Dependence of icosahedral-like short range order on the cooling rate in a bulk metallic CuZrAl glass - theoretical and experimental analysis

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The preparation of the bulk metallic glass Cu$_{47.5}$Zr$_{47.5}$Al$_5$ is simulated by molecular dynamics. The temperature of the initial liquid state and the cooling rate are varied. It appears that the fraction of icosahedral atomic arrangements depends significantly on the cooling rate. The question is considered whether or not such structural differences could be observed experimentally by diffraction. We prepared Cu$_{47.5}$Zr$_{47.5}$Al$_5$ samples at different cooling rates and analyzed them by means of X-ray scattering. The scattering intensities of the simulated samples are calculated and compared to the experimental data. The experimental diffraction patterns of the samples prepared at different cooling rates show similar differences as the simulated ones which confirms the reliability of the molecular dynamics simulations.