A Surrogate for Debye-Waller Factors from Stokes Shifts\textsuperscript{1} \textsc{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 $\alpha$ relaxation and the Debye-Waller factor:

$$\tau_\alpha = \tau_\infty \exp \left[ \frac{a^2}{2\langle u^2 \rangle} + \frac{\sigma_{u^2}^2}{8 \langle u^2 \rangle^2} \right].$$

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.

\textsuperscript{1}We acknowledge funding from NIH/NIBIB under grant R01 EB006398-01A1