First International Workshop on Complex Glasses 17-19 October 2023 Warsaw

Tuesday 17 October 2023 - Thursday 19 October 2023

Warsaw

Book of Abstracts

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Density functional - molecular dynamics simulations of amorphous materials

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Density functional (DF) simulations of electronic structure are limited to small (nanometer) system sizes and extremely short (picosecond) time scales when in combination with molecular dynamics (MD). Nevertheless, we have applied the DF formalism to various amorphous materials and glasses in the past to investigate their structural, dynamical and electronic properties. In this talk, I shall briefly review our work on amorphous-to-crystalline transition and polyamorphism in functional chalcogenides (phase-change materials), dynamical properties of liquid pnictogens (Sb, Bi), field-driven ionic migration in a glassy GeS2 solid-state electrolyte, and novel electronic properties of oxide glasses. I shall also discuss how the advent of neural-network force-fields has changed the field and made the DF-MD approach obsolete in many occasions.

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Simplest ‘complex’ glassforming liquids… A bridge between theories and experiments or applications

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From applications point of view, pharmacology to electrochemistry or optics, the most interesting glasses are ‘complex systems’ made from the cooling of a liquid, i.e., a material whose properties will strongly depend on the method of preparation, and the ‘complexity of the phenomenon’ involves concomitantly Thermodynamics, Dynamics and Structure. A good glassformer exhibit an amorphous, disordered structure obtained on reasonable cooling rather than crystallizing into a well-ordered structure. Bulk and nanosized metallic glasses belong to this category; most often, several atomic components are required to avoid crystallization during normal liquid cooling, but the search of simplicity and monoatomic system remains very active provided ultrahigh cooling rate could be used against spontaneous crystallization. Molecular glasses belong to another category composed of organic or small inorganic molecules and not single atoms. However, the quest for simplicity remains the same considering their chemical shape, local organisation and their intermolecular interactions. This presentation looks at the key ingredients to form a molecular or metallic glass, their limits and differences, in terms of structure and dynamics, with a special emphasis on icosahedral order and high temperature activation energy.

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Simulated multi-component metallic glasses akin to experiments

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We study a three-component metallic glass system by means of a hybrid Monte Carlo and Molecular Dynamics algorithm which allows the generation of equilibrated samples for temperatures below the conventional glass transition accessible by conventional methods. Using a realistic potential for the atomic interactions we explore the kinetics, thermodynamics, and rheology of a Cu-Zr-Al metallic glass composition in the ultrastable glass regime, showing in particular how the configurational entropy depends on the temperature, and compare it to the ubiquitous Cu-Zr one. Our results pave the way for theoretical studies of complex metallic glasses and comparisons with experiments.

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The effect of composition on the thermodynamics, structure and atomic motion of (Pd-Pt)$_{42.5}$Cu$_{27}$Ni$_{9.5}$P$_{21}$ alloys

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According to basic hard sphere models Pt should replace Pd in the $Pd_{42.5}Cu_{27}Ni_{9.5}P_{21}$ alloy. But $Pt_{42.5}Cu_{27}Ni_{9.5}P_{21}$ shows significant structural differences compared to the Pd based alloy. To study the differences, we prepared a series of (Pd-Pt)$_{42.5}$Cu$_{27}$Ni$_{9.5}$P$_{21}$ alloys replacing Pd by Pt. We assess the thermodynamic functions revealing that the driving force for crystallization increases with the increase of the Pt content, which is in line with the decreasing critical casting thickness. The Pt-richer alloys are thermodynamically more fragile than the Pd-rich alloys, which is revealed by a larger specific heat capacity and a faster drop of the configurational entropy in the Pt-richer alloys. We conclude that the structure of the Pt rich alloys is dominated by its change in medium range o-rder whereas the Pd-rich alloy is dominated by extraordinary short range. Since the two alloys show similar kinetic fragilities but different thermodynamic and structural fragilities we used XPCS to study the atomic dynamics of the two extreme cases of the series, namely the alloy $Pd_{42.5}Cu_{27}Ni_{9.5}P_{21}$ and the alloy $Pt_{42.5}Cu_{27}Ni_{9.5}P_{21}$ as a function of temperature and wave vector.

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Unsupervised learning of amorphous structure

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Unsupervised learning of amorphous structure

I will assess the ability of unsupervised learning techniques to identify collective variables that capture structural heterogeneity in dense, amorphous materials. These structural variables can be used to provide a coarse-grained definition of locally favored structures or to identify structure-property relationships in glassy liquids and amorphous solids. I will focus on applications in simple models of glassy binary mixtures - possible extensions to more complex glasses will be discussed.

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Recent developments in the study of physical aging

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This talk presents recent accurate experimental data for aging following a temperature jump [1], which definitively confirm the Narayanaswamy concept of a material time controlling aging, which is now more than 50 years old [2]. Specifically, the data show that even though aging is highly nonlinear, it conforms to a standard linear-response description if time is replaced by material time. If time allows, I will also present simulation data attempting to identify the material time [3].

[1] B. Riechers et al., Sci. Adv. 8, eabl9809 (2022).
[2] O. S. Narayanaswamy, J. Amer. Ceram. Soc. 54, 491 (1971).
[3] I. M. Douglass and J. C. Dyre, Phys. Rev. E 106, 054615 (2022).

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Structure – dynamics – property correlations in complex metallic glasses

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The structure of metallic glasses determines their properties. X-ray diffraction nano-tomography can provide accurate details of the internal structure, as shown for phase-separated glasses.

Besides, nano-beam electron diffraction reveals that the local hardness of microscale domains decreases with increasing size and volume fraction of atomic clusters with higher local medium-range order (MRO). This allows to propose a model of ductile phase softening will enable the design of metallic glasses with optimized properties b-y tuning the MRO size and distribution.

In-situ X-ray diffraction can also reveal structural rearrangements upon annealing. The configurational entropy calculated from X-ray pair correlation functions gives a structural footprint of rejuvenation, and the changes in atomic configuration can be correlated with calorimetric signals and α-, β- and γ-relaxations, thereby crosslinking structure with property changes.

Altogether, these examples show how modern structure characterization techniques allow deep insights into the atomic structure, thus providing guidelines for alloy design and tailoring of properties.

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Simulation-Informed Models for Amorphous Metal Additive Manufacturing

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My research group is currently engaged in a collaboration to develop computational tools to enable design of additively manufactured amorphous metal parts with desired mechanical properties, including strength and toughness. Amorphous metals, also termed metallic glasses, have potential as a transformative material for additive manufacturing applications. Unlike crystalline materials that solidify through the growth of anisotropic grains, typically resulting in grain boundaries and complex textures, rapid cooling causes MGs to solidify without crystal structure. Amorphous metal additive manufacturing is promising both for superior structural homogeneity compared to crystals and for overcoming cooling-rate limitations for casting larger MG structures. However, reheating associated with layer-by-layer processing results in material with a complex thermal history and spatially varying mechanical properties. We are pursuing simulation-informed modeling as an integral component of a simultaneous design approach for amorphous metals and additive manufacturing processes targeting mechanical performance. Beyond describing this collaboration, I will discuss two computational investigations that underpin our computational approaches. The first deploys computer modeling to quantify of the local yield surface of simulated binary glass-forming systems in two- and three-dimensions. This work extends classical macro-scale plastic approaches down to the nanoscale. We relate features of the resulting yield surface to underlying defect-scale processes in the glass. The second approach interrogates an atomistic representative volume element to harvest simulation data for the quantification of plastic constitutive response in a 3D binary glass. The resulting data quantifies the stress drops characteristic of metallic glass mechanical response in terms of state variables related to the stress and the structural state of the glass. This data informs a stochastic finite state automata model that can reproduce aspects of the mechanical response and the associated evolution of the material's structural state. This serves as a constitutive model for a high-resolution continuum model able to achieve predictions of mechanical response on significantly larger length scales. I will discuss the prospects for harnessing such computational techniques to develop computational tools suitable for prediction of the mechanical properties of additively manufactured amorphous metal parts.

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Size dependent vitrification and vitrification decoupling from α-relaxation in metallic glasses

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We have recently observed by means of fast scanning calorimetry (FSC) that reducing the sample size can profoundly impact glass formation of bulk metallic glass-forming liquids [1,2]. In samples prepared in identical conditions, we have investigated in a wide range of time scales both atomic mobility that is the rate of spontaneous fluctuations taking place in the unperturbed supercooled liquid at equilibrium, and the vitrification kinetics.

The atomic mobility remains bulk-like for all investigated sample sizes, ranging from bulk dimensions to several microns. In contrast, we observe pronounced size dependent vitrification kinetics more evident for the smallest samples and at low cooling rates. As a result, vitrification of metallic glasses takes place at temperatures lower than bulk samples for samples size below 10 μm. The glass transition is reduced up to 40 K in small samples.

The important implication of this outcome is that mild reductions of the sample size in metallic glasses allow exploring thermodynamic states, in terms of fictive temperature, deep down in the energy landscape.

[1] V. Di Lisio, I. Gallino, S. S. Riegler, M. Frey, N. Neuber, G. Kumar, J. Schroers, R. Busch, D. Cangialosi, Nature Commun. 14 (2023) 4698.
[2] X. Monnier, D. Cangialosi, B. Ruta, R. Busch, I. Gallino, Sci. Adv. 6, eaay1454 (2020).

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Predicting the failure of twodimensional silica glasses

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The key to constructing successful continuum models lies in identifying the fundamental underlying governing mechanisms. In the case of metals, dislocations, grain boundaries, and similar defects have been identified as such. Researchers have developed a hierarchical scaling approach by systematically coarse-graining these entities. However, in glasses, the underlying mechanisms governing plasticity have not yet been successfully identified.

In our study, we employ two machine learning techniques, residual neural networks (ResNet) and support vector machines (SVC) based on local symmetry functions, to detect the initiation of plasticity in two-dimensional silica samples subjected to uniaxial tension in simulations. These samples are generated using a Monte Carlo procedure and athermal quasi-static simulation conducted with LAMMPS, utilizing a potential that accurately represents the structure and mechanics of silica.

Both machine learning methods utilize features derived from the initial unstressed configuration. ResNet employs images of the entire sample, while the SVC relies solely on information from the local atomic neighborhood. ResNet demonstrates high accuracy in identifying the location of the initial bond break and predicting the crack path. To further analyze ResNet's performance, we employ attention maps generated through Gradient-weighted Class Activation Mapping (Grad-CAM). These maps correlate with topological defects and local potential energies, revealing qualitative differences in samples failing at low versus high strains. In the former case, the attention map focuses on a smaller section of the sample, whereas in the latter case, it spreads more widely.

Conversely, the SVC excels in identifying atoms involved in the first bond break, achieving a specificity of approximately 96% and an overall sensitivity of approximately 99%. However, it exhibits a false positive rate of about 4%. Given that only about 0.1% of atoms in each sample undergo the first irreversible deformation, this results in a highly imbalanced classification problem, and the false positive rate is not unexpected. Therefore, the SVC can be effectively used as a subset selection method, successfully identifying nearly all particles involved in irreversible deformation while disregarding the vast majority of elastically deforming atoms.

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Computer simulation of a polydisperse model glassformer: Localization, length scales and response to external fields

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The dynamics of a polydisperse model glassformer are investigated by augmenting molecular dynamics (MD) simulation with swap Monte Carlo (SMC) (the details of the model with a deterministic choice of particle diameters can be found in Ref. [1]). SMC leads to a drastic speed-up of structural relaxation and allows to obtain fully equilibrated liquid samples at very low temperatures, i.e. far

below the critical temperature of mode coupling theory, T_c. We elucidate the microscopic mechanism for this speed-up. It manifests in a stepwise increase of the mean squared displacement when the time scale between the application of swap sweeps is significantly larger than a characteristic microscopic time scale [2]. Compared to Newtonian dynamics, with the hybrid MD-SMC dynamics the glass transition shifts to a lower temperature and a different temperature dependence of the localization length is found. Far below $T_c%, the systems are in a transient amorphous
solid state, associated with the possibility of brittle yielding, as manifested by a sharp stress drop in the stress-strain relation and shear banding [3].

[1] N. Küchler and J. Horbach, Phys. Rev. E **106**, 064103 (2022).
[2] N. Küchler and J. Horbach, Phys. Rev. E **108**, 024127 (2023).
[3] K. Lamp, N. Küchler, and J. Horbach, J. Chem. Phys. **157**, 034501 (2022).

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Ion-irradiation-induced amorphization of high-entropy ceramic thin films

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The high-entropy materials are newly intriguing materials showing superb properties. They show both remarkable mechanical properties and radiation resistance. Particularly interesting is its incredible radiation resistance tolerance, which unfortunately remains open to debate. In this work, the radiation damage mechanism and mechanical properties of CoCrFeNiSiN high-entropy ceramic films with various nitrogen contents were studied using HRTEM and nanoindentation. The results show that, ion-irradiation-induced amorphization dominates the radiation damage mechanism. Such amorphization replaces the irradiation-induced hardening failure of most other developed high-entropy materials.

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Rayleigh scattering and disorder-induced mixing of polarization in structural glasses: theoretical developments and experimental verification

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Topological disorder leads to uneven elastic moduli on meso/nanoscale. Glasses can thus be modeled as random media with spatially fluctuating elastic moduli, linked to a stochastic Helmholtz equation and related Dyson Equation (DE). The DE yields system's elastodynamic response to impulsive force, potentially giving its full dynamics characterization, though unsolvable in state-of-the-art. We propose a DE approximate solution, the Generalized Born Approximation (GBA) [1,2]. By involving second-order terms in the self-energy's perturbative expansion, GBA surpasses Born approximation's local inhomogeneity domains-scattering treatment. GBA conveys unprecedented results in modeling acoustic-like excitations in glasses i) providing a realistic estimation of Rayleigh scattering-related attenuation strength, beyond reproducing its typical forth-power wavevector dependence; ii) describing polarization features, including the polarization mixing observed in the dynamic structure factor. Inelastic X-ray Scattering test on a complex ionic glass returned excellent agreement.
[1]Phys. Rev. B 102, 214309 (2020)
[2]Front. Phys. 6, 108 (2018)

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Tuning brittleness in multi-component metallic glasses: insights into chemical complexities and aging effects

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Shear localization in slowly-driven bulk metallic glasses (BMGs) is typically accompanied by sharp (often discontinuous) features associated with the bulk stress response as a signature of plastic yielding transition. It is well-established that the dynamical transition and its sharpness alters with the extent of local chemical ordering and microstructural complexities, being highly composition-dependent in multi-component BMGs, but also exhibit significant variations depending on the protocols used for glass preparation (i.e. thermal annealing). Here we report on atomistic simulations of six Ni-based multi-element BMGs and demonstrate that the degree of strain localization is largely controlled by compositional features as well as annealing process. By varying the glass age and chemical ingredients, we observe a distinct cross-over in strain patterns shifting from diffuse features to localized (yet system-spanning) patterns in BMGs, in a close analogy with the ductile-to-brittle transition observed in a wide spectrum of solid materials. We argue that such influence arises from the inherent interplay between aging-induced, composition-dependent icosahedral ordering and co-operative formation of shear transformation zones. The observed cross-over is quantified by measuring the susceptibility of atoms to undergo plastic rearrangements which exhibits strong (anti-)correlations to the local ordering features. Notably, the spatial correlation length tends to show certain divergence prior to yielding with a remarkable dependence on the annealing process and elemental ingredients.

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The origin of the density scaling exponent for polyatomic molecules and the estimation of its value from the liquid structure.

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In glass science, density scaling has aroused the broad attention of researchers because it expresses the complex thermodynamics of a supercooled liquid as a function of a single variable using only one parameter, the so-called scaling exponent directly related to the intermolecular potential. Accordingly, the readily available macroscopic properties could provide difficult-to-obtain information about microscopic interactions. However, so far, a complete understanding of the origin of the density scaling exponent has only been achieved for simple monoatomic molecules. Therefore, the precise interpretation of the density scaling exponent for real molecules, consisting of many different atoms and characterized by a prominent structural anisotropy, is still missing. In this study, based on molecular dynamics simulations of model systems, we provide an exact definition of the density scaling exponent value for systems composed of polyatomic molecules whose atoms interact by purely repulsive potentials. Consequently, we boldly say that our studies are a step toward explaining the origin of the scaling exponent for realistic molecules, which is necessary to take advantage of all the merits of the density scaling for real materials.

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Predicting plastic events in glasses from the topology of the vibration field

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The plastic deformation of crystals can be understood from structural defects such as disclinations and dislocations. Although also glasses are solids, their structure resembles closely the one of a liquid and hence the concept of structural defects becomes ill-defined. Rationalizing on a microscopic level the mechanical properties of glasses close to the yielding point and to relate plastic events to structural properties is therefore very challenging. Here we investigate the topological characteristics of the eigenvector field of the vibrational excitations of a simple glass model, notably its topological defects as a function of vibrational frequency. We find that if the system is subjected to a quasistatic shear, the location of the resulting plastic events correlates strongly with the topological defects that have a negative charge. Our results provide thus a direct link between the structure of glasses prior their deformation and the plastic events during deformation.

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Properties of borophosphate glasses of different compositions

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In our daily surroundings, we are used to the presence of glass to the point that its existence is barely noticeable. This universal material can be applied in various areas like telecommunication, information technology, memory storage and optics. As a consequence, the interest in glasses and their properties is increasing in recent years. Researchers all over the world investigate different kinds of glasses, including sodium borophosphate (NBP) glass, which is the subject of the presented study. We examine how different compositions and time or temperature of synthesis affect this specific kind of glass. The main goal of the research is to obtain the material with a decreased melting temperature, using micro-pulling down method. This will open the opportunity to dope glasses with different nano- and micromaterials, including those with lower melting point. It will expand the range of applications possible to achieve.

Acknowledgements:
The authors thank ENSEMBLE3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and Teaming Horizon 2020 programme of the European Commission.

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Thermodynamic and dynamic properties of a simple ellipsoidal model near the glass transition

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For the first time, the single-component ellipsoidal Gay-Berne model has been successfully used to the simulation study of the supercooled liquid state and the glass transition at elevated pressure[1]. Contrary to the single-component Lennard-Jones liquid model, the GB supercooled liquid has turned out to be characterized by the sufficient glass formation ability in the thermodynamic range giving the possibility of quite convenient investigations of the translational and rotational molecular dynamics near the glass transition. We have thoroughly explored the density scaling properties in the supercooled liquid state in the anisotropic GB model. We have confirmed the validity of the density scaling of translational and rotational relaxation times. We have investigated the molecular anisotropy effect on the role of entropy in the thermodynamic evolution of the time scale of molecular dynamics near the glass transition[2]. Also, considering the total system entropy S, the configurational system entropy Sconf, and the excess system entropy Sex, which is an excess of the ideal gas entropy in the same thermodynamic conditions as the GB liquid is examined, we gain a new insight into the linkage between molecular dynamics and thermodynamics near the glass transition.

[1] K. Liszka, A. Grzybowski, K. Koperwas, M. Paluch, Density Scaling of Translational and Rotational Molecular Dynamics in a Simple Ellipsoidal Model near the Glass Transition, 4546. https://doi.org/10.3390/ijms23094546
[2] K. Liszka, A. Grzybowski, K. Grzybowska, K. Koperwas, and M. Paluch, Entropy Scaling of Molecular Dynamics in a Prototypical Anisotropic Model near the Glass Transition. https://doi.org/10.1021/acs.jpcb.3c02429

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The role of the Eshelby back-stress in amorphous plasticity

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We study an elasto-plastic automaton model of an amorphous solid subject to athermal quasi-static shearing. Most contemporary approaches in the statistical physics community to elasto-plastic modeling of amorphous matter assume that after a region in the material yields the region will find itself in a state of zero stress. However, in the Eshelby problem, an inclusion, after it undergoes a plastic transformation, will find itself under a non-negligible negative stress, σ_c. The magnitude of σ_c depends on the Poisson ratio and the shape of the inclusion, but for a disk-shaped inclusion in two dimensions in an incompressible material, the inclusion will be under a stress of $(-1/2)$ times the shear modulus; clearly a non-negligible amount. The magnitude of σ_c monotonically decreases as the material becomes more compressible. We show that σ_c has a profound impact on yielding both in cyclic and steady shear. In both cases, the probability distribution of local stresses, $P(\sigma)$, shows a pronounced signature of σ_c. For the cyclic shear case, we show that it determines the critical cycling amplitude below which the final steady states are trivially elastic. For the steady shear case, we show that it determines the value of the flow stress for varying Poisson ratio.

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X-ray induced photoplasticity

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A solid loaded beyond the yield stress looses its elastic properties and becomes plastic. This limit for glasses is abrupt, which makes experimental investigations challenging. Here, the yield point is reached by the alternative approach of increasing the density of plastic regions by generation of point defects during X-ray irradiation. For the case of a glass of $LiBO_2$, we show that at low-dose, i.e. for a low-density of defects, the defects behave as isolated stress sources which induce atomic displacements typical of an elastic solid. As the density of defects increases, the mechanical response of the glass at the local scale changes from elastic to more and more plastic, until reaching the limit where it becomes that characteristic of a flowing system, which signals that the yield point is reached.

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Shaping the structure of material layers using pulse plasma technology

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The forming the properties of materials consists in fulfilling the sequence of different energy states. First, one should obtain the state of increased free energy, as the excited initial state for subsequent treatments and then conduct controlled relaxation of this energy excess in or-der to reach a lower level of non-equilibrium energy state of material - defined as a new degree of structure metastability, both in phase and morphological terms. This grade determines the usable properties of the material as a synthesis product. Effectiveness in implementation the above sequence, which is crucial for obtaining the desired properties of materials, is directly dependent on recognition of the synthesis environment. In the case of plasma surface engineering methods, this effectiveness is conditioned by ensuring of high levels of the energy and the degree of non-equilibrity of plasma at the same time. Additionally these conditions create a unique chance for freezing of metastable states of synthesis products on cold substrates, difficult or impossible to achieve by other means. This work will give an overview of research results concerning of use pulse magnetron sputtering method in case of synthesis of multicomponent alloy layers.

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Elasticity, Facilitation, Avalanches of Relaxation, and Dynamic Heterogeneity in Glass-Forming Liquids

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We study the role of elasticity-induced facilitation on the dynamics of glass-forming liquids by coarse-grained two-dimensional models in which local relaxation events, taking place by thermal activation, can trigger new relaxations by long-range elastically-mediated interactions. By simulations, we show that the models reproduces the main salient facts associated with dynamic heterogeneity and offers a mechanism to explain the emergence of dynamical correlations at the glass transition [1]. Moreover, we provide a theoretical description of dynamical heterogeneities, based on the premise

that relaxation occurs via local rearrangements coupled by elasticity. We find that the dynamical correlation length and correlation volume are controlled by a critical point at vanishing temperature, and predict their singular behavior in terms of the distribution of local energy barriers at T=0. We show that a decoupling between particle diffusion and relaxation time (the so-called Stoke-Einstein violation) must occur, which diverges at T=0. Our description makes a direct connection between dynamical heterogeneities and avalanche-type response [2].

[1] Ozawa and Biroli, Phys. Rev. Lett., 130, 138201 (2023)
[2] Tahaei, Biroli, Ozawa, Popovic, and Wyart, in preparation

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Zero-parameter theories for low-temperature melting lines of repulsive particles

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Short-ranged repulsive pair-potentials, such as harmonic-repulsive and Hertzian spheres in two and three dimensions [1-3], are commonly used in models of metallic alloys, colloids, and coarse-grained models of molecular systems. This study aims to develop and assess the accuracy of zero-parameter theories for the melting lines. We provide closed-form expressions for the shape of the fcc-fluid coexistence line by i) mapping particle interactions to hard spheres (HS) and ii) utilizing the more recent isomorph theory of melting [4,5]. The results suggest that the general framework of isomorph theory provides an attractive alternative to the classic HS theories [2].

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Enhanced optical performance of nanoplasmonic cavity glasses

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Plexcitonic systems combine plasmonic properties and excitonic emission which results in improved performance of the system by e.g. fast and intense luminescence, desirable in optoelectonic devices, ultrafast optical switches and quantum information science.

Here, we demonstrate optically active volumetric materials obtained with micro-pulling down method. By applying NanoParticle Direct Doping Method, nanocomposites with plasmonic properties are fabricated, which allows us to observe enhanced optical features. New generation of plasmonic materials are manufactured by NanoParticle-Direct Doping method developed in our laboratory. The possibility of direct introduction of plasmonic particles lets us easily dope glasses with nanoparticles of various electromagnetic properties, thus tuning LSPR to enhance the targeted effects, e.g. PL of quantum dots.
Combining research on both fabrication and characterization of the novel materials with unusual electromagnetic properties may result in development of low-cost photonic devices with enhanced functionalities.

Acknowledgements:
The authors thank ENSEMBLE3 Project (MAB/2020/14) which is carried out within the International Research Agendas Programme (IRAP) of the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund and Teaming Horizon 2020 programme of the European Commission.

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Yielding, avalanches and clusters in silica and other model glasses

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Results from computer simulations will be presented concerning the yielding of the BKS model of silica, in comparison with other atomic glasses that have been investigated, under cyclic shear deformation. The nature of avalanches and clusters associated with plastic rearrangements and the nature of structural change. Although qualitative aspects of yielding in silica are similar to other glasses, the statistics of clusters exhibits significant differences, which we associate with differences in local structure. Across the yielding transition, anomalous structural change and densification, associated with a suppression of tetrahedral order, is observed to accompany strain localization.

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Analogies between growing dense active matter and soft driven glasses

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We develop a minimal model to describe growing dense active matter such as biological tissues, bacterial colonies and biofilms, that are driven by a competition between particle division and steric repulsion. We provide a detailed numerical analysis of collective and single particle dynamics. We show that the microscopic dynamics can be understood as the superposition of an affine radial component due to the global growth, and of a more complex non-affine component which displays features typical of driven soft glassy materials, such as aging, compressed exponential decay of time correlation functions, and a crossover from superdiffusive behaviour at short scales to subdiffusive behaviour at larger scales. This analogy emerges because particle division at the microscale leads to a global expansion which then plays a role analogous to shear flow in soft driven glasses. We conclude that growing dense active matter and sheared dense suspensions can generically be described by the same underlying physics.

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Investigation of Plasmon induced luminescence enhancement on Eu3+ doped sodium borophosphate glasses for optical application

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Influence of noble metal nanoparticles assisted luminescence enhancement on the co-doped glasses gathered more attention on recently due to its versatile application in the field photonics, plasmonics and photovoltaics. Present case, we prepared rare-earth Eu3+ ions and 20-30 nm sized silver nanoparticles (Ag NPs) doped sodium borophosphate (NBP) glasses by nano particle direct doping method (NPDD) [1,2]. The nano silver (Ag NPs) concentration was varied between the samples (0.1, 0.3 and 0.5 wt%), while the concentration about rare-earth ion (Eu3+) was kept constant (0.5 wt%). Further, here we investigated the impact of plasmon induced luminescence characterises on co-doped samples. The localized surface plasmon resonance (LSPR) band at 404 nm & 3.07 eV in both absorption, optical extinction spectra clearly describe the success of distribution of silver nanoparticles over the glass matrix. The luminescence characteristics of NBP: Eu and NBP: Eu, Ag NPs were performed with different laser excitations 325, 473 and 532 nm, respectively. The luminescence regarding 5D0-7FJ transitions from Eu3+ ion was observed in the emission spectra. The observed emission enhancement in the material co-doped with Eu and Ag NPs can be interpreted as the plasmonic effect coming from metallic nanoparticles in the vicinity of Eu3+. In addition, the photometric parameters were calculated for the co-doped samples; which elucidates that the samples having prominent red emission. It would be useful as a sufficient red emitter for tri-color converted white emitter applications.

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Decoupling of Ion Transport and Structural Dynamics in Ionic Glassformers

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Since the discovery of the so-called superionic glass in 1972, which shows anomalously high ionic conductivity in a glassy state, the origin and the mechanism of this fast ionic transport have been studied for around 50 years. The first cornerstone was laid by C. A. Angell in 1983, which suggested the breakdown of the Stokes-Einstein law and introduced the Decoupling index R defined as the ratio of conductivity relaxation time to structural relaxation time. After that, various experimental evidences have been accumulated to convince the importance of the decoupling index R in various glass-forming systems. This talk will discuss the molecular origin of a decoupling phenomenon in different ionic glass-forming liquids and solids. Specifically, the cases of protic and aprotic ionic liquids, polymerized ionic liquids, and ionic nanocomposites will be presented. The importance of pressure behavior of the decoupling index will also be highlighted.

This research was funded in whole by National Science Center, Poland [Opus 21,2021/41/B/ST5/00840].

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Recent developments in additive manufacturing of metallic glasses and their composites

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Although metallic glasses (MG) have extraordinary mechanical and chemical properties, their industrial use still needs to be improved due to the low number of glass-forming alloys with high glass-forming ability (GFA), toughness, and processability.
However, the dynamic growth of laser-based Additive Manufacturing (AM) can provide a cost-effective way of producing MGs in bulk form regardless of their GFA. Although the process optimization compromises both porosity and crystallinity reduction, the non-equilibrium nature of MGs can be maintained in bulk material through high heating and cooling rates.
This trade-off has been overcome by a new AM scanning strategy and post-processing methods, which achieved high amorphous phase content with good density by finetuning double laser exposure in a key-hole mode and separating scanning lines. With selective devitrification in the heat-affected zone, fiber-like glassy-crystalline composites have been formed with full control over the microstructure.
To eliminate residual porosity without visible crystallization, hot isostatic pressing (HIP) was performed on amorphous and composite samples. This method has been successfully applied to process Zr-, Fe-, and Mg-based MGs with high and low GFA via AM. Comprehensive guidelines for MGs and their composite formation via AM are provided, including procedures for quick process optimization.