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Polyamorphic transitions in network glasses and glass-forming liquids

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Over the past two decades, we have witnessed increasing evidence for the occurrence of polyamorphism, i.e., the existence of more than one thermodynamically and structurally distinct non-crystalline state of a given substance. This concept is manifest predominantly through the transitions between different polyamorphic states, as we are still not able to unequivocally describe a given amorphous structure. However, if substantiated, the concept of polyamorphism should facilitate such a description, since it implies that polyamorphic states are uniquely defined and a distinctive structural character must exist for each state. We have observed polyamorphic transitions in a number of glass-forming systems, e.g., when probing their high-frequency visco-elastic response as a function of temperature,[1] or when compacting such systems at high pressures. We have carried out molecular dynamics simulations to reveal explanations for the phenomena observed in experiments.[2] In this presentation we discuss reversible and irreversible transitions in silica glass, their relation to the anomalous thermo-mechanical properties of this material, and the effects of permanent densification on structure and properties. We present an unusual transition in boron oxide glass, which is continuous upon compression and discontinuous upon decompression.[3] We show how the manifestations of polyamorphic transitions and their are related to structural transformations in the crystalline counterparts of these materials, and how this can even lead to the discovery of previously unknown metastable crystalline phases. [1] J. Kieffer, J.E. Masnik, O. Nickolayev, and J.D. Bass, Phys. Rev. B **58**, 694 (1998). [2] L. Huang, and J. Kieffer, Phys. Rev. B **69**, 224203 and 224204 (2004). [3] J.D. Nicholas, S.V. Sinogeikin, J. Kieffer, and J.D. Bass, Phys. Rev. Letters **92**, 215701 (2004).