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Structural studies on pressure-quenched $Sc_2(WO_4)_3$

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Introduction

Following the report of negative thermal expansion (NTE) in ZrW_2O_8 and HfW_2O_8 over a wide range of temperature [1], NTE was also reported in many of the $A_2(MO_4)_3$ where A is a trivalent cation such as Sc, Al, Y etc. and M = W, Mo [2]. These compounds crystallize in either an orthorhombic structure as in $Sc_2(WO_4)_3$ that exhibits NTE or in a monoclinic structure that has positive thermal expansion behavior. High pressure investigation on the structural stability of these compound have shown that most of these exhibit intermediate structural transitions and subsequently amorphize irreversibly above 10 GPa [3-6]. The intermediate crystalline phases were found to be quenchable as in the case of $Sc_2(WO_4)_3$ [7] and $Ga_2(WO_4)_3$ [8], however these structures have not been fully understood in relation to the parent structure. Further, calorimetric studies on the enthalpy and entropy of formation from the oxides A_2O_3 and MO_3 suggested that many of these $A_2(MO_4)_3$ compounds may be metastable / entropically stabilized [9]. We have carried out structural studies on $Sc_2(WO_4)_3$ pressure quenched from 5 and 10 GPa in search of finding a new polymorph as reported in earlier work [7,8].

Ex-situ angle dispersive x-ray diffraction (ADXRD) measurement was carried out on the recovered sample after subjecting it to uniaxial compressions of 5 and 10 GPa. using 0.4270 Å line from synchrotron source, photon factory, beam line BL13A. No significant amorphous background was found and the pattern (a) closely resembled that of the orthorhombic phase. While the pattern of the sample p-quenched from 10 GPa was also predominantly that of parent crystalline phase, few new peaks are also found as shown in Fig. 1. The pattern was analyzed in the light of possible decomposition into (Sc_2O_3 + $3WO_3$). However no strong lines of crystalline WO_3 are found. Further analysis is in progress.

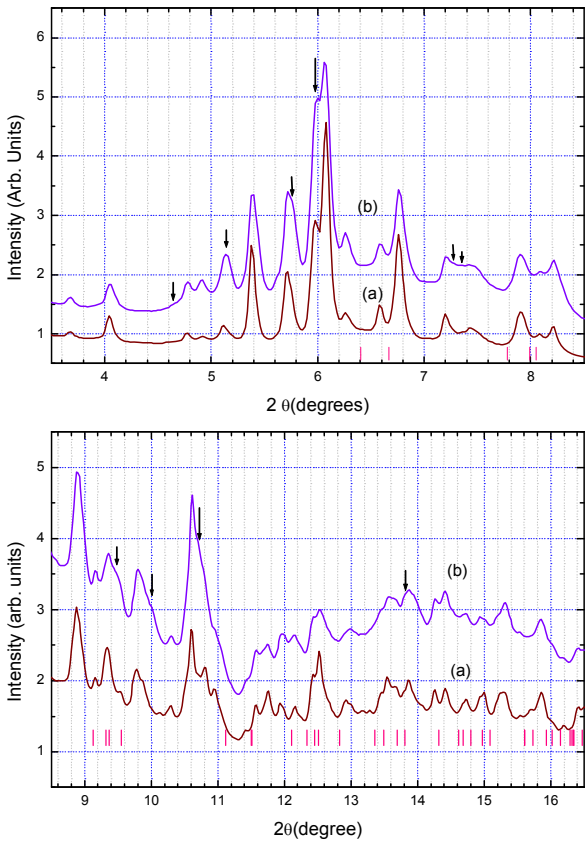

Fig. 1. X-ray diffraction pattern of the $Sc_2W_3O_{12}$ p-quenched from (a) 5 and (b) 10 GPa. The pattern (a) is very similar to the orthorhombic phase of $Sc_2W_3O_{12}$. New lines are identified by arrows in (b). Tic pattern corresponds to crystalline WO_3.

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