X-ray diffraction study of oxygen deficient $Y_2Ti_2O_{7-\delta}$ pyrochlore powders synthesized by high-energy ball milling (HEBM)

Supplementary information

Rietveld refinements were performed on XRD data collected on $Y_2Ti_2O_{7-\delta}$ pyrochlore powders. Experimental details of the refinement method are given here: list of the refined parameters, and the CIF files of two of the powders studied.

1. List of refined parameters

- Cell parameter a
- Lorentzian components of pseudo-Voigt peak-shape function (*Lx*, *Ly*)
- Berar-Baldinozzi correction of asymmetry (four terms)
- Legendre polynomial approximation of background (five terms)
- Sample position correction shift parameter
- Scale factor
- Debye-Waller coefficient of Y atoms
- *O*_{48f} site occupancy
- *O*_{48f} reduced atomic position *x*

2. CIF files

Cristallographic Information Files of the stoichiometric and the most substoichiometric $Y_2 Ti_2 O_{7-\delta}$ pyrochlore powders are given as attached files. They provide the description of the refined structure of these two materials.

ACCEPTED MANUSCRIPT/ CLEAN COPY