Symposium Amorphous materials: structure, dynamics, properties (SYAM)

jointly organised by
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Metal and Material Physics Division (MM)

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A wide variety of materials are not in a crystalline state but rather resemble a frozen liquid, in which constituent particles lack long range spatial order. This class of materials includes "hard" glassy metals and polymers, but also "soft" glasses such as suspensions, emulsions, foams, colloidal and granular assemblies. Although these systems differ widely in their length, time, and energy scales, many of their dynamical and rheological properties are universal owing to their disordered nature. These systems are endowed with a hierarchy of relaxation times that are key to understanding their response to external driving. While the yielding transition in the limit of slow athermal driving has hallmarks of critical behavior typical for a dynamical phase transition, new (thermal) effects come into play when glasses are operated closer to their glass transition temperature. This symposium invites experimental, theoretical, and computational explorations of all facets of glassy behavior in amorphous materials. This includes in particular approaches to characterize and predict the slowing down of the dynamics (vitrification) at the glass transition in the bulk and under confinement, the ensuing nonequilibrium relaxation dynamics in the glassy state, and studies of the structural, thermal and mechanical properties of such materials.

Overview of Invited Talks and Sessions

(Lecture hall Audimax 1)

Invited Talks

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Sessions

SYAM 1.1–1.5	Tue	13:30–16:15	Audimax 1	**Amorphous materials: structure, dynamics, properties**

SYAM 1: Amorphous materials: structure, dynamics, properties

Time: Tuesday 13:30–16:15 Location: Audimax 1

Invited Talk SYAM 1.1 Tue 13:30 Audimax 1

Glassy dynamics of vitrimers — •Liesbeth Janssen — Eindhoven University of Technology, The Netherlands

Vitrimers are a promising new type of polymer glasses that combine the recyclability of thermoplastics with the high mechanical performance of thermosets. At the heart of their exceptional material properties lies highly unusual glass-forming behavior. In this talk I will discuss how we can model and understand this behavior, using coarse-grained simulations and first-principles-based theory [1].

[1] S. Ciarella, R.A. Biezemans, L.M.C. Janssen, Understanding, predicting, and tuning the fragility of vitrimeric polymers, Proc. Natl. Acad. Sci. USA 116, 25013 (2019).

Invited Talk SYAM 1.2 Tue 14:00 Audimax 1

Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films — •Zahra Fakhraai — Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104

Physical vapor deposition can produce glasses with near-equilibrium properties at low temperatures. This phenomenon is enabled by the enhanced mobility at the surface region, which enables access low-energy states in the energy landscape that are otherwise kinetically inaccessible. In thin films (For TPD molecule, h˜20-50 nm), where surface mobility is further enhanced, we observe a liquid-liquid phase transition to a high-density supercooled liquid (HD-SCL) phase. The HD-SCL is formed when vapor deposition is performed below the phase transition temperature (T_LL). Above T_LL films of the same thickness follow the supercooled liquid (SCL) state. Films deposited in the HD-SCL state have densities that exceed even the crystal density. The kinetic stability of these films, measured using solvent vapor-annealing, also shows a sharp change at T_LL, further confirming the liquid-liquid phase transition phenomenon. The HD-SCL is only energetically favored in the thin film regime and rapidly transforms to the ordinary SCL or glass upon further deposition (h $>$ 60 nm). This rapid transition is a sign that the specific boundary conditions of thin films can enable the observation of phases that are otherwise unstable in bulk glasses. We discuss how this phenomenon may be related to the observation of low Tg in liquid-quenched thin films of molecular and polymeric glasses and how it may more generally elucidate the nature of phase transitions in glasses.

Invited Talk SYAM 1.3 Tue 14:30 Audimax 1

Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest — •Beatrice Ruta[1], Nico Neuber[2], Isabella Gallino[2], and Ralf Busch[2] — [1]Univ Lyon 1, CNRS, Institut Lumière Matière, Villeurbanne, France — [2]Chair of Metallic Materials, Saarland University, Saarbrücken, Germany

Glass-formers are considered as archetypes of complex systems and the glass transition keeps fascinating scientists since decades. Although the impressive works done in the last year, still little is known on the mechanism of atomic motion governing the dynamics in ultra-viscous liquids close to the dynamical arrest, due to the difficulty to prove the slow collective particle motion of glass formers.

Thanks to the use of intense coherent X-ray beams available in third generation synchrotrons, we have performed the first experimental investigations of the temperature and wavelength dependence of the atomic motion in supercooled alloys close to the glass transition [1-3]. We find that the dynamics is strongly influenced by the underlying structure which can lead to peculiar oscillations of the microscopic relaxation time in correspondence to structural features [3]. This behavior is accompanied by dramatic changes in the shape of the intermediate scattering functions and suggests the presence of large dynamical heterogeneities at the mesoscopic scale.

[1] S. Hechler et al. Phys. Rev. Mat., 2, 085603, 2018
[2] B. Ruta et al. Phys. Rev. Lett. 125, 055701 2020
[3] N. Neuber et al. In preparation

15 min. break

Invited Talk SYAM 1.4 Tue 15:15 Audimax 1

Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids — •Celine Ruscher[1,2], Daniel Korchinski[2], and Joerg Rottler[2] — [1]Institut Charles Sadron, Strasbourg, France — [2]Stewart Blusson Quantum Matter Institute, The University of British Columbia, Vancouver, Canada

Amorphous solids are yield stress materials whose flow consists of periods of elastic loading interrupted by rapid stress drops, or avalanches, coming from microscopic rearrangements known as shear transformations (STs). From the microscopic point of view, the density of STs, or density of local residual stresses, $P(x)$, governs the statistical properties of global collective failure events at the yielding transition.

Using atomistic simulations, we reveal the evolution of $P(x)$ upon deformation. A pseudogap form $P(x) \sim x^{\theta}$ is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however, $P(x)$ starts to develop a system size dependent plateau in the small x limit. To explain the origin of the plateau we consider a mesoscopic elastoplastic approach. Our results show how the spatial extent of avalanches in the stationary regime has a profound effect on the distribution of local residual stresses x. While the entrance into the plateau is set by the lower cutoff of the mechanical noise produced by individual STs, the departure from the usually assumed power-law pseudogap form comes from stress fluctuations induced by collective avalanches.

Invited Talk SYAM 1.5 Tue 15:45 Audimax 1

Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment — •Olfa D'Angelo[1] and W. Till Kranz[2] — [1]Inst. Materialphysik im Weltraum, DLR-Köln — [2]Inst. Theoretische Physik, Uni. Köln

The variety in granular materials' behaviour makes them fascinating materials, but also difficult to encompass into a globalised theory. Recently, Kranz et al. described granular fluids close to the glass transition using mode coupling theory, and extended this theory towards the non-linear rheology of granular fluids submitted to finite shear rates [1]. This approach allows to embrace in a single theoretical framework the variety of rheological responses observed in dense granular fluids, as it predicts and delineates rheological regimes comprising Newtonian, shear thinning, and shear thickening (Bagnoldian).

We provide the first experimental validation of this theory [2], through flow curves spanning six orders of magnitude in shear rate, over a wide range of packing fractions. As we uncover the predicted rheological regimes in an air-fluidised granular bed of glass beads, we explore the areas of uncertainties in comparing our careful measurements to the theory. Experimental results and theory compare very favourably; besides the predicted regimes, experiments reveal an additional regime at high Peclet number, where Bagnold scaling is lost.

[1] W.T. Kranz, F. Frahsa, A. Zippelius, M. Fuchs, and M. Sperl, Phys. Rev. Fluids **5**, 024305 (2020).
[2] O. D'Angelo, A. Shetty, M. Sperl, and W.T. Kranz, in preparation (2021).