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Fine Structure of $Zr_{80}Pt_{20}$ Amorphous Alloy Determined from Anomalous X-ray Scattering (AXS) Data by Applying Reverse Monte-Carlo (RMC) Simulation Method

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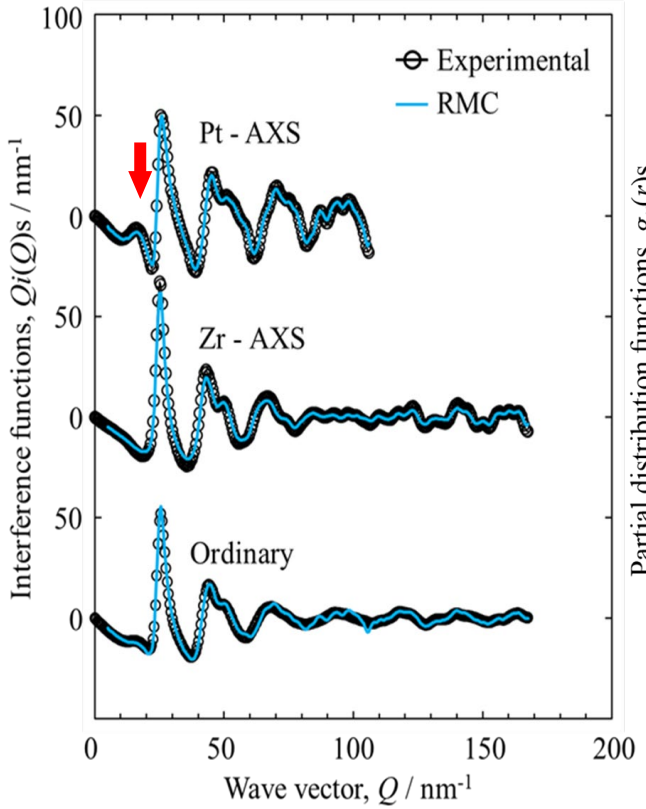

Fig. 1 Experimental interference functions, $Q\Delta i_{Pt}(Q)$, $Q\Delta i_{Zr}(Q)$, and $Qi(Q)$, and corresponding values obtained from RMC simulation.

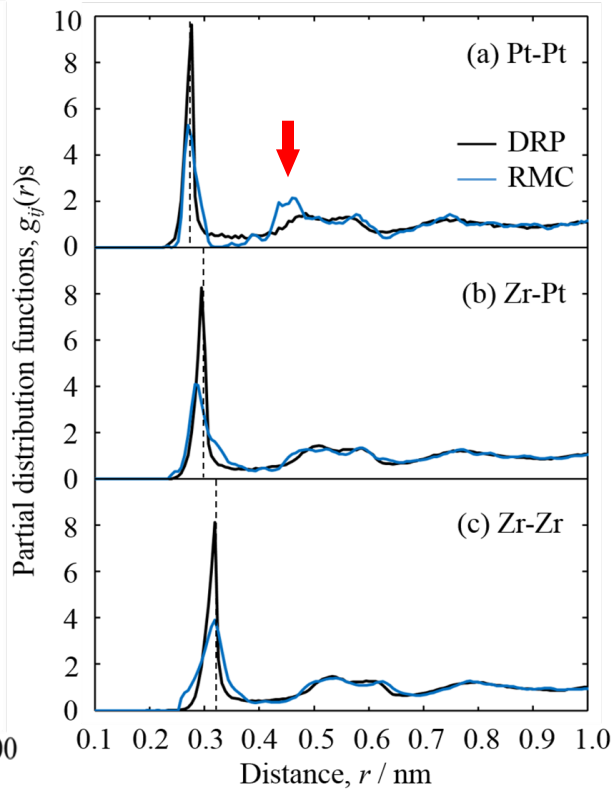

Fig. 3 Partial pair distribution functions, $g_{ij}(Q)$s, calculated from 3-D structural model obtained by RMC simulation. The corresponding functions for the DRP structure are also illustrated for comparison.

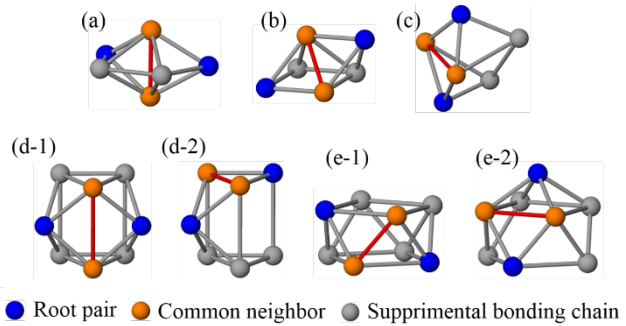

Fig. 7 Schematic diagrams of Bernal polyhedra corresponding to $[211]_{CN}$, (a) face shared tri-tetrahedra (FSTT), (b) capped half-octahedron (CHO), (c) partial tetragonal dodecahedron (PTD), (d-1,2) partial tri-capped trigonal prism (PTTP), and (e-1,2) partial bi-capped tetragonal anti-prism (PBTA).

- The structure of $Zr_{80}Pt_{20}$ amorphous metal with developed medium-range ordering (MRO) was analyzed by combining AXS (Anomalous X-Ray Scattering) and RMC (Reverse monte-Carlo) simulation.
- The origin of the pre-peak signal is associated with unique Pt-Pt pairs with the correlation distance about 0.45nm
- RMC model suggests that MRO develops in the Pt-Pt correlation, and that this unique MRO are composed of the Zr-rich tetrahedral linkage and the Pt-rich non-Bernal polyhedral linkage.

T. Kawamata et al., (2021)