PAUL SCHERRER INSTITUT

PSI

CONDENSED MATTER THEORY SEMINAR

Shear deformation in a model binary glass

Dr. Peter Derlet, PSI (LSM/CMT)

Thursday, Aug 23, 2018, 14:00-15:00

OVGA/407 (PSI-East)

Abstract:

Molecular dynamics simulations are performed for a model binary glass to investigate the relationship between atomic structure, density and cohesive energy, and the amorphous material's response to an applied load. Time scales spanning six order of magnitude are considered. Relaxation is found to induce a local densification which may be quantitatively connected to the creation of icosahedral structure that minimizes bond energy frustration and maximizes local atomic packing, establishing a robust link between the structural state and its free volume content. Under load, collective system-spanning plasticity is observed without significant structural damage for the slowest strain rates. Such collective plasticity is localized to a plane spanning the simulation cell. The nature of such "shear bands" is found to depend strongly on the amorphous structure prior to loading and the rate at which the mechanical load is applied.

Contact: Markus Müller, WHGA/136, Markus.Mueller@psi.ch, tel: 056 310 44 30