

Local structural analysis for a Pd₄₀Ni₄₀P₂₀ BMG with thermally induced chemical short-range order by anomalous X-ray scattering

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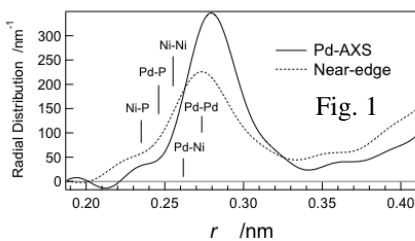
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Introduction

It is well established[1,2] that the relaxation event, which is called chemical short-range order (CSRO) process, is occurred in as-quenched and/or pre-annealed Pd₄₀Ni₄₀P₂₀ metallic glasses in a temperature range of 100-150 K under the glass transition temperature, T_g . The CSRO process is usually interpreted as energetically preferential atomic rearrangement between specific species mediated by free volume. Then, it is believed that the amorphous network structure reminds almost unchanged during the formation of chemical order, because the CSRO process has a remarkable short relaxation time compared with the relaxation due to free volume.

We will report the change in the local amorphous structure during the enhancement of ordered degree induced in a Pd₄₀Ni₄₀P₂₀ bulk metallic glass (BMG) by anomalous X-ray scattering (AXS) technique near a Pd-K absorption edge. This method allows us to take out three kinds of atomic correlations, Pd-P, Pd-Ni, Pd-Pd, from six atomic correlations included. Therefore, more reliable conclusion is expected to be extracted from diffraction data compared to conventional X-ray diffraction method.

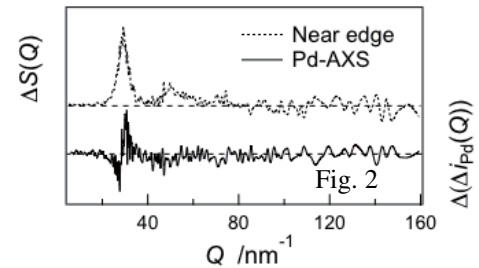
Experimental results



A Pd₄₀Ni₄₀-P₂₀ bulk metallic glass in a rod shape with a size of 8 mm in diameter and 20 mm in length was prepared by

water-quenching method with a dehydrated B₂O₃ flux. Thermal analysis showed that the glass had $T_g=573$ K. The pre-annealing was performed at 573 K for 1.8×10^3 s to unify the distribution of free volume in as-quenched BMG. After that, the sample was further annealed at 445 K for (a) 1.2×10^3 and (b) 1.2×10^5 s to enhance the chemical order in the pre-annealed sample. The diffraction experiments were conducted for these two states by AXS at NW10A station. Used X-ray energies were 24.316 and 24.041 keV for near and far edge experiments, respectively. The detail of experimental configuration and data correction was presented in ref. [3]. The interference function, $Qi(Q) = Q\{S(Q)-1\}$ of near edge experiment and AXS counterpart, $Q\Delta i_{Pd}(Q)$, were estimated for the sample in the state (a). By Fourier

transformation of these quantities, the radial distribution functions, $RDF(r)$ and $RDF_{Pd}(r)$, were calculated and the result is shown in Fig. 1. Similar analysis was carried out for the sample in the state (b), where the chemical order is enhanced further. The differences, $\Delta S(Q) = S_b(Q) - S_a(Q)$, between the state (a) and (b) was calculated for near edge experiments, and the result is shown in Fig. 2 along with AXS counterpart, $\Delta(\Delta i_{Pd}(Q)) = (\Delta i_{Pd}(Q))_b - (\Delta i_{Pd}(Q))_a$. The change in first peak intensity of $S(Q)$ is similar to that reported in the literature[4], while it is



quite different from AXS's result. The AXS experiment indicates that the principal peak of $\Delta i_{Pd}(Q)$ shifted to a higher Q position during the enhancement of chemical order. In the real space, this corresponds to the increase of atomic correlation with a shorter distance. The first peak of $RDF_{Pd}(r)$ was deconvoluted by a linear combination of three Gaussians denoting P-Pd, Ni-Pd and Pd-Pd atomic correlations, and the coordination numbers, N_{PPd} , N_{NiPd} and N_{PdPd} were calculated. The result is summarized in Table 1. The N_{NiPd} decreased with increasing times, while the N_{PdPd} , on the contrary, increased. This means that the enhancement of chemical order resulted in the variation of local amorphous structure similar to micro-phase separation.

Table 1: Coordination numbers

State	N_{PPd}	N_{NiPd}	N_{PdPd}
(a)	0.7	4.8	6.1
(b)	0.7	2.8	7.4

References

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