MM 10: Topical Session Glass Dynamics III

Time: Monday 14:45-15:30

Topical TalkMM 10.1Mon 14:45H16Transport Processes in Dense Melts near and far from Equi-
librium — •THOMAS VOIGTMANN — Institut für Materialphysik im
Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170
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Mass transport in densely packed liquids is characterized by slow dynamical processes and a strong sensitivity of the transport coefficients to control parameters and/or external fields. I will give an overview of recent theoretical developments based on the mode-coupling theory of the glass transition and some of its nonequilibrium generalizations. I will in particular focus on the relation between tagged-particle properties as measured, e.g., through self-diffusion processes, and the collective dynamics probed for example in the inter-diffusion of concentration fluctuations in multicomponent glass formers and metallic melts. Mixtures that exhibit strong decoupling between the individual species demonstrate the similarities and differences in these processes quite clearly. Externally applied forces allow to probe the underlying dynamical processes in the nonlinear, nonequilibrium regime, and thus provide much more detailled information than just the equilibrium transport coefficients. As an example, I will discuss the relation between local, microscopic friction and its macroscopic counterpart, viscosity.

Location: H16

MM 10.2 Mon 15:15 H16 Structure conserving correlations, inherent structure dynamics, and the Kohlrausch-Williams-Watts behaviour of simulated metallic-glass forming Ni0.5Zr0.5 — •HELMAR TEICHLER — Inst. f. Materialphysik, Univ. Göttingen, 37077 Göttingen, Germany

In glass forming melts near the glass temperature, the alpha-decay reflects relaxation processes with Kohlrausch-Williams-Watts behaviour on macroscopic time scales. Microscopic explanation of these fundamental features is a challenging open question, which needs understanding emergence of extreme slow dynamics with non-exponential response from atomic motions in the melt. Regarding this, we here present an analysis of microseconds-scale molecular dynamics simulation results for glass forming Ni0.5Zr0.5. The concept of "strongly effective particles" (SEPs) is used to relate the properties of macro-scale correlation functions to the atomistic processes in the melt. We show in particular that the Kohlrausch-Williams-Watts behaviour reflects structure conserving correlations (SCC) in the formation and annihilation of SEPs. The SCC make that there are long-time memory-effects in the inherent structure dynamics. Details are discussed concerning the microscopic picture behind the SCC and how to generate for relevant correlators equations of motions that take care of the SCC.