

Dual medium-range order structures in $Zr_{80}Pt_{20}$ metallic glassesSiyuan Zha¹ & Akihiko Hirata¹¹*Department of Materials Science, Waseda University, 3-4-1 Ohkubo, Shinjuku, Tokyo 169-8555, Japan*

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Numerous studies have revealed that Zr-based metallic glasses exhibit high glass-forming ability and possess excellent mechanical and physical properties. At the atomic level, it has been suggested that Zr-based metallic glasses predominantly form icosahedral local structures as their primary short-range order (SRO) due to their high atomic packing density [1]. Additionally, a geometry-based model has been proposed in which SRO atomic clusters, centered around solute atoms, overlap with each other to form medium-range order (MRO) structures [2]. In this study, we focus on the $Zr_{80}Pt_{20}$ alloy, which is known to contain a large number of icosahedral atomic clusters [3,4]. By investigating the dominant solute-centered (Pt-centered) atomic clusters and their spatial distribution, we elucidate the dual nature of the MRO structures formed in this alloy.

Molecular dynamics (MD) simulations were performed to study the cooling and isothermal relaxation processes of the $Zr_{80}Pt_{20}$ alloy. Initially, 32,000 atoms (Zr: 25,600 atoms, Pt: 6,400 atoms) were arranged on an FCC lattice and equilibrated at 3000 K for 40 ps. The system was then cooled to 300 K at a rate of 1.0×10^{11} K/s, followed by a 10 ns isothermal relaxation. The Embedded Atom Model (EAM) interatomic potential was used, and calculations were performed under periodic boundary conditions with the NPT ensemble. Structural analysis was conducted using the partial pair distribution function and Voronoi polyhedral analysis.

For the glass state, Voronoi polyhedral analysis revealed that the dominant atomic clusters were $\langle 0,0,12,0 \rangle$ and $\langle 0,2,8,1 \rangle$, centered around Pt atoms, which together accounted for approximately 44.4% of all Pt-centered atomic clusters. To examine the spatial distribution of these atomic clusters, we calculated the partial pair distribution function between Pt atoms at the center of these clusters (Figure 1).

The results indicate that Pt atoms at the center of $\langle 0,0,12,0 \rangle$ icosahedral atomic clusters are frequently linked at the first nearest-neighbor distance, forming interpenetrating MRO structures. In contrast, the spatial distribution of Pt atoms in $\langle 0,2,8,1 \rangle$ distorted icosahedral-like atomic clusters closely resembles that of all Pt atoms. These results suggest a dual nature of the MRO in the glass. Furthermore, a prominent pre-peak is formed in the calculated Pt-Pt partial structure factor for the central Pt atoms of $\langle 0,2,8,1 \rangle$ atomic clusters, suggesting that those Pt atoms are considered to be the primary origin of the pre-peak in the structure factor of the system.

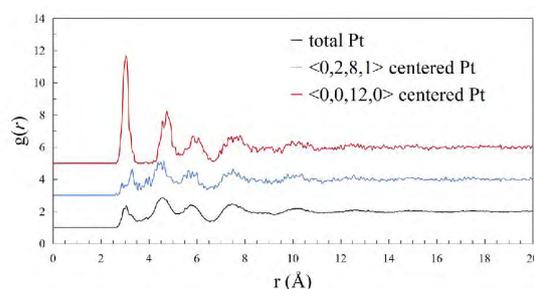


Fig. 1 Pt-Pt partial pair distribution function

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