13A/2006G047

Structural analysis of pressure-amorphized zirconium tungstate

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Introduction

There is considerable current interest in materials that exhibit negative thermal expansion (NTE) from the point of view of synthesizing composites and solid-solutions with desired coefficient of thermal expansion including zero thermal expansion. $Zr(WO_4)_2$ is found to turn amorphous at high pressure and the amorphization is irreversible [1]. The *a*-$Zr(WO_4)_2$ recovered after releasing the pressure is found to be substantially denser than the starting cubic α-phase [2]. In the present work we have investigated the structure of pressure-amorphized $Zr(WO_4)_2$ using synchrotron radiation at Photon Factory. The scattered intensity was analyzed to obtain the structure factor $S(q)$.

Results and discussion

$Zr(WO_4)_2$ powder samples were soaked at 5.5, 7.5 and 10.5 GPa for 2 hours in a diamond-anvil cell and then the pressure was released. The recovered gaskets, with the sample embedded in the gasket hole, were used as such in the x-ray diffraction measurements using synchrotron radiation (λ = 0.4270(2) Å) from 13A beam-line at Photon Factory, KEK. An image plate was used as the detector. The 2-D image plate data was integrated to convert it to 1-D intensity versus 2θ data.

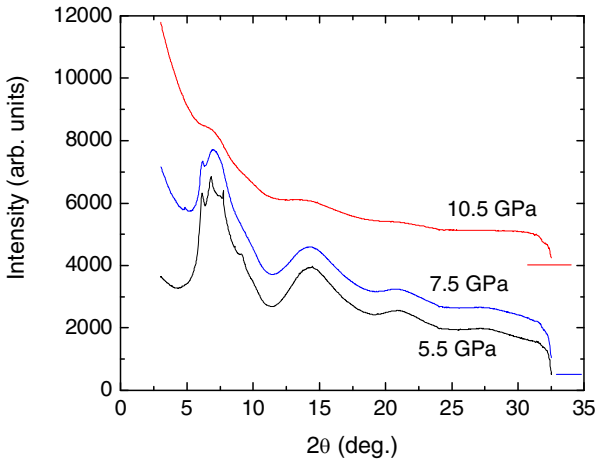

Fig. 1 Measured diffraction pattern from *p*-amorphized $Zr(WO_4)_2$ recovered from different pressures.

Figure 1 shows the as-measured data as a function of scattering angle 2θ. One can see typical amorphous-like scattering pattern for all the samples. Weaker scattering pattern for 10.5 GPa sample is due to smaller sample thickness. In order to remove the weak diffraction peaks riding over the amorphous scattering pattern the data was filtered using OmitSpot software. The rising background at low 2θ arises from air scattering. In order to obtain the structure factor the data was first corrected for air-scattering and θ-dependent attenuation factor. The coherent scattering was obtained after subtracting the incoherent scattering using Krogh-Moe procedure [3].

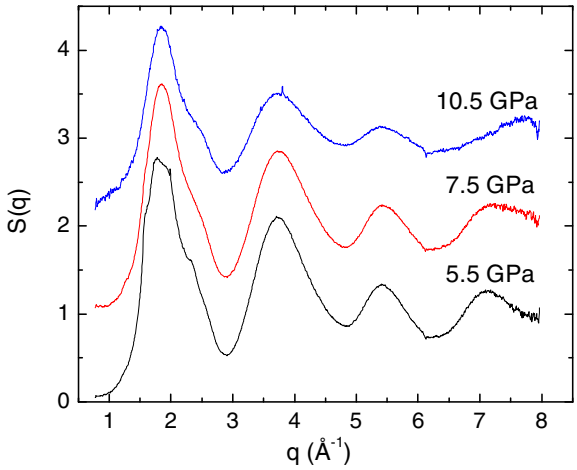

Fig. 2 Structure factor of *p*-amorphized $Zr(WO_4)_2$.

Figure 2 shows the structure factor of amorphous $Zr(WO_4)_2$ recovered from different pressures. The height of the first peak is found to reduce gradually at successively higher pressures suggesting weaker structural correlations at high pressure. Furthermore, there is a small shift of the position of the first peak to larger q in 7.5 and 10.5 GPa recovered samples as compared to the 5.5 GPa sample. As the average nearest-neighbour distance is inversely correlated to the position of the first peak in $S(q)$, the present results suggest that amorphous samples recovered from higher pressure could more dense as compared to that recovered from 5.5 GPa.

References

[1] T.R. Ravindran et al., Phys. Rev. Lett. 84, 3879 (2000).
[2] A.K. Arora et al., J. Phys. Condens. Matter 16, 1025 (2004).
[3] J. Krogh-Moe, Acta Crystallalogr. 9, 951 (1956)

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