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Dynamical Susceptibility of Glass Formers: Contrasting the Predictions of Theoretical Scenarios

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Recommended and a Commentary by Peter G. Wolynes, University of California, San Diego

If the problem of the glass transition remains open, it is not because of a lack of theoretical imagination. On the contrary the area suffers from a multiplicity of hypotheses and a relative dearth of detailed comparisons of the consequences of these hypotheses, with quantitative observations. In this climate you will find the paper by Toninelli et al. refreshing.

These authors discuss evidence for growing dynamical length scales in computer simulations of classical fluids, using data of Reichmann and Denny. A growing length scale in this temperature regime is predicted by mode coupling theory which gives good agreement with the results. Unfortunately, as the authors point out the data do not extend deeply into the super cooled regime where they could test the nature of strongly activation-limited processes. Thus at this point there is no contradiction with theories based on random first order transitions which contain the mode-coupling regime as a crossover. Greater computer power (and perhaps some now unforeseen algorithm advances) may allow such computational tests in the future using the strategy presented here.

In contrast to these pictures that invoke strong cooperativity, Toninelli et al. show that one can discard models based on freely diffusing point defects in this regime. Likewise they observe qualitative differences from the simplest three-dimensional models that invoke facilitated diffusion.

Perhaps the most important fruit of the study is the impetus it should provide to laboratory experimentalists to measure these dynamical susceptibilities in the time-temperature regime of deeply super cooled liquids. X-ray speckle techniques come to mind as challenging possibilities.