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Localization model for relaxation in glass-forming materials[1]
DAVID S. SIMMONS, MARCUS T. CICERONE, JACK F. DOUGLAS, National Institute of Standards and Technology — As a material approaches its glass transition, its structural relaxation time τ rapidly increases as its particles become localized. A model relating this relaxation time increase to an experimentally accessible measure of localization (e.g. the Debye-Waller factor $\langle u^2 \rangle$) would have a fundamental impact on our understanding of glass formation and would be practically useful in the design of new materials. After examining such a relationship proposed by Leporini and coworkers and finding it to be inadequate, we develop an activated transport model that accurately describes relaxation data from a variety of simulated and experimental glass-forming materials. This model naturally extends the Hall-Wolynes and free volume models relating τ to $\langle u^2 \rangle$ (or free volume). The model parameters are physically meaningful and reflect the anharmonicity and anisotropy of particle localization. The Vogel-Fulcher-Tamman relation also describes relaxation in the simulated and experimental glass-forming materials we considered, and by exploring consistency between these two relations we gain new insight into the characteristic temperatures of glass formation in terms of the extent of particle localization.

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