Understanding how glasses 'relax' provides some relief for manufacturers

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(PhysOrg.com) -- Researchers at the National Institute of Standards and Technology and Wesleyan University have used computer simulations to gain basic insights into a fundamental problem in material science related to glass-forming materials, offering a precise mathematical and physical description* of the way temperature affects the rate of flow in this broad class of materials -- a long-standing goal.

Manufacturers who design new materials often struggle to understand viscous liquids at a molecular scale. Many substances including polymers and biological materials change upon cooling from a watery state at elevated temperatures to a tar-like consistency at intermediate temperatures, then become a solid "glass" similar to hard candy at lower temperatures. Scientists have long sought a molecular-level description of this theoretically mysterious, yet common, "glass transition" process as an alternative to expensive and time-consuming trial-and-error material discovery methods. Such a description might permit the better design of plastics and containers that could lengthen the shelf life of food and drugs.

A fundamental question is why many materials behave differently when temperature changes. In some "fragile" glass-forming materials, a modest variation in temperature can make the material change from highly fluid to extremely viscous, while in "strong" fluids this change in viscosity is much more gradual. This effect influences how long a manufacturer has to work with a material as it cools. "For decades, material scientists have heavily relied on empirical rules of thumb to characterize these materials," says NIST theoretician Jack Douglas. "But if you want to design a material that does precisely what you want, you need a molecular understanding of the underlying physical processes involved."

According to Douglas, the increasingly viscous nature of glass-forming liquids is related to molecules that move together in long strings around other atoms that are almost frozen in their motion. The growth of these snake-like structures leads to an increase in the viscosity of the liquid: the lower the temperature, the longer the chains, and the more viscous the fluid. The team found that the rate at which these spontaneously organizing snake-like strings grow in size as the material cools is quantitatively related mathematically to the fluid fragility—confirming intuitive arguments made nearly half a century ago by physicists G.

Adams and J.H. Gibbs, but now bolstering them with a firm computational underpinning.

Douglas and his collaborator Francis Starr of Wesleyan University achieved a large variation of fluid fragility through use of a computer model, which mimics a polymer fluid that includes tiny nanometer-sized particles. Portraying the addition of various amounts of nanoparticles and varying their interaction with the polymers, Starr says, gave the team a sort of "knob to tweak" to reveal how the fluidity changed with temperature and how the motion of the clusters was quantitatively related to changes in the fluid's properties. This tuning of cooperative motion in glass-forming liquids and fragility should be crucial in material design. Douglas says.

More information: F.W. Starr and J.F. Douglas. Modifying fragility and collective motion in polymer melts with nanoparticles. *Physical Review Letters*, week ending March 18, 2011, Vol. 106, 115702 pp. 1-4, DOI: 10.1103/PhysRevLett.106.115702

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