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Temperature Dependence of Structural Relaxation: From "Super-fragile" Polymers to "Super-strong" Behavior of Water

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The microscopic mechanism of the steep temperature dependence of structural relaxation upon approaching Tg still remains a puzzle in the field of dynamics of polymers and soft materials in general. The steepness of the temperature behavior and its deviation from classical Arrhenius law is usually characterized by the fragility index m. This contribution presents an overview of several models proposed to connect molecular parameters to the fragility. We emphasize the Generalized Entropy Theory [1] and its prediction on the role of chain packing in fragility of polymers. Based on this theory and many experimental studies we unravel the role of chain structure, intermolecular interactions and molecular weight in polymer fragility [2,3], providing a qualitative explanations of why many polymers exhibit extremely fragile behavior. Next we show that similar qualitative ideas about frustration in packing might be applicable to other glass forming systems. In the last part we discuss the recent discovery of "super-strong" behavior of deeply supercooled water and the role of quantum effects in this anomalously low fragility.

[1] Stukalin, E. B.; Douglas, J. F.; Freed, K. F. **J. Chem. Phys. 131**, 114905 (2009).
[2] K. Kunal, et al., **Macromolecules 41**, 7232 (2008).
[3] A. Agapov, et al., **Macromolecules 45**, 8430 (2012).