

Publication Highlights:

[N. V. Priezjev](#), “The effect of cryogenic thermal cycling on aging, rejuvenation, and mechanical properties of metallic glasses”, *Journal of Non-Crystalline Solids* **503**, 131 (2019). [DOI](#)

The development of novel processing routes including thermal and mechanical treatments of metallic glasses is important for numerous structural and biomedical applications. In the first of several papers on the topic, I studied the influence of *repeated heating and cooling* on mechanical properties, structural relaxation, and evolution of the potential energy in metallic glasses using molecular dynamics (MD) simulations. Interestingly, I found that poorly-annealed glasses are relocated to progressively lower levels of potential energy over consecutive cycles, whereas well-annealed glasses can be rejuvenated at sufficiently large thermal amplitudes. Moreover, it was shown that the structural transition to different energy states proceeds via collective *nonaffine displacements* of atoms that are organized into clusters, whose typical size becomes larger with increasing cooling rate or thermal amplitude. The main conclusion is that the elastic modulus and the peak value of the stress overshoot exhibit distinct maxima at the thermal amplitude, which corresponds to the minimum of the potential energy. [Online presentation](#).

[N. V. Priezjev](#), “The yielding transition in periodically sheared binary glasses at finite temperature”, *Computational Materials Science* **150**, 162 (2018). [DOI](#), [PPT](#)

In a series of recent papers, I investigated the structural relaxation and dynamic behavior of amorphous materials subjected to periodic shear deformation. In general, the mechanical response depends sensitively on the strain amplitude, preparation history, loading conditions, and temperature. More specifically, I showed that below yield, rapidly quenched glasses can be *mechanically annealed* toward lower potential energy states, and the energy levels that can be accessed after hundreds of shear cycles become deeper at larger strain amplitudes. At the critical strain amplitude, the transition from slow to fast relaxation dynamics is associated with the largest number of *dynamically correlated* atoms, as indicated by the peak value of the dynamical susceptibility. Furthermore, it was demonstrated that after a certain number of transient cycles, the yielding transition at finite temperature is accompanied by the formation of a system-spanning shear band of large nonaffine displacements in both well and poorly annealed glasses. On the other hand, below the yielding point, binary glasses start to deform reversibly after a number of transient cycles and nonaffine displacements become organized into compact clusters.

[N. V. Priezjev](#) and [M. A. Makeev](#), “Strain-induced deformation of the porous structure in binary glasses under tensile loading”, *Computational Materials Science* **150**, 134 (2018). [DOI](#)

In the last few years, my colleague and I published 7 papers on structural transformations and mechanical properties of porous glasses under various loading conditions. We considered vitreous systems obtained in the process of phase separation taking place after a rapid isochoric quench of a glass-forming liquid to temperatures well below the glass transition. The porous structure in undeformed samples varies from a connected porous network to a random distribution of isolated pores with increasing average density. We generally find that during compressive (or tensile) loading, the porous structure is linearly transformed in the elastic regime, and the elastic modulus follows a power-law increase as a function of the average glass density. Upon further loading, the

pores become significantly deformed and coalesce into larger voids that leads to formation of system-spanning empty regions associated with failure of the material. These results are important for design of porous absorbent materials and structural applications. [Online presentation](#).

T. Darvishzadeh and N. V. Priezjev, “Effects of crossflow velocity and transmembrane pressure on microfiltration of oil-in-water emulsions”, *Journal of Membrane Science* **423**, 468 (2012). [DOI](#)

In collaboration with my Ph.D. student T. Darvishzadeh, we have focused on the problem of oil removal from water using hydrophilic porous membranes. In practice, the efficient separation of oil-in-water dispersions should involve high flux of water through the membrane and, at the same time, high rejection rate of the oil phase. In our first study, the effects of transmembrane pressure and crossflow velocity on rejection of oil droplets and thin oil films by pores of different cross-section were investigated numerically by solving the Navier-Stokes equation. We found that in the absence of crossflow, the critical transmembrane pressure, which is required for the oil droplet entry into a circular pore of a given surface hydrophilicity, agrees well with analytical predictions based on the Young-Laplace equation. With increasing crossflow velocity, the shape of the oil droplet is strongly deformed near the pore entrance and the critical pressure of permeation increases. As a result, we determined numerically the *phase diagram* for the droplet rejection, permeation, and breakup depending on the transmembrane pressure and shear rate. The insights that our study offers into droplet behavior at the membrane surface might have important implications for the design of novel membranes. [Online presentation](#). *Over 80 citations*.

A. Niavarani and N. V. Priezjev, “Rheological study of polymer flow past rough surfaces with slip boundary conditions”, *Journal of Chemical Physics* **129**, 144902 (2008). [DOI](#)

With my Ph.D. student A. Niavarani, we have studied the slip phenomena in thin polymer films confined by periodically corrugated surfaces using MD and continuum simulations. We found that for rough surfaces with wavelength larger than the polymer chain size, the effective slip length decays monotonically with increasing amplitude of the surface roughness. At small amplitudes, this decay is reproduced accurately by the numerical solution of the Navier-Stokes equation with the local slip condition. When the corrugation wavelengths are comparable to the chain size, polymer chains stretch in the direction of shear flow above the crests of the surface corrugation, while the chains located in the grooves elongate perpendicular to the flow. In this regime, the continuum approach fails to describe accurately the rapid decay of the effective slip length with increasing wavenumber.

N. V. Priezjev, A. A. Darhuber, S. M. Troian, “Slip behavior in liquid films on surfaces of patterned wettability: Comparison between continuum and molecular dynamics simulations”, *Physical Review E* **71**, 041608 (2005). [DOI](#), [PPT](#)

While at Princeton University, we have investigated the behavior of the *effective* slip length in simple fluids, which are subject to planar shear in a cell with mixed surface boundary conditions (BC). The shear flow was induced by translating the upper wall with a constant velocity, while the lower stationary wall with mixed BC was patterned by a periodic array of stripes representing alternating regions of finite slip and no-shear, *i.e.*, perfect slip. Such a surface provides an approximation to a periodic array of experimentally observed flat *nanobubbles* attached to the

wall. A detailed comparison between continuum analysis and MD simulations at low shear rates indicated that there is excellent agreement between the velocity profiles and the effective slip lengths when the characteristic length scale of substrate inhomogeneities is larger than approximately 30 molecular diameters. Remarkably, these results demonstrated that molecular level simulations can successfully reproduce hydrodynamic predictions provided that the length scales of surface patterns are large compared to the liquid molecular size. [Online presentation](#). *Over 300 citations*.

[N. V. Priezjev](#) and S. M. Troian, “Molecular Origin and Dynamic Behavior of Slip in Sheared Polymer Films”, *Physical Review Letters* **92**, 018302 (2004). [DOI](#)

During my postdoctoral appointment at Princeton, I investigated transport properties of simple and polymeric liquids in nanofluidic systems using molecular dynamics simulations. I performed a detailed statistical mechanical analysis of the two-dimensional ordering of a liquid film parallel to a solid wall for a confined polymer melt in order to explore the characteristics of slip behavior at the interface. There is strong evidence that the molecular origin and dynamic behavior of slip, which has been described for simple fluids, is more generally applicable to polymeric systems even when the fluids exhibit non-Newtonian behavior. In addition, our studies have shown that beyond a polymer chain length of about ten constitutive units, the molecular weight dependence of the slip length correlates strongly with the fluid viscosity. *Over 200 citations*.

[N. V. Priezjev](#) and R. A. Pelcovits, “Surface extrapolation length and director structures in confined nematics”, *Physical Review E* **62**, 6734 (2000). [DOI](#)

During my doctoral study, I investigated surface-induced director structures in nematic liquid crystals confined to cylindrical cavities with homeotropic (perpendicular) anchoring using Monte Carlo simulations. In this particular geometry there exists an interesting interplay between bulk and surface energies, which results in different director configurations inside the cylindrical pore. This work reconciled the apparent contradictions between the results of earlier simulations and approximate analytic theories. We demonstrated that care must be taken in comparing the parameters used in the two approaches; in particular, the parameters of the analytic theories are strongly temperature dependent. It was also found that the rate at which we cooled the system from the isotropic to nematic phase played a crucial role in the development of the final director structure, because of a large free energy barrier separating different director structures. *Over 30 citations*.

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