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Negative thermal expansion and pressure induced amorphization in Zirconium tungstate as studied by 181Ta TDPAC

181Ta Time differential perturbed angular correlation study carried out in zirconium tungstate shows the occurrence of four distinct Zr sites. Based on the values of quadrupole parameters, it is interpreted that one site represents the probe atoms associated with regular ZrO6 while the other three sites of probe atoms are understood to be associated with contracted and distorted ZrO6. Effective decrease in Zr-O bond length is understood to be due to an increase in the fractions of ZrO6 octahedra which undergo contraction with temperature, thus explaining negative thermal expansion of the system. This system undergoes amorphization with the application of pressure exceeding 2 GPa. Results of PAC studies on this system will also be discussed with respect to amorphous - crystalline transition with isochronal annealing treatments.

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REQUESTING FOR AN INVITED TALK

Summary

Negative thermal expansion and pressure induced amorphization in Zirconium tungstate as studied by 181Ta TDPAC

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Zirconium tungstate ZrW_2O_8 is a cubic compound with three dimensional network of corner-linked ZrO_6 octahedra and WO_4 tetrahedra. Each WO_4 has one nonbridging W-O bond. ZrO_6 occupy face centered positions in the unit cell. This system exhibits negative thermal expansion isotropically over the temperature range 4–1050 K. Results of 181Ta TDPAC study in zirconium tungstate imply the occurrence of four distinct Zr sites. It is interpreted that one site represents regular ZrO_6 and the other three sites are associated with contracted and distorted ZrO_6 . Effective decrease in Zr-O bond length is understood to be due to an increase in the fractions of ZrO_6 octahedra which undergo contraction with temperature, thus explaining negative thermal expansion of the system [1]. Evolution of structures of ZrO_6 octahedra with isochronal annealing treatment has also been studied in zirconium tungstate amorphized by the application of a pressure of 5 GPa aiming at understanding pressure induced amorphization in the system [2].

Figure 1. (a) and (b) correspond to Time dependent anisotropy spectra obtained in untreated reference Zirconium tungstate sample at 300 K and 433 K respectively, while Figs (c), (d) and (e) refer to time dependent anisotropy spectra obtained in as pressure amorphized and subsequent to annealing at 875 and 975 K respectively. Shown on the right hand side is the crystal structure of zirconium tungstate with ZrO_6 tetrahedal and WO_4 octahedral units.

References:

1. Atomic scale study of negative thermal expansion in zirconium tungstate R. Govindaraj ,C. S. Sundar and A. K. Arora, Phys. Rev. B76, 012104 (2007)

2. Studies of local structure at Zr sites in pressure amorphized zirconium tungstate R Govindaraj, C S Sundar and A K Arora, J. Phys.: Condens. Matter 21 (2009) 235402

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