ATOMISTIC SIMULATIONS OF AMORPHOUS METALS IN THE ELASTOPLASTIC REGIME FOR UNIAXIAL COMPRESSION

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Amorphous Metals

- No crystalline structure.
- High hardness and moldability, high resilience, high mechanical strength and high wear resistance, among other properties. Great potential as advanced engineering materials.
- Many details of the mechanical behavior are still unknown. Molecular Dynamics (MD) simulations were used to obtain the results presented in this poster.

Simulation Details

- Lammps software was used.
- $Cu_{46}Zr_{54}$ prismatic sample, with 160000 atoms. The quenching rate c the sample was 10^{12} K/s, and the strain rate 10^{9} /s (Arman et al., 2010
- The interactions between atoms was describes with an embedded ator method (EAM) potential (Daw, 1984).
- We use 3D periodic boundary conditions.

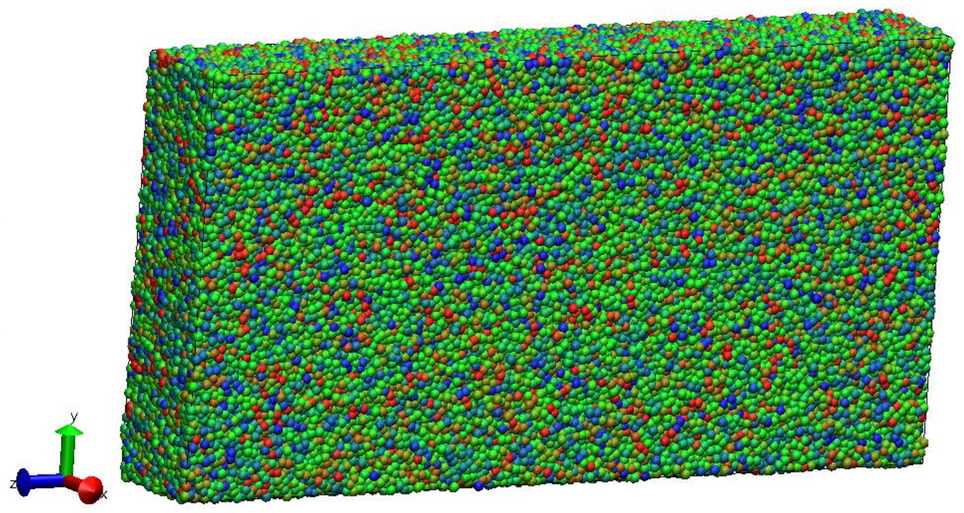

Figure 1

Results

Figure 1: sample at ε=6% and T=300K, under uniaxial compression. No shear bands observed.

Figure 2: von Mises stress versus strain at all the simulated temperatures. After the purely elastic deformation there is a decrease in von Mises tension, suggestive of plasticity.

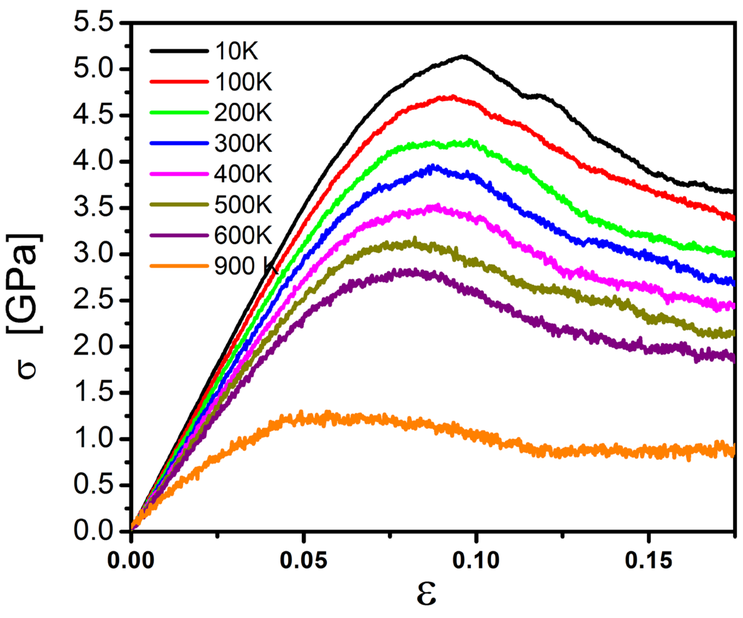

Figure 2

Figures 3 and 4: peak von Mises stress and Young Modulus fitted against temperature with the following equation:

$$y = A_1 e^{(-T/To)}$$

Both of them decrease with increasing temperature, as expected.

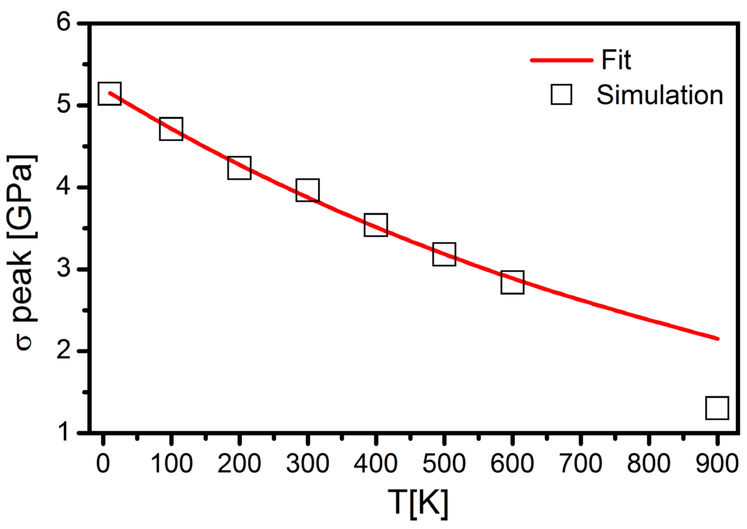

Figure 3

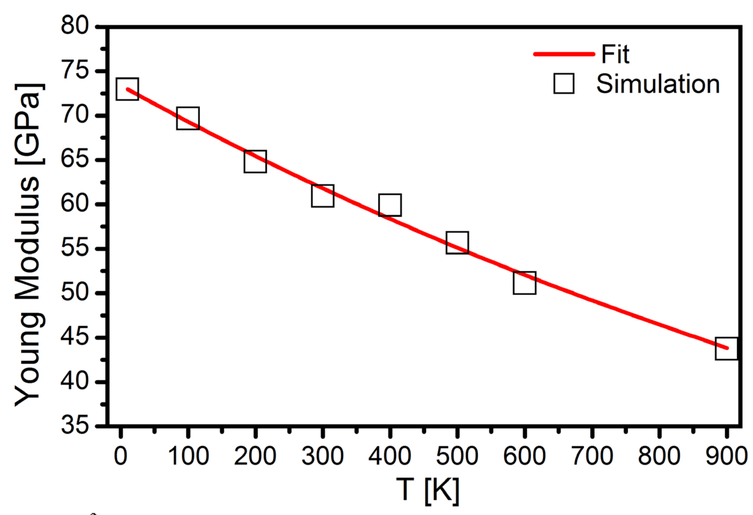

Figure 4

Figure 5: To verify that the absence of shear bands is not due to periodic conditions during deformation, simulations were carried out with free lateral boundary conditions. Buckling is observed. Still no shear bands.

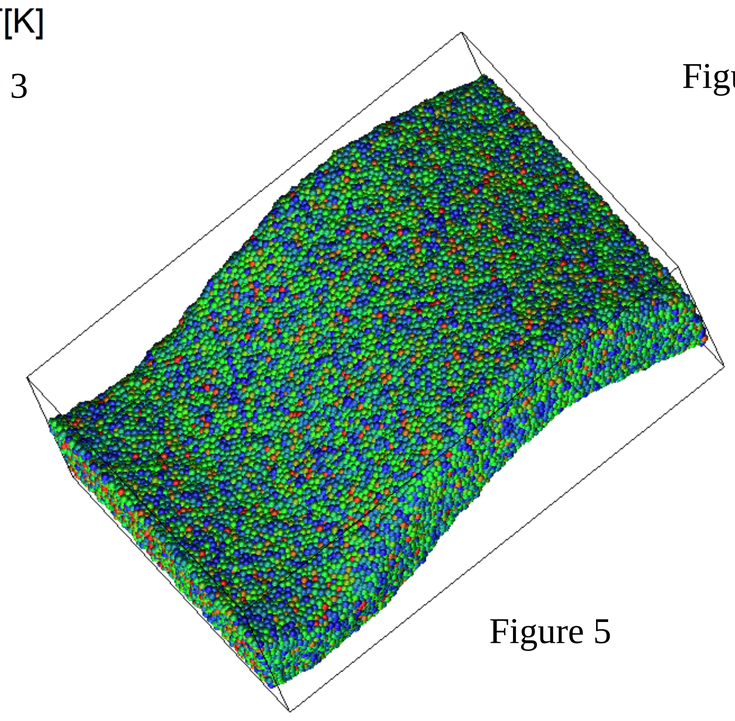

Figure 5

Conclusions

- No shear bands are observed, which is to be expected given that our glass was generated with very high quenching rates (Xiao et al., 2012).
- The behavior with temperature can be adjusted reasonably well with an exponential decay with temperature, typical of thermal activated phenomena.

Acknowledgements

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References

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