

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

A Surrogate for Debye-Waller Factors from Stokes Shifts¹ MARCUS CICERONE, QIN ZHONG, MADHUSUDAN TYAGI, NIST — We show that short-time relaxation behavior characteristic of the intermediate scattering function at q near the peak in the static structure factor can be obtained from time-resolved Stokes shifts (TRSS) in glassforming materials. We extract Debye-Waller factor ($\langle u^2 \rangle$) analogs from the TRSS data from four glassforming liquids and apply these to a proposed relationship between α relaxation and the Debye-Waller factor; $\tau_\alpha = \tau_\infty \text{Exp} \left[\frac{a^2}{2\langle u^2 \rangle} + \frac{\sigma_a^2}{8\langle u^2 \rangle^2} \right]$. This putative relationship has previously been evaluated using experimental Debye-Waller factors obtained in the time range (40 to 2000) ps. We show that the relation yields physically meaningful fit values only when relaxation on a 1 ps timescale is considered. We also observe an unexpected dependence of short-time Debye-Waller factors on fragility.

¹We acknowledge funding from NIH/NIBIB under grant R01 EB006398-01A1

Marcus Cicerone
NIST

Date submitted: 29 Nov 2010

Electronic form version 1.4