Pressure-Dependence of the Glass Transition Temperature of Low- and High-Density Amorphous Ice

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ABSTRACT

Water has multiple glassy states, often called amorphous ices. Low-density (LDA) and high-density (HDA) amorphous ice are separated by a dramatic, first-order like phase transition. It has been argued that the LDA-HDA transformation connects to a first-order liquid-liquid phase transition (LLPT) above the glass transition temperature T_g. Direct experimental evidence of the LLPT is challenging to obtain, since the LLPT occurs at conditions where water rapidly crystallizes. In this talk, we will explore the implications of a LLPT on the pressure dependence of $T_g(p)$ for LDA and HDA by performing computer simulations of two water models---one with a LLPT, and one without. In the absence of a LLPT, $T_g(p)$ for all glasses nearly coincide. We will show that when there is a LLPT, different glasses exhibit dramatically different $T_g(p)$ which are directly linked with the LLPT. Available experimental data for $T_g(p)$ are only consistent with the scenario including a LLPT, which lead us to predict the behavior of $T_g(p)$ for LDA.