Binary Cu-Hf metallic glasses investigated by the reverse Monte Carlo simulation and Voronoi analysis

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The special interest in Cu-Hf metallic glasses (MGs) is driven by their excellent glass forming ability and extraordinary mechanical properties such as the high fracture compression strength (~ 2260 MPa) combined with a large plastic elongation (~ 2.2 %) [1]. However, only limited effort has been invested in revealing their local atomic structure. Therefore as-prepared states of the quenched binary $Cu_xHf_{(100-x)}$ x = 54, 61 and 69 alloys were characterized by the high energy X-ray diffraction (HEXRD) at 80 keV, anomalous X-ray diffraction (AXRD) near the Hf absorption *K*-edge (65.351 keV), neutron diffraction (ND) and Cu *K*-edge X-ray absorption fine structure spectroscopy (EXAFS). Three-dimensional (3D) models were developed by the reverse Monte-Carlo (RMC) simulation technique using HEXRD, ND and Cu *K*-edge EXAFS experimental datasets and analysed in detail by pair distribution functions and Voronoi analysis. Furthermore in this work the obtained Hf differential pair distribution functions, $DPDF_{Hf}(r)$, using the AXRD technique are confronted with ones obtained from a RMC simulated configuration box of atoms.

Figure 1 shows partial pair distribution functions, g(r), extracted from the 3D RMC models for all the investigated samples. The closest interatomic distances for the first coordination shell do not depend on Cu content however interatomic distances shift to lower *r* values for higher coordination shells as the amount of Cu content increases in investigated Cu-Hf MGs. Figures 2 shows identified Voronoi polyhedra with the frequency of at least 2 %. The results are obtained by normal and radical Voronoi analysis and the influence of constrains on Voronoi analysis is discussed.

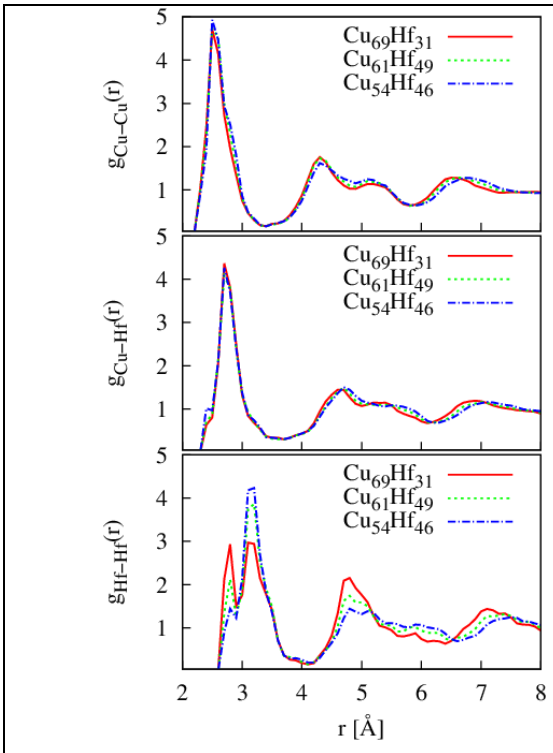

Figure 1. Partial pair distribution functions of the Cu-Hf MGs obtained by the RMC simulation.

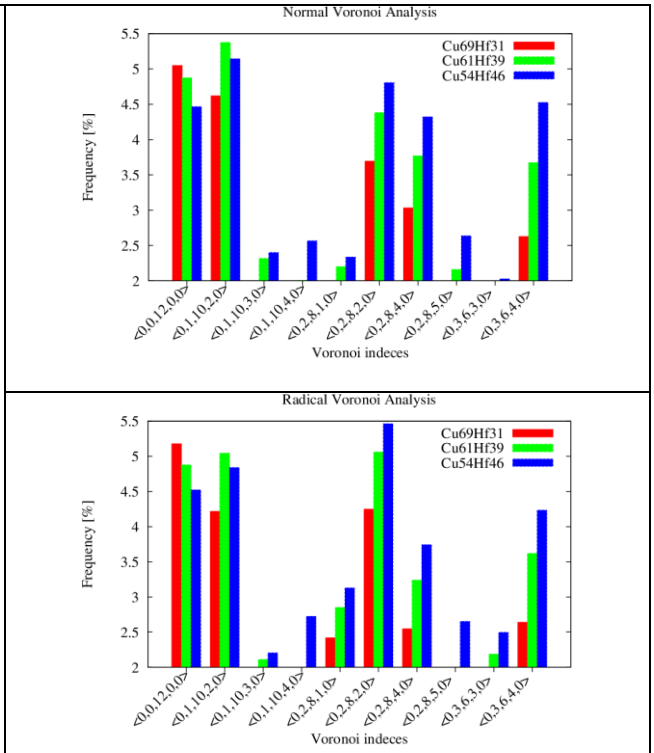

Figure 2. Voronoi polyhedral statistics of 3D models obtained by the RMC simulation using Voronoi normal (top) and radical (bottom) analysis.

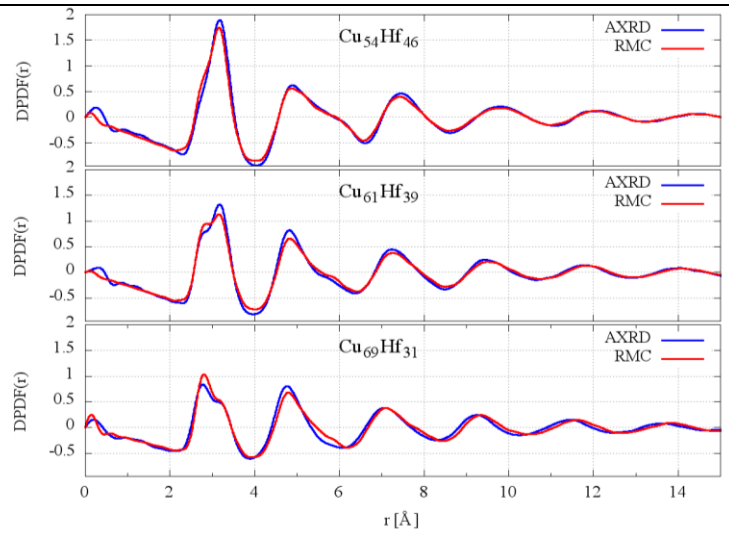

Figure 3. Comparison of Hf differential pair distribution function $DPDF_{Hf}(r)$ extracted by AXRD and from the 3D RMC configuration box.

Reference

1. A. Inoue and W. Zhang, *Mater. Trans.* **45**, 584-587 (2004).