Applications of XAFS to metallic glasses under high pressure

Przemyslaw Dziegielewski,

Faculty of Physics, Warsaw University of Technology, Poland

Metallic glasses (MGs) are amorphous solids with a liquid-like atomic structure, i.e. lacking the transitional symmetry of crystals. Their local atomic arrangement can be described in terms of densely packed atomic clusters [1]. Hydrostatic compression of the order of tens of gigapascals induces significant modifications of geometry and arrangement of those clusters and affects the properties of MGs. XAFS technique provides a unique opportunity for experimental studies of MGs and resolving their complex, non-periodic atomic structure. During the past decade, there has been an increased interest in high-pressure structural studies of solids, in particular in XAFS experiments involving diamond anvil cells. Those experimental studies are often supplemented by computational techniques such as molecular dynamics simulations and *ab-intio* calculations.

In this seminar, some examples of the application of high-pressure EXAFS to investigate the characteristic features of the local atomic structure of Ce-AI [2] and Zr-Cu metallic glasses [3, 4] will be presented. We demonstrate significant changes in the local atomic order, "polyamorphic" transition and pressure-induced devitrification. Moreover, we will present the significant role of simulations for understanding experimental results of studies of MGs atomic structure.

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[4] Antonowicz, J. et al., Atomic-level mechanism of elastic deformation in the Zr-Cu metallic glass, Phys. Rev. B 93, 144115, 2016

Dr Przemyslaw Dziegielewski, Faculty of Physics, Warsaw University of Technology, Poland. Her scientific interests focus on the physics of amorphous metals. Her research involves XAFS analysis, molecular dynamics simulation, and ab-initio calculations of their atomic and electronic structure, particularly, in high-pressure conditions.