Abstract Submitted for the MAR13 Meeting of The American Physical Society

Coarse grained dynamics in the glass phase ANTON SMESSAERT, JORG ROTTLER, University of British Columbia — Atomic scale dynamics in glasses is dominated by extended periods of localized vibration, where the crowded surroundings of a particle act as a cage. Collective motion is necessary to escape the cage, and the succession of particle jumps or hops leads to diffusion. Each jump is an elementary relaxation event since the local structure is stable until a jump occurs. The link between local dynamics and structural properties has become of increasing interest in recent years. Aging of the mechanical response has been tied to a power-law distribution of persistence times in the cages, and concentration of hops into dynamical heterogeneities (DH) was observed in granular media and simulations of supercooled liquids in 2D. These studies were limited to small systems or hop detection in subsets, because of the post processing requirements. We present results based on a new algorithm that allows us to detect the hops of all particles during a molecular dynamics simulation. This complete coarse-grained "map" of the dynamics allows us to directly investigate temporal and spatial correlations between relaxation events. Furthermore, we can readily identify DH using a cluster algorithm and we explore the impact of aging and deformation on the size and shape of DH.

> Anton Smessaert University of British Columbia

Date submitted: 12 Dec 2012

Electronic form version 1.4