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Kinetically controlled glass transition measurement of organic aerosol thin films using broadband dielectric spectroscopy

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Havriliak-Negami Equation and Fitting Principles

The real part of the Havriliak-Negami equation, $\varepsilon'(\omega)$, is shown as:

$$\varepsilon'(\omega) = \varepsilon_\infty + \Delta\varepsilon(1 + 2(\omega\tau)^\alpha \cos\left(\frac{\pi\alpha}{2}\right) + (\omega\tau)^{2\alpha})^{-\beta/2}\cos(\beta\varphi) \qquad \text{(S1)}$$

where ε_∞ is the permittivity at the high frequency limit, α, β are fitting parameters, and τ is the characteristic relaxation time of the medium.

The imaginary part of the Havriliak-Negami, $\varepsilon''(\omega)$, is shown in Eq. (2). Sometimes, when there are ionic impurities in the supercooled liquid, a dc-conductivity term that follows strickly through ω^{-1} can contribute to the imaginary part as well (Adrjanowicz et al., 2009). The imaginary part of the of the Havriliak-Negami equation is re-written as:

$$\varepsilon''(\omega) = \frac{\sigma_{dc}}{\varepsilon_o\omega} + \Delta\varepsilon(1 + 2(\omega\tau)^\alpha \cos\left(\frac{\pi\alpha}{2}\right) + (\omega\tau)^{2\alpha})^{-\beta/2}\sin(\beta\varphi) \qquad \text{(S2)}$$

where σ_{dc} is the conductivity of the supercooled liquid, ε_o is a permittivity constant.

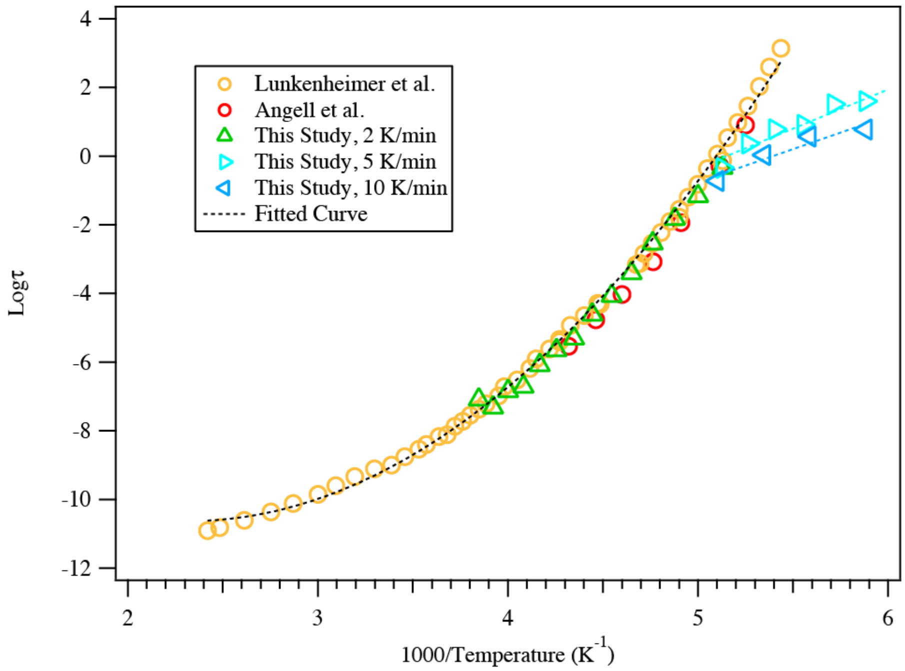

Figure S1. The logarithm of the relaxation timescale as a function of the inverse temperature derived from glycerol. The circles are from Lunkenheimer et al. (1999) and Angell (1995). The triangular points are experimental measurements from this work with different cooling rates. The dashed lines are the fitted curves for the super-Arrhenius and Arrhenius regions. The results show that the Tg values from this work match very well with previous studies.

References

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