ATOMISTIC SIMULATIONS OF AMORPHOUS METALS UNDER UNIAXIAL TENSION AT DIFFERENT TEMPERATURES

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- **Amorphous metals** are increasingly used in modern life, showing great potential as advanced engineering materials, due to some of its characteristic properties such as high hardness, high resilience, high mechanical strength and high wear resistance.

- Many details of the mechanical behavior are still unknown, and the currently used models and theories are far from predictive.

- In this poster, we present the results obtained with molecular dynamics (MD) simulations of an amorphous metal (***CuZr***).

- The results obtained are relevant for understanding the mechanical behavior of the material, such as stress-strain and temperature-strain relationships. In our simulations it is possible to observe the ***nucleation and growth of a void*** due to high stress and strain rate values.

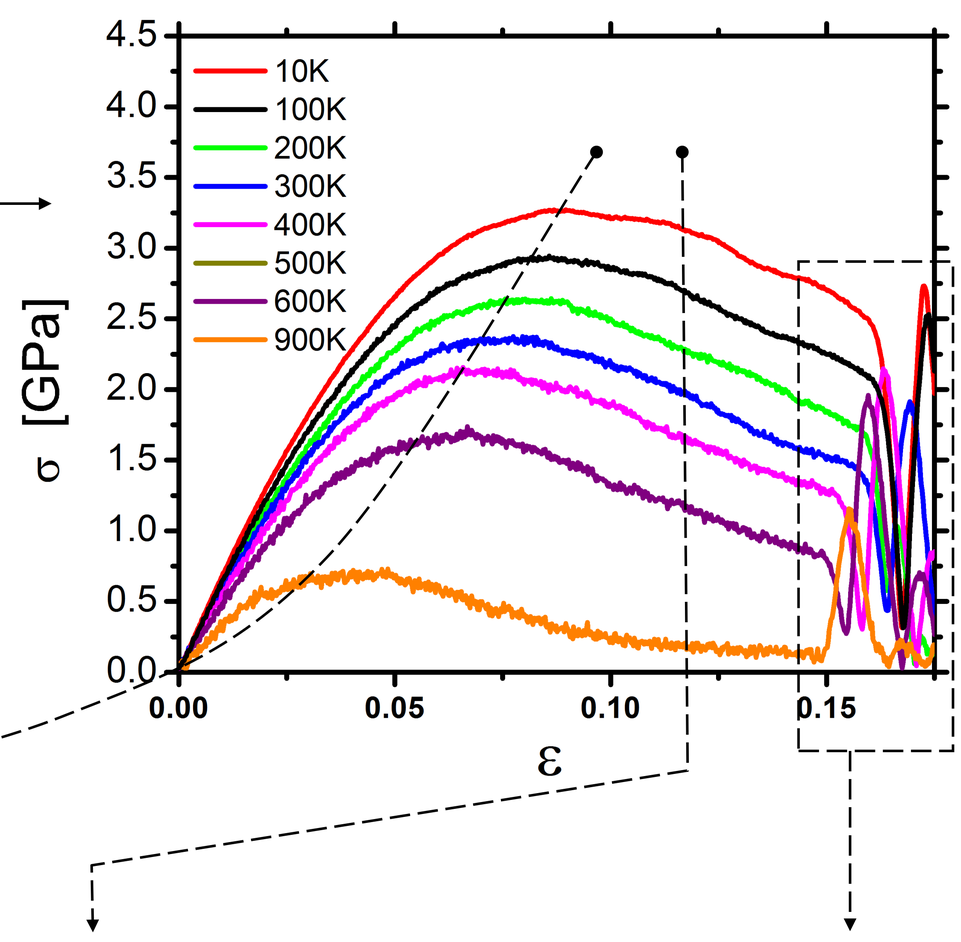
MD Simulation of $Cu_{46}Zr_{54}$

Stress-Strain

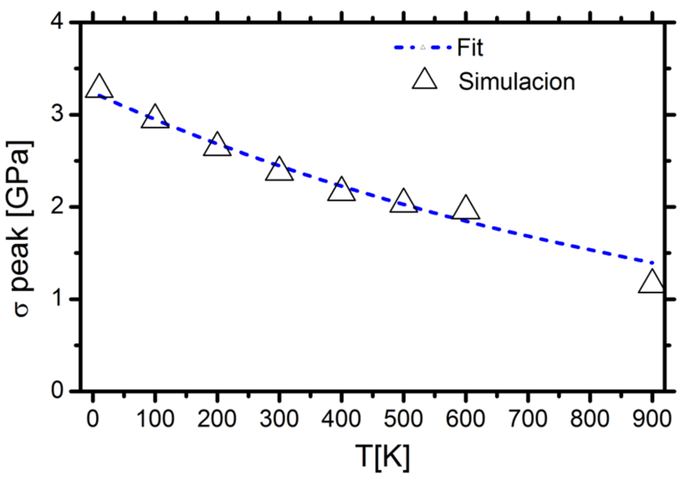
Simulations carried out using the LAMMPS software

Prismatic $Cu_{46}Zr_{54}$ sample, with a total of about 160,000 atoms.

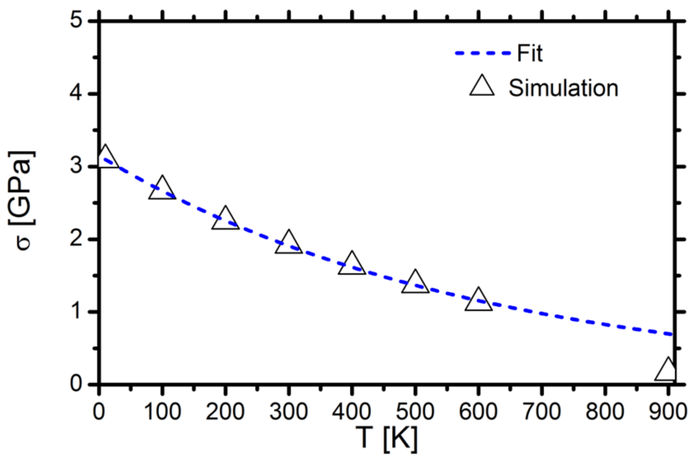
Quenching rate of 10^{12} K/s



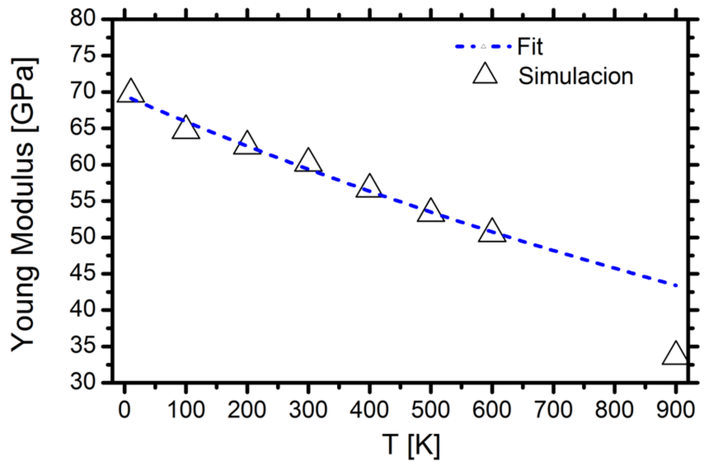
Peak von Mises Stress vs T



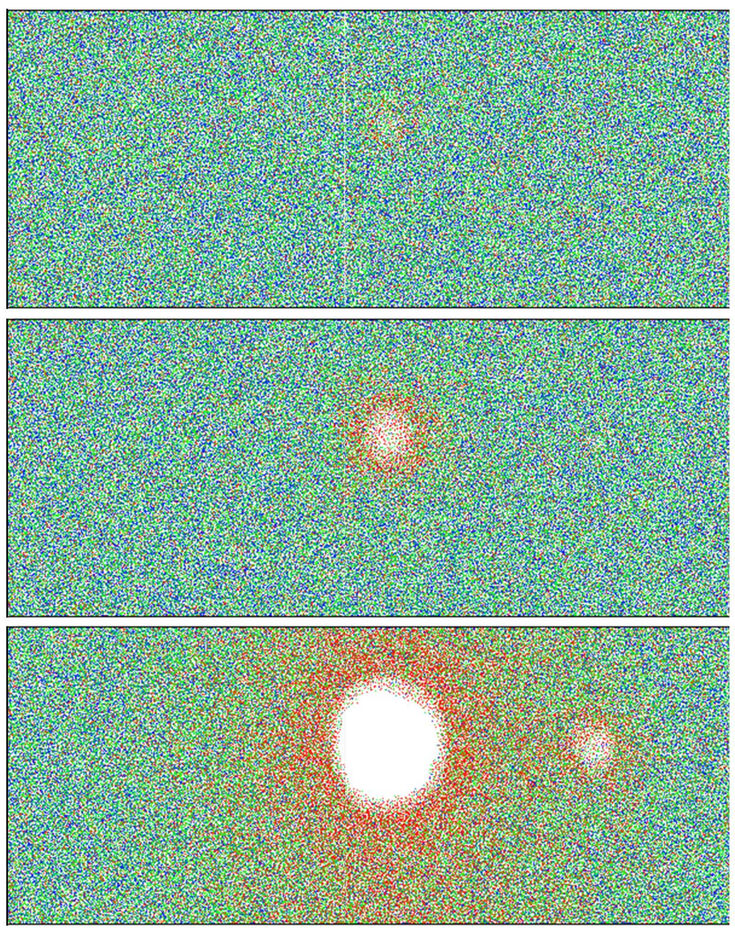
Stress at ε = 0.12 vs T



Young Modulus Fit vs T



Void Nucleation and Grow



Conclusion: A detailed understanding of the influence of temperature, quenching rates, etc., in the mechanical properties of metallic glasses will allow obtaining necessary properties for their application in new technologies, including applications under extreme conditions, such as aerospace missions or materials in nuclear reactors. Studies like the one presented here will contribute to this understanding and accelerate novel material development.