Microstructure formation of metallic nanoglasses and their mechanical properties

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Background and motivation

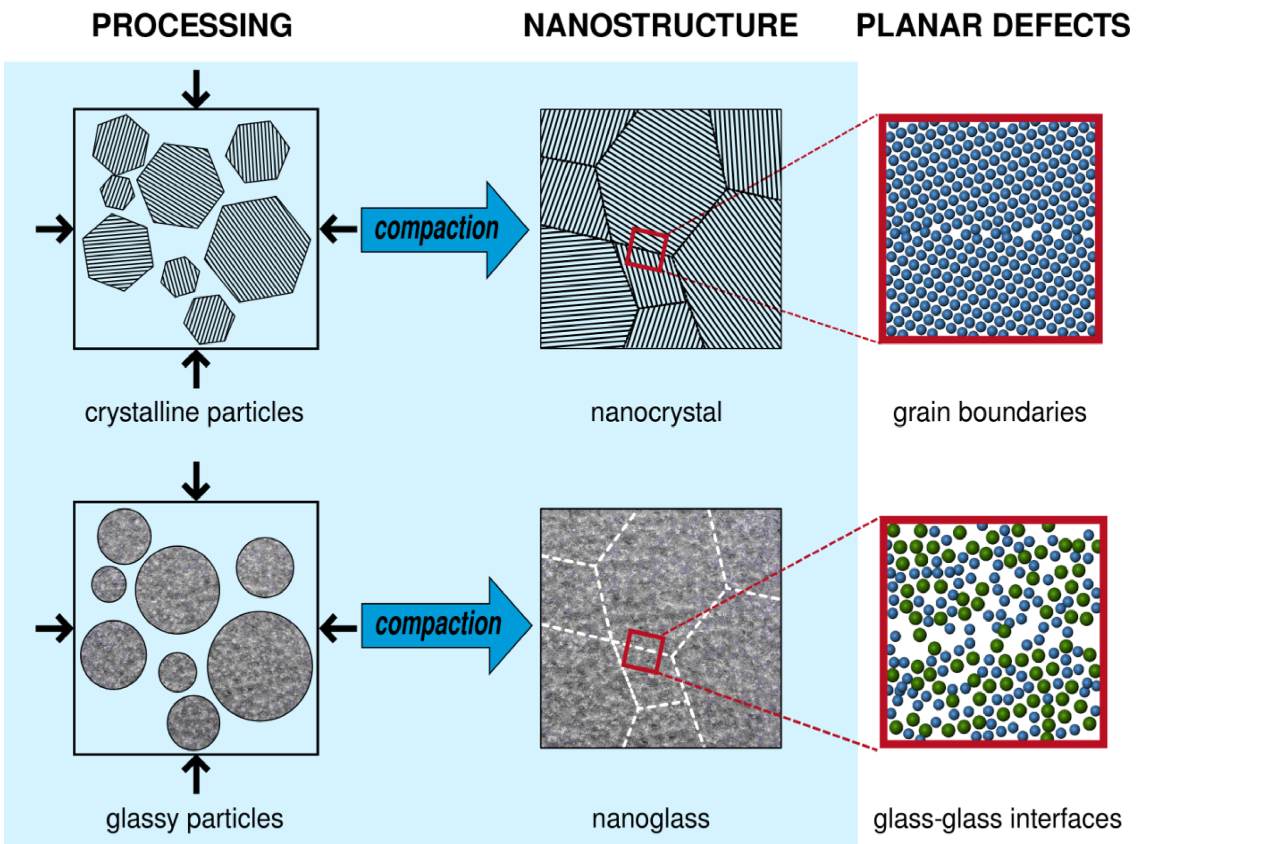
Bulk metallic glasses combine unique mechanical properties, such as high strength and hardness with substantial fracture toughness. However, their strong tendency towards shear localization results in macroscopically brittle failure at room temperature.
One promising way to improve the plasticity is to use metallic nanoglasses. Metallic nanoglasses consist of glassy grains connected with glass-glass interfaces [1].

Objectives: Investigate the microstructure of nanoglasses and their mechanical properties.

Method

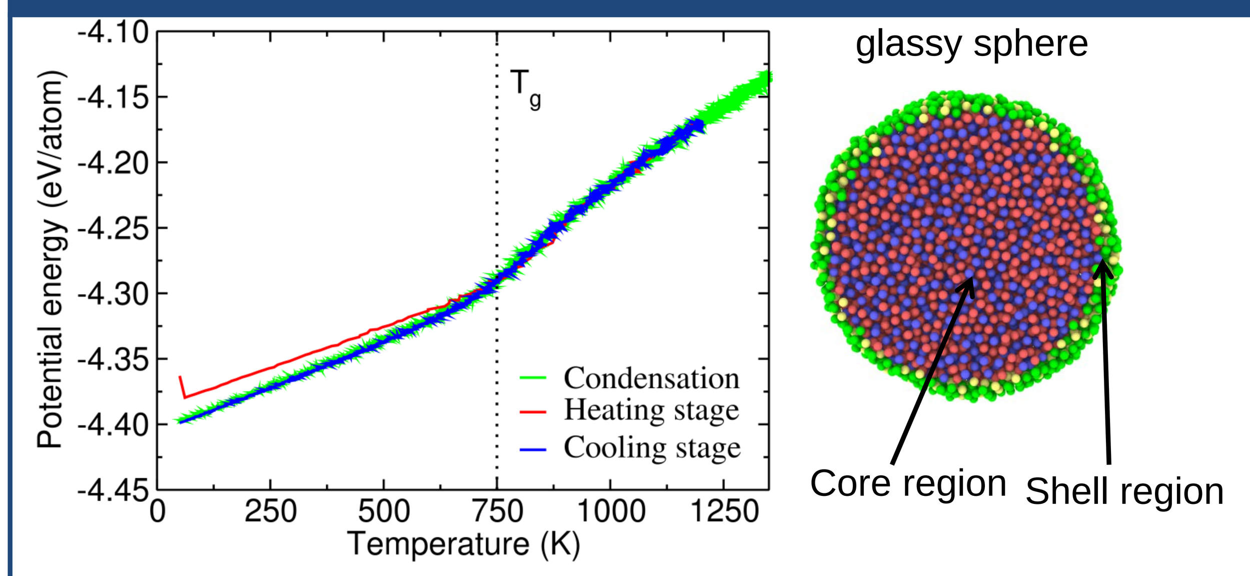
- Classical molecular dynamics (MD), LAMMPS. System size is about 3.10^6 atoms.
- Interatomic potential: Finnis-Sinclair-type potential for Cu-Zr
- Sample preparation by melt quenching (dT/dt = 0.01 K/ps)
- Nanoglass: Cold-compaction of nanometer-sized glassy spheres which are prepared by inert-gas condensation technique
- Atomic scale deformation mechanisms : Local atomic von Mises strain η

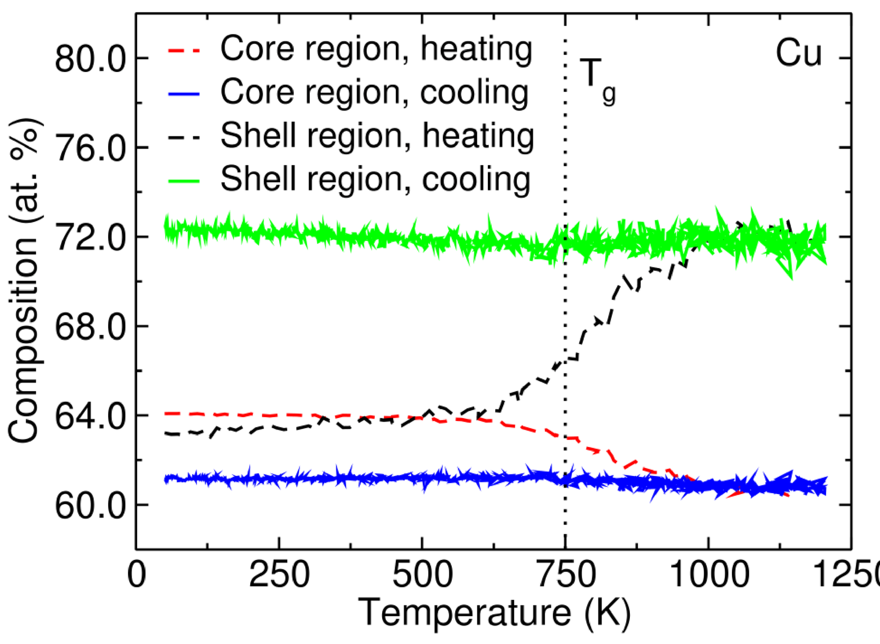
The concept of nanoglass



The basic idea is to generate a new kind of glass with a possibility to modify the defect and/or the chemical microstructures of glasses in a way comparable to the methods that are used today for crystalline materials [1].

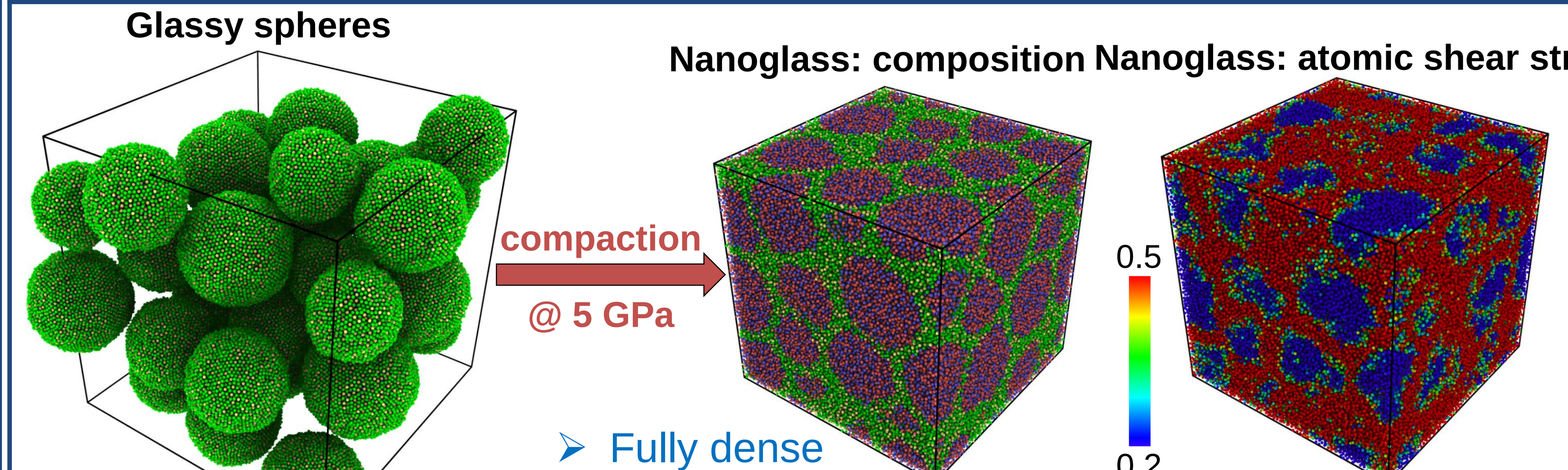
Glassy particle in inert-gas condensation



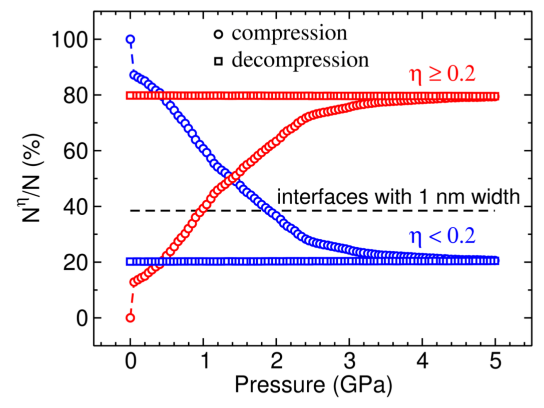


- Compositional variations result from surface segregation effects already present in the primary glassy particles [2].

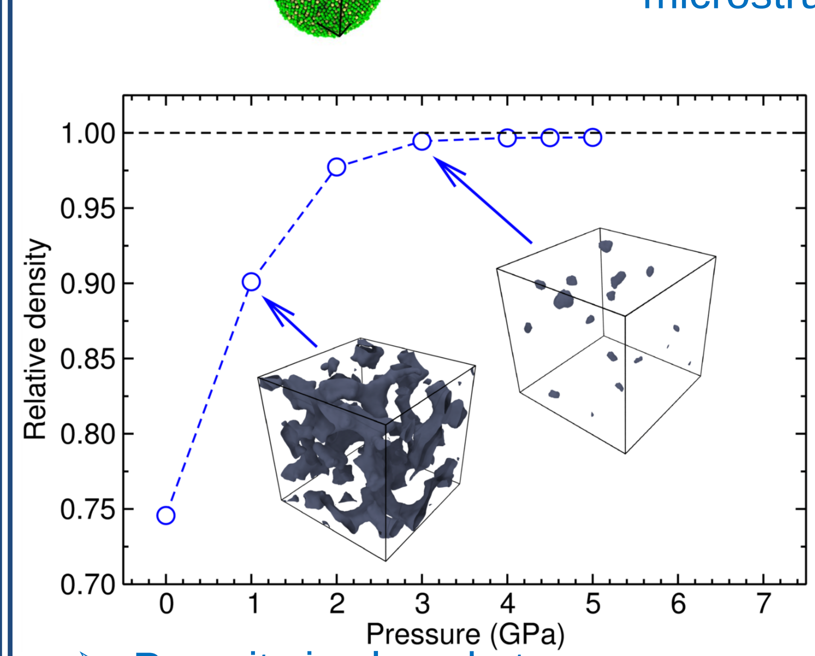
Formation of nanoglass microstructure



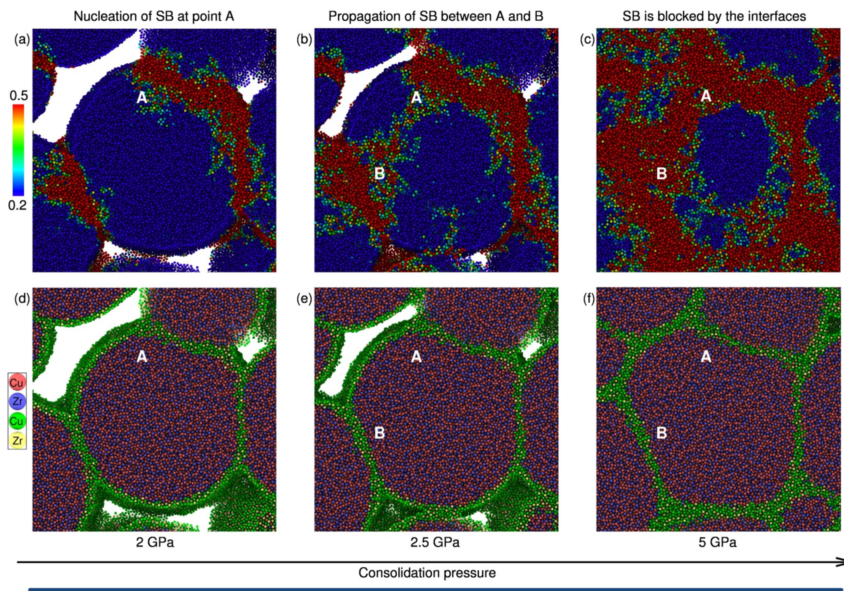
- Fully dense microstructure



- 80% of atoms are massively sheared: defective short-range order [3].



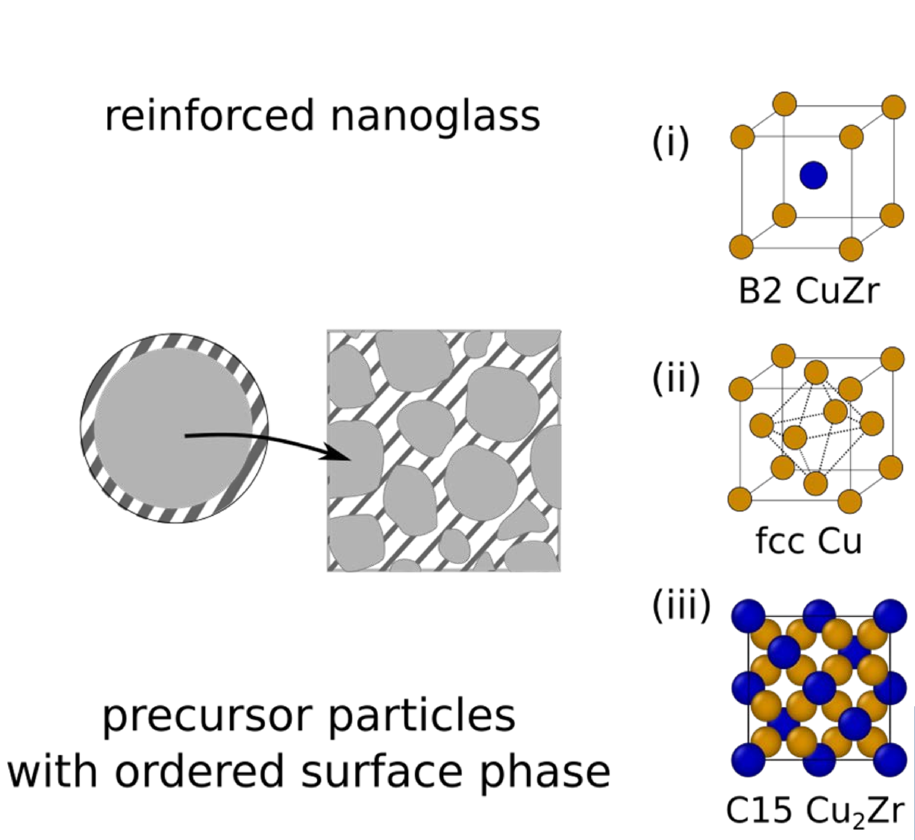
- Porosity is closed at pressure of 5 GPa [3].



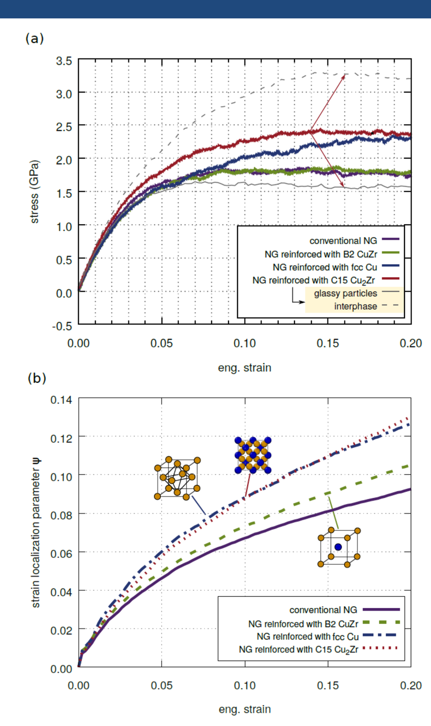
Shear band (SB) formation in a glassy sphere during the consolidation [3].

- At 2 GPa (image (a)), a SB nucleates from the interfaces, point A, and with further loading the SB propagates to point B. SB is blocked by the interfaces: the interfaces do not mix with the glassy regions (images (c) and (f)).

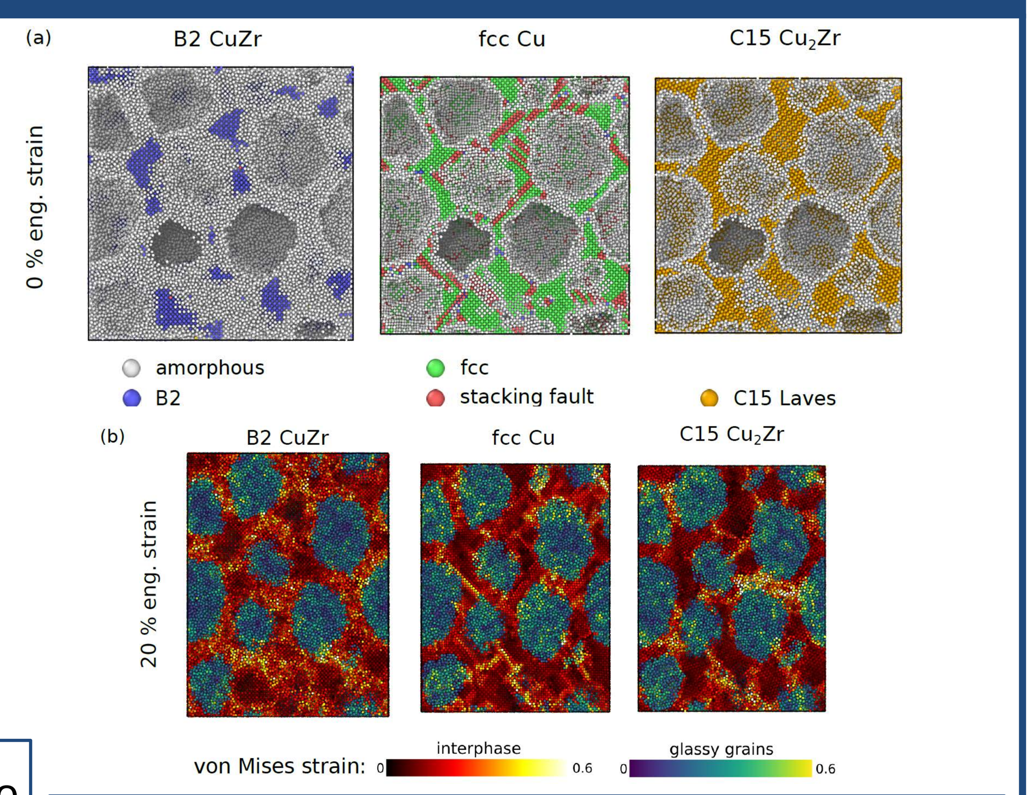
Mechanical properties: Reinforcement of nanoglasses by interface strengthening



To reinforce the conventional nanoglass (NG), the glassy interface interphase is replaced by a crystalline phase. This can be single crystalline (i) B2 CuZr, (ii) fcc Cu or (iii) the C15 Laves phase [4].



Tensile tests of the conventional NG and three NG composites reinforced with B2 CuZr, fcc Cu and C15 Cu_2Zr (Laves). (a) Stress-strain curves. (b) Evolution of the strain localization parameter.



Reinforcement of nanoglasses. (a) nanoglass-composites before tensile testing: The glass atoms have been removed for visualization; the atoms are color coded according to their atomic structure. (b) Snapshots of the atomic configurations at 20% macroscopic strain show the local atomic von Mises strain [4,5].

- Increasing yield strength by introducing the C15 Cu_2Zr Laves-phase into the nanoglass.

Conclusion

- Compositional variations between interfaces and glassy grains result from surface segregation effects already present in the primary glassy particles.
- During the consolidation process the glassy spheres deform by homogeneous plastic flow and shear bands.
- Porosity close at pressures exceeding 4 GPa.
- Interfaces have a width of about 1nm in terms of composition and at least 2 nm in terms of defective short-range order.
- Analogous to grain boundary strengthening in crystalline materials, it is possible to reinforce the nanoglass without compromising its ductility.

References

[1] K. Albe et al., Mech. Mater. 67, 94-103 (2013).
[2] O. Adjaoud et al., Acta Mater. 113, 284-292 (2016).
[3] O. Adjaoud et al., Acta Mater. 145, 322-330 (2018).
[4] C. Kalcher et al., Scr. Mater. 141, 115-119 (2017).
[5] C. Kalcher et al., Acta Mater. 141, 251-260 (2017).

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We acknowledge the financial support of the DFG through SPP1594 and the computing time granted by Jülich Supercomputing Center through Project HDA22