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Predicting the Viscosity of Multicomponent Glass-Forming Liquids

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The quantitative design of glassy materials with tailored properties is a longstanding problem in the glass science community. One of the most technologically important properties is the shear viscosity, since all stages of industrial glass production require careful control of shear viscosity. Here, we show that topological constraint theory holds the key to understanding the temperature and composition dependence of the viscosity of glass-forming liquids. Using this approach, we derive detailed topological representations of soda lime borate and borosilicate systems that enable the accurate prediction of glass transition temperature and liquid fragility. The implications of the glass topology are discussed in terms of both the temperature and thermal history dependence of the atomic bond constraints and the influence on relaxation behavior. We also present a phenomenological model offering an improved description of the composition and temperature dependence of the shear viscosity of multicomponent liquids, for which the existing analytical models currently do not apply. The model predicts the isokom temperatures of 7141 viscosity measurements for 760 different compositions with a root-mean-square error of only 6.55 K.