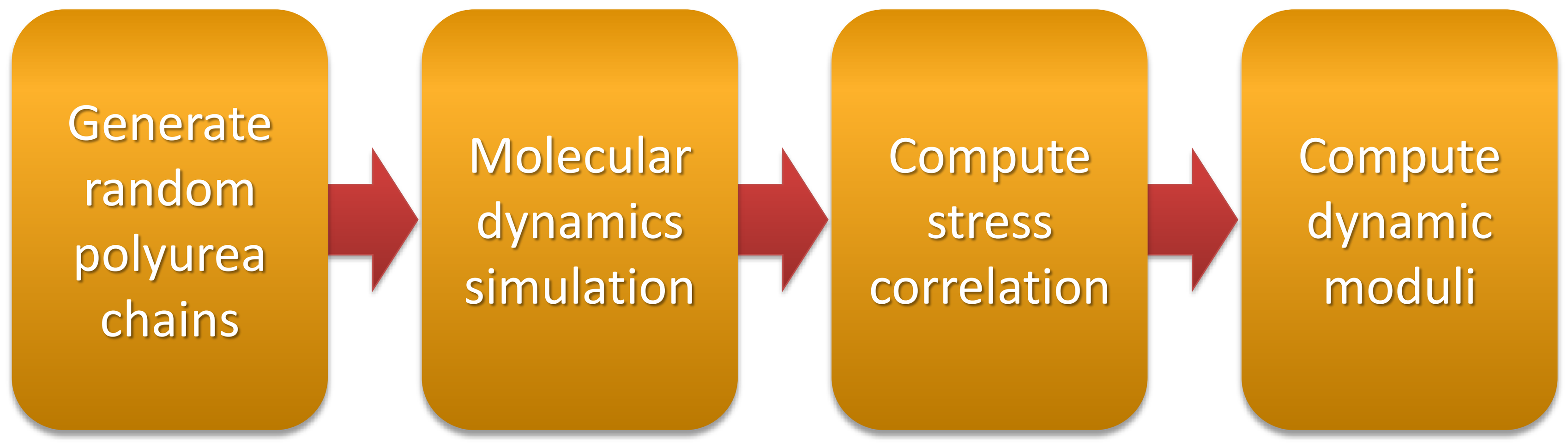
Application:

Improved materials to protect military personnel from blast-related traumatic brain injury.

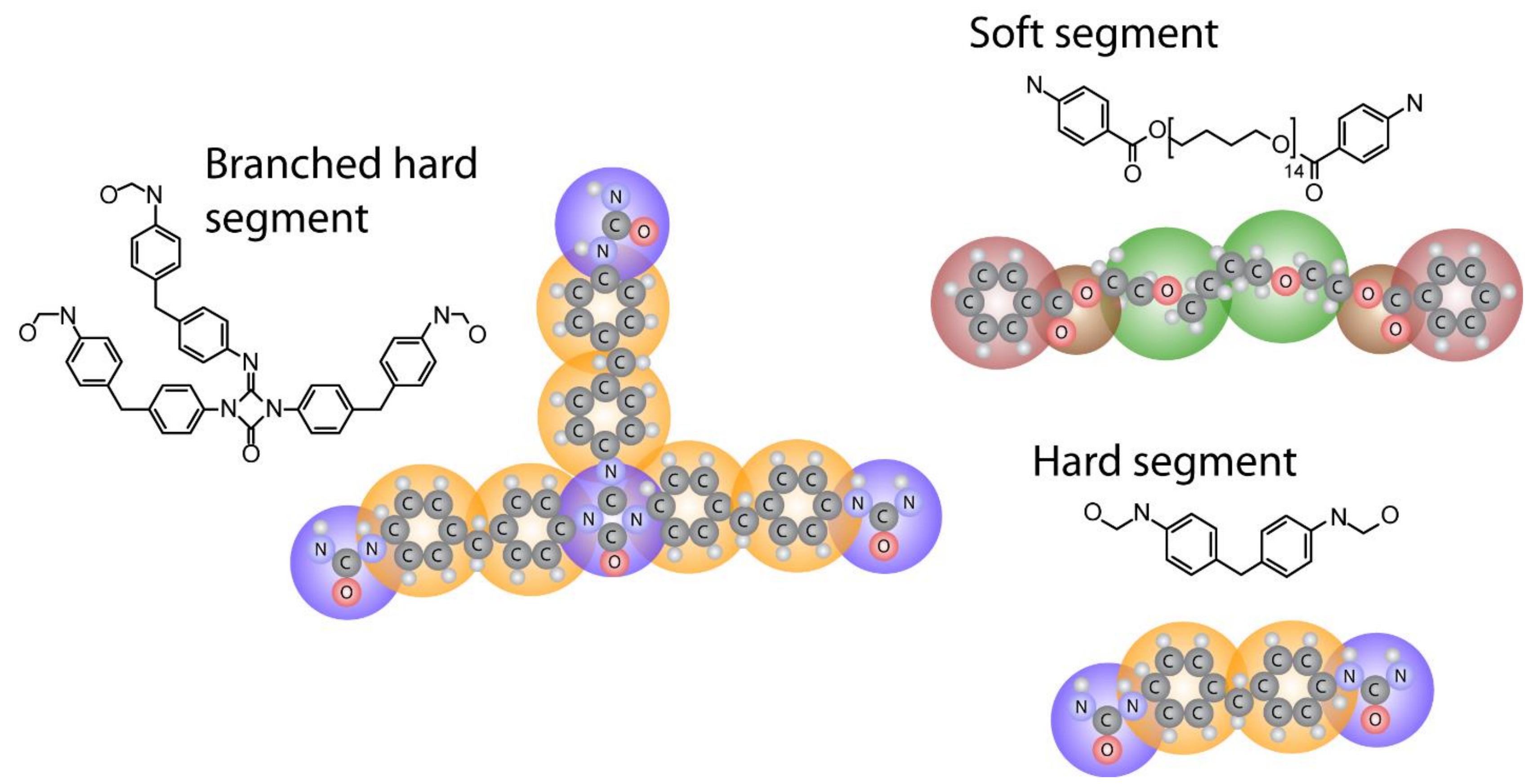
Explosive ordinance detonation in Afghanistan *(photo by Cpl. Jeff Drew, US Marine Corps)*

Advanced Combat Helmet

Method:



Coarse-grained polyurea components:



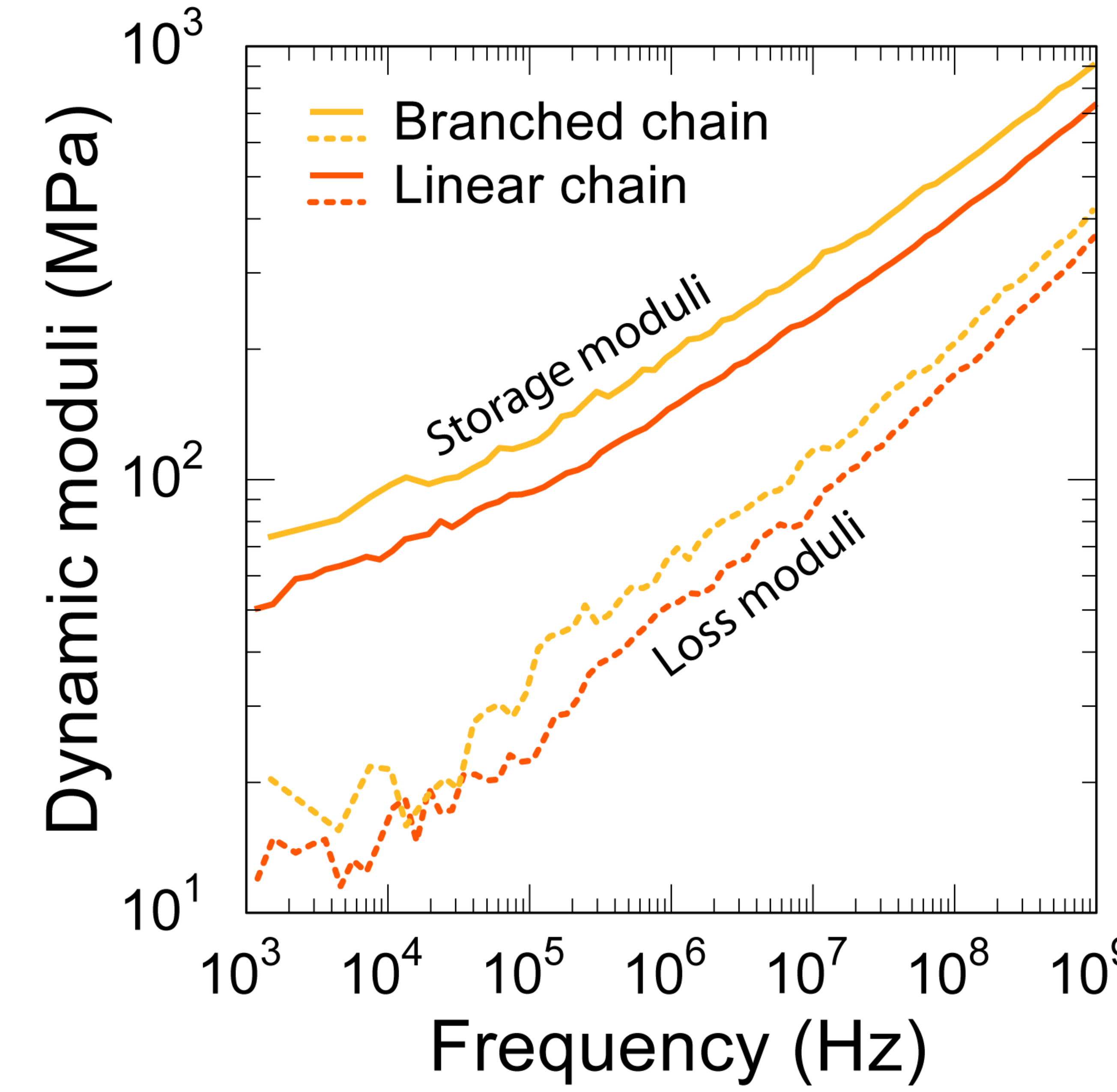
Coarse-grained building blocks of polyurea.

Computing Macroscopic Properties:

- **Stress:** $\sigma_{\alpha\beta} = \frac{1}{V}\left(\sum_i m_i v_{i\alpha} v_{i\beta} + \sum_i \sum_j r_{ij\alpha} F_{ij\beta}\right)$ V: volume, m: mass, r: pair distance, F: pair force, v: velocity
- **Stress relaxation:** $G_{\alpha\beta}(t) = \frac{V}{k_B T}\left\langle \sigma_{\alpha\beta}(t)\sigma_{\alpha\beta}(0)\right\rangle$
- **Dynamic Moduli:** $G^*(\omega) = i\omega\int_0^\infty e^{-i\omega t} G_{\alpha\beta}(t)\,dt$

Results:

Branched polyurea chains exhibit 50% higher stiffness and a smaller increase in loss modulus.



Dynamic moduli of branched and linear polyurea predicted by coarse-grained molecular dynamics simulation.

Conclusions:

- Coarse-grained models can link polymer chemistry to mechanical behavior.
- Increase to chain branching leads to higher stiffness and more dissipation in polyurea.