Abstract Submitted
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Twinkling Fractal Theory of the Glass Transition.[1] RICHARD WOOL, Department of Chemical Engineering, University of Delaware — A new approach to the glass transition temperature T_g considers the interaction of particles with an anharmonic potential U(x), and Boltzmann population $\phi(x) \sim \exp -U(x)/kT$. As T_g is approached from above, solid clusters of atoms form and percolate at T_g. However, the solid percolation cluster is in dynamic equilibrium with its surrounding liquid and "*twinkles*" as solid and liquid atoms interchange. The *twinkling* frequency $F(\omega)$ is related to the vibrational density of states $G(\omega) \sim \omega^{df}$ and the energy difference $\Delta U \sim (T^2-T_g^2)$ via $F(\omega) \sim G(\omega) \exp -\Delta U/kT$, where $d_f = 4/3$ is the fracton dimension. $F(\omega)$ controls the rate dependence of T_g, physical aging, yield stress, heat capacity C_p, T_g of thin films, etc. When $T < T_g$, the non-equilibrium volume development ΔV, is determined by the fractal structure at T_g.The thermal expansion coefficients in the liquid and glass are related via $\alpha_g = p_c\alpha_L$. For a Morse potential $U(x) = D_o[1\text{-}\exp ax]^2$, we predict that $T_g = 2D_o/9k$, and $\alpha_L = 3k/[4D_o a R_o]$. For atoms with $R_o \approx 3$ Å, bond energy $D_o \approx$ 2-10 kcal/mol and anharmonicity factor $a \approx 2$/Å, we obtain $\alpha_L T_g \approx 0.03$, and modulus $E \sim 1/\alpha_L$, which were found for a broad range of polymers. The yield stress σ_y is determined by the onset of the twinkling fractal state as $\sigma_y = \{0.16\ E\ [p_s\text{-}p_c]\ D_o/V_m\}^{1/2}$ where V_m is the molar volume.

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