

Polymorphisms and early-stage crystallization of Zr-based glasses induced by high pressure and temperature

L. Rogal^{1*}, D. Laniel², G. Weck³, G. Garbarino⁴, Z. Kobylarz¹, U.A. Wdowik⁵ and J. Dutkiewicz¹

¹*Institute of Metallurgy and Materials Science Polish Academy of Science, 30-059 Krakow, Poland*

²*Centre for Science at Extreme Conditions, School of Physics and Astronomy, University of Edinburgh, King's Buildings, EH9 3FD Edinburgh, United Kingdom*

³*DIF/DPTA, CEA 91680 Bruyères-le-Châtel, France*

⁴*European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France*

⁵*IT4Innovations, VSB – Technical University of Ostrava, 708 00 Ostrava- Poruba, Czech Republic*

*e-mail: l.rogal@imim.pl

Cu₄₃Zr₄₃Ag₇Al₇ (at. %) metallic glasses were annealed above the glass transition temperature (497 °C) under 7.8–73 GPa. Two high-pressure systems were employed: (i) a Bridgman toroidal-type apparatus with resistive heating and (ii) a Diamond Anvil Cell (DAC) equipped with double-sided YAG laser heating.

In situ Pair Distribution Function (PDF) measurements at the European Synchrotron Radiation Facility (ESRF) reveal a decrease in atomic distances associated with the densification of the metallic glasses, indicating polymorphic transitions and subsequent early-stage crystallization induced by high pressure and temperature. Post-annealing high-resolution transmission electron microscopy (HRTEM) analyses, performed at atomic resolution, distinguish multiple glassy states. Inverse and Fast Fourier Transform (FFT and IFFT) of selected HRTEM micrographs demonstrate a progressive reduction in nearest-neighbor spacing with increasing pressure and the development of ordered microdomains within the amorphous matrix at higher temperatures (Fig. 1). These findings imply a structural reorganization that precedes crystallization reorganization preceding the onset of crystallization.

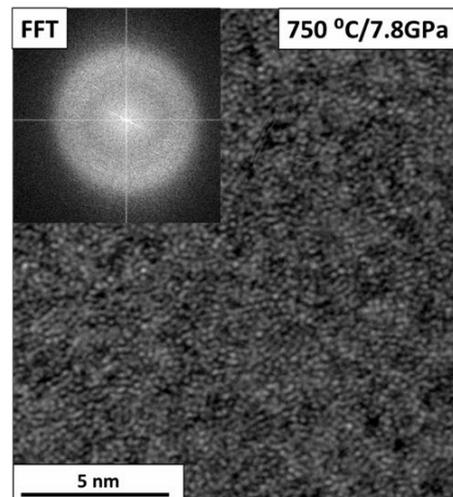


Fig. 1 Representative HRTEM image and corresponding Fast Fourier Transform (FFT) showing a diffuse ring characteristic of an amorphous structure with incipient ordering.

Additionally, a notable decrease in the effective glass transition temperature was observed at higher sintering temperatures, implying a correlation between densification mechanisms and the stability of the amorphous phase. The combined results provide new insights into pressure-driven polymorphic transformations and the fundamentals of crystallization kinetics in Zr-based metallic glasses under extreme conditions.

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