Atomistic Study of the Mechanical Properites of a Sintered Bulk Metallic Glass (Nanoglass)

Franco Ardiani[a] (francoamg@gmail.com), Andrés A. Manelli[a], Carlos J. Ruestes[b,c], Claudio A. Careglio[a] and Eduardo M. Bringa[b,c]

[a]Facultad de Ingeniería, Universidad Nacional de Cuyo
[b]FCEN, Universidad Nacional de Cuyo
[c]CONICET

April 24, 2015

Acknowledgements:
We thank support from SeCTyP-UNCuyo grant B008. EMB and CJR also thank support from PICT-PRH 0092.

Contents

Introduction

- Metallic Glass: amorphous metal (without crystalline order).
- Has advantages over crystalline metals, like elasticity combined with high resistance, strength and moldability.
- Plasticity in these materials occurs by nucleation of shear transformation zones which grow into shear bands.
- Shear bands may lead to brittle failure (heterogeneous deformation): importance of **preventing their propagation**.
- A more homogeneous deformation may be achieved by adding **porosity**.

Introduction

- Metallic Glass: amorphous metal (without crystalline order).
- Has advantages over crystalline metals, like elasticity combined with high resistance, strength and moldability.
- Plasticity in these materials occurs by nucleation of shear transformation zones which grow into shear bands.
- Shear bands may lead to brittle failure (heterogeneous deformation): importance of **preventing their propagation**.
- A more homogeneous deformation may be achieved by adding **porosity**.

- Example applications for MGs: amorphous structural steels, biomedical materials, aerospace materials, etc.
- Production of MGs: techniques which include high quenching rates, low volumes and composition control.
- STZs and SBs: STZs are small zones of intense shearing strain, consisting of a few atoms. A SB contains more atoms and has a different aspect ratio.
- Porosity to evitate the propagation of SBs: related to the way of preventing dislocation motion in metals.
- MD (Molecular Dynamics): solves problems with many atoms, interacting through an interatomic potential or force field.

Simulation details

- Software: Lammps (lammps.sandia.gov) for simulation, Ovito (www.ovito.org) and Gnuplot for analysis.
- Sample: based on Cu_{46} Zr_{54} described by Arman et al. (2010).
  - Cooling rate 10^{12} K/s.
- EAM (Embedded Atom Method; Daw, 1984) alloy potential adopted (Cheng, 2008).

Arman B., Luo S.-N., Germann T.C. and Cağin T., *Phys. Rev. B.*, **81**, 144201 (2010).
Daw M. and Baskes M.I., *Phys. Rev. B.*, **29**:6443-6453 (1984).
Cheng Y.Q., Sheng H.W. and Ma E., *Phys. Rev. B.*, **78**, 014207 (2008) https://sites.google.com/site/eampotentials/

Simulation details

- Software: Lammps (lammps.sandia.gov) for simulation, Ovito (www.ovito.org) and Gnuplot for analysis.
- Sample: based on Cu_{46} Zr_{54} described by Arman et al. (2010).
  - Cooling rate 10^{12} K/s.
- EAM (Embedded Atom Method; Daw, 1984) alloy potential adopted (Cheng, 2008).

EAM

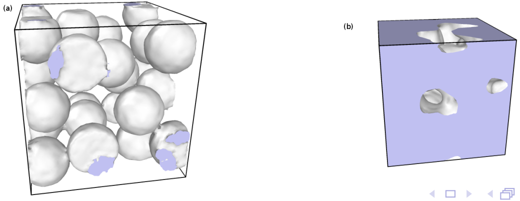
$$E_i = F_\alpha\left(\sum_{i\neq j}\rho_\beta(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j}\phi_{\alpha\beta}(r_{ij})$$

- EAM: the total energy E_i of an atom i is given by this equation, where F is the embedding energy which is a function of the atomic electron density ρ, ϕ is a pair potential interaction, and α and β are the element types of atoms I and J. The multi-body nature of the EAM potential is a result of the embedding energy term. Both summations in the formula are over all neighbors J of atom I within the cutoff distance.

Porous sample preparation

Procedure

1. Random placement of 2.5 nm radius spheres.
2. Relaxation @ 650K (constant volume, few ps).
3. Up to 10 ps of compressive pressure (400 bar).
4. Repeat two previous steps.
5. Further relaxation: cooling to zero T, barostat to zero pressure, heating to simulation temperature and, barostat to zero pressure (5 ps, constant T)



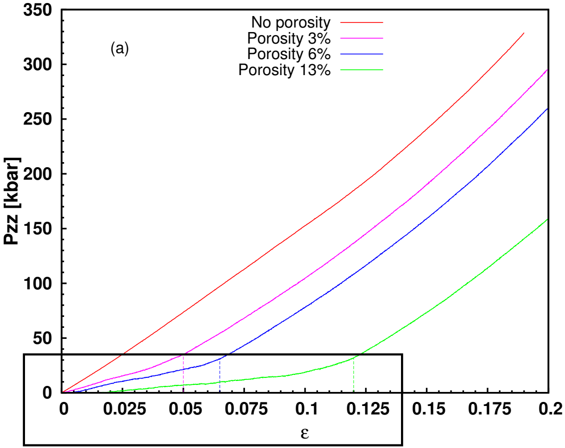
Results

Samples and loading

- Took samples of different initial porosities (3.3%, 5.8% and 13.1%).
- Loading at a strain rate of $10^9/s$, appropiate for shock compression experiments.
- Purely uniaxial strain.
- Periodic boundary conditions.

Results

Compression

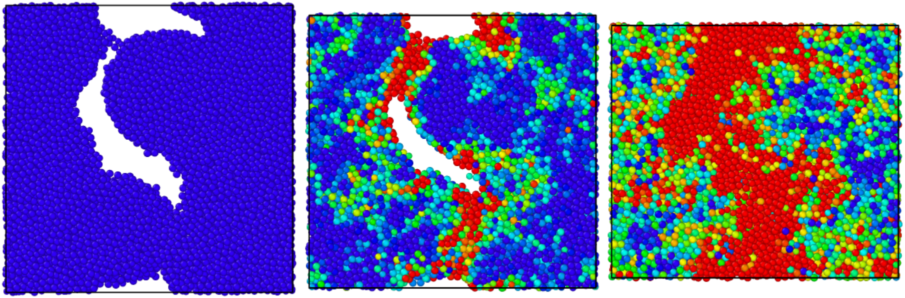


After pore closure, curves are similar to the one for no porosity. There is significant hardening after pore closure.

Before pore closure, strain increases while maintaining low stress levels.
Porosity produces shear concentration, and pores start to collapse.

Results

Compression

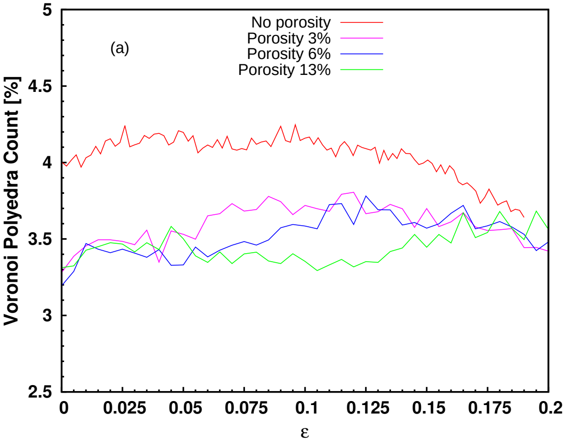


Shear strain coloring for a thin slice of the 13% porosity sample. Strains are 0, 5 and 12%
Blue correspondes to shear strain lower than 10%, and red to shear strain greater than 30%

Pores act as stress concentrators.
They also impede incipient shear band formation.
Accumulation of strain along diagonal directions, as in incipient shear banding.

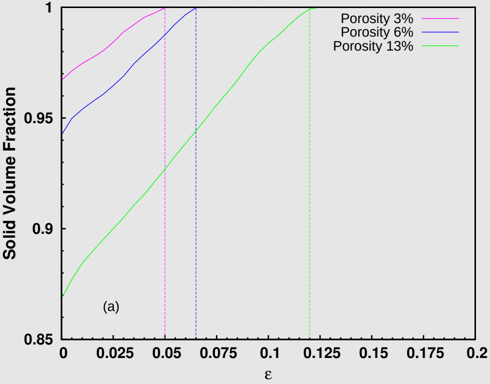
Results

Compression



The fall in the number of Type 3 atoms after a constant stage has been thought to be an indicator of the onset of plasticity (Arman, 2010).

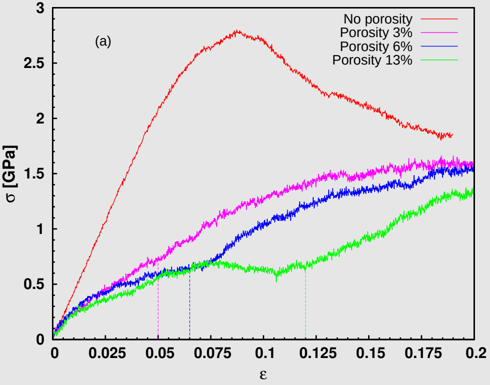
Counter-intuitive result. Here we do have plasticity but there is almost no change in Voronoi polyhedra.
Other processes involved?



Solid volume fraction versus strain.

The dashed lines show when pores totally close. The values are:

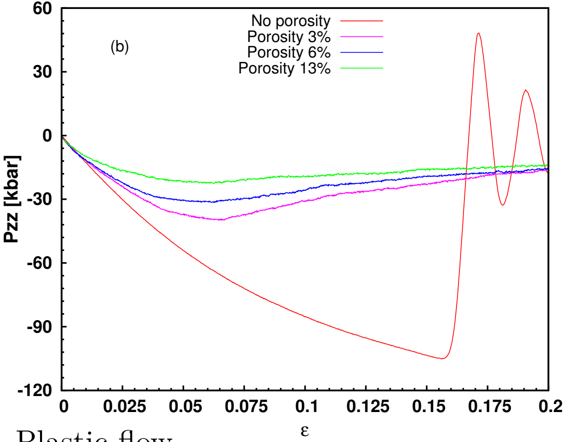
$3\% \rightarrow 0.05, 6\% \rightarrow 0.065, 13\% \rightarrow 0.12$

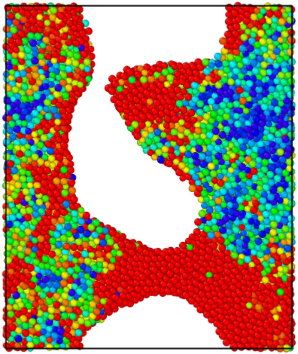


Von Mises stress versus strain.

Results

Tension





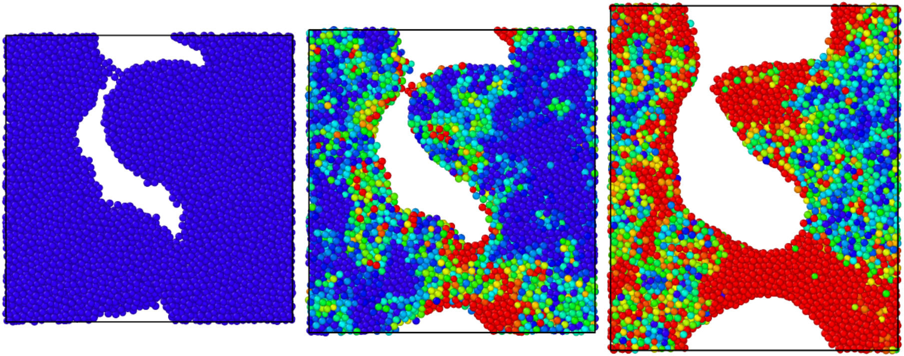
Shear strain coloring of the 13% porosity sample's slice at 20% strain.

Plastic flow.

The use of periodic boundary conditions precludes the closing of the voids (there is no necking).

Results

Tension

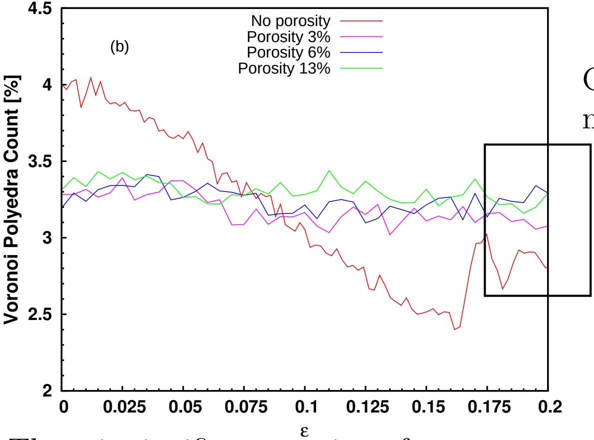


Shear strain coloring of a thin slice of the 13% porosity sample. Strains are 0, 6 and 20%
Blue correspondes to shear strain lower than 10%, and red to shear strain greater than 30%

Shear strain is mostly concentrated around the pores.

Results

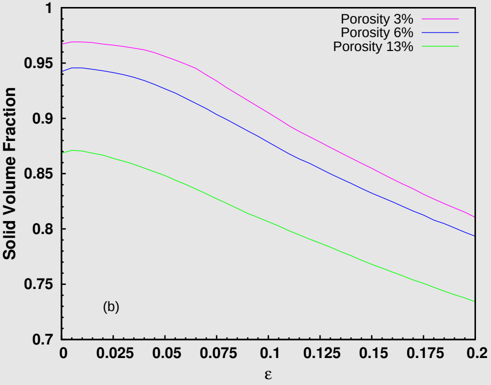
Tension



Constant after void nucleation.

There is significant motion of atoms around pores, preventing the formation of STZs other than the ones around the pores.

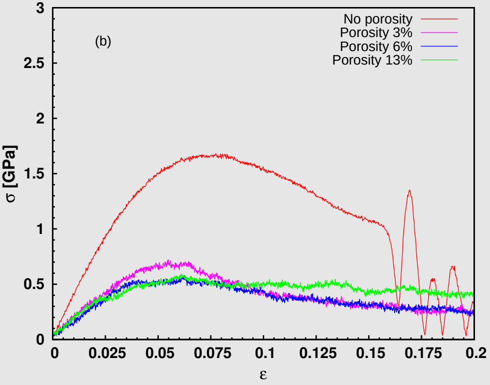
└─Results



Solid volume fraction versus strain.

Study of Sintered BMG
└─Results

└─Results



Von Mises stress versus strain.

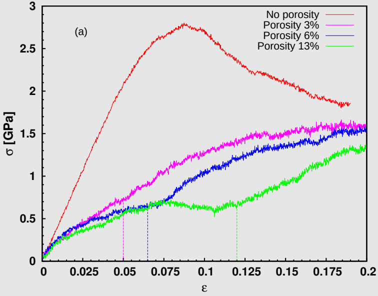
Conclusions

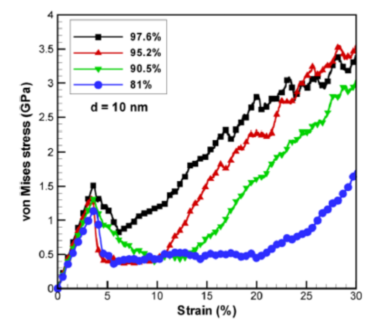
- Sintering process leads to glass with taylored porosity values.
- Under compression: pores act as stress concentrators but also delay nucleation of SBs. After closure, there is hardening.
- Under tension: pores do not close and they concentrate plastic flow around them, also impeding formation of STZ and SBs.
- Results under strain were somewhat comparable to the ones by Yuan et al. (2014), where a single crystal sample with voids was studied.

Yuan F. and Wu X., *AIP ADVANCES*, **4**, 127109 (2014).

Conclusions

- Sintering process leads to glass with taylored porosity values.
- Under compression: pores act as stress concentrators but also delay nucleation of SBs. After closure, there is hardening.
- Under tension: pores do not close and they concentrate plastic flow around them, also impeding formation of STZ and SBs.
- Results under strain were somewhat comparable to the ones by Yuan et al. (2014), where a single crystal sample with voids was studied.

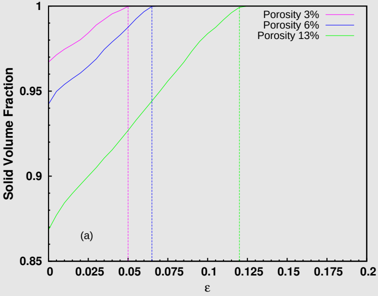


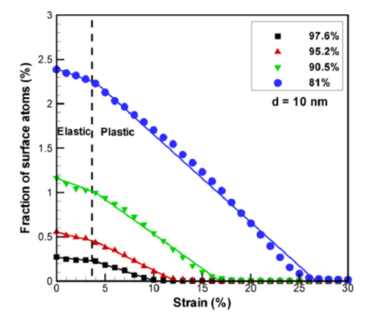


Yuan F. and Wu X., *AIP ADVANCES*, **4**, 127109 (2014).

Conclusions

- Sintering process leads to glass with taylored porosity values.
- Under compression: pores act as stress concentrators but also delay nucleation of SBs. After closure, there is hardening.
- Under tension: pores do not close and they concentrate plastic flow around them, also impeding formation of STZ and SBs.
- Results under strain were somewhat comparable to the ones by Yuan et al. (2014), where a single crystal sample with voids was studied.





Yuan F. and Wu X., *AIP ADVANCES*, **4**, 127109 (2014).

Atomistic Study of the Mechanical Properites of a Sintered Bulk Metallic Glass (Nanoglass)

Franco Ardiani[a] (francoamg@gmail.com), Andrés A. Manelli[a], Carlos J. Ruestes[b,c], Claudio A. Careglio[a] and Eduardo M. Bringa[b,c]

[a]Facultad de Ingeniería, Universidad Nacional de Cuyo
[b]FCEN, Universidad Nacional de Cuyo
[c]CONICET

April 24, 2015

Acknowledgements:
We thank support from SeCTyP-UNCuyo grant B008. EMB and CJR also thank support from PICT-PRH 0092.