# Synopsis

Metallic glasses (MGs), which are metals solidified in an amorphous state, have shown attractive mechanical properties such as high strength (up to 5 GPa), yield strain (around 2%) and good corrosion resistance. They exhibit heterogeneous plastic flow by formation of shear bands (SBs) at temperatures well below the glass transition temperature. However, they can be very brittle with $K_{Ic} \sim 1$ - 15 MPa$\sqrt{m}$ or very tough ($K_{Ic} \sim 80$ MPa$\sqrt{m}$). Experiments and MD simulations suggest that failure in the brittle MGs occurs by cavitation with little shear banding and can be traced to nanoscale fluctuations in atomic density. Also, notwithstanding their high $K_{Ic}$, MG samples lack tensile ductility and fail catastrophically by crack propagation in a dominant SB. However, nano-sized MG samples and a novel architecture called as nanoglass (NG) composed of nano-grains of MGs separated by fine free volume rich interfaces do exhibit tensile ductility. Relatively few continuum simulations have been undertaken to understand the deformation and fracture behavior of MGs and NGs from a mechanics standpoint. Therefore, continuum finite element analysis of cavitation and cavitation induced fracture in brittle MGs are performed in this work. In addition, tensile deformation behavior of nano-scale notched MG and NG samples are analyzed.

Brittle MGs are modeled as heterogeneous elastic-plastic solid containing doubly periodic distribution of weak zones with lower yield strength. The presence of the weak zones mimics the density/strength fluctuation in brittle MGs as observed in experiments and atomistic simulations. Finite element simulations are performed by subjecting a square unit cell containing a circular weak zone to different (biaxiality) stress ratios under 2D plane strain conditions. A tiny void is introduced in the weak zone to trigger

cavitation. The results show that the critical hydrostatic stress at cavitation is reduced due to the presence of the weak zones and is governed by yield properties of the weak zone and the prevailing stress state. Moreover, unlike in a homogeneous plastic solid, the cavitation stress of the heterogeneous aggregate does not reduce appreciably as the stress ratio decreases from unity when the yield strength of the weak zone is low. The volume fraction of the weak zones and stress ratio influence the nature of cavitation bifurcation. This includes the possibility of snap cavitation wherein a void of finite size suddenly forms in the intact material which does not happen in a homogeneous plastic solid.

Further, continuum simulations of crack initiation under mode-I plane strain, small scale yielding conditions in a heterogeneous elastic-plastic solid having a distribution of weak zones are performed. The results show that a three-step process is involved in the catastrophic fracture observed in brittle MGs. First, cavities nucleate in weak zones ahead of the crack tip and start growing rapidly. Secondly, curved shear bands form linking the current crack tip with the nearby cavity. Thirdly, as plastic strain and free volume accumulate within these shear bands, failure takes place facilitating further extension of the crack. The proposed fracture mechanism explains the formation of nano-corrugations in brittle MGs. The results also predict a correlation between notched fracture toughness and Poisson's ratio and brittle-ductile transition which is qualitatively similar to that observed in experiments.

the deformation behavior of nano-sized notched MG samples subjected to plane strain tensile loading is modeled through finite element simulations using a non-local plasticity theory for MGs. The results show that a plastic zone first develops around the notch root and grows to a critical size before a dominant shear band emanates from this zone that would lead to failure. The SB width and the saturation notch root plastic zone size scales with an intrinsic material length $l_c$ associated with interaction stress between flow defecrs. Also, the ratio of the ligament length to saturation plastic zone size governs the transition from shear banding to necking.

The deformation behaviour of NGs subjected to plane strain tensile loading is investigated through finite element simulations using the above non-local plasticity theory. It is found that the ratio of the material length $l_c$ to nano-grain size governs the deformation behavior of NGs. Also, SB width scales in same manner with $l_c$ both in MG and NG specimens and moderate changes in specimen size have little effect on mechanical response of NGs.