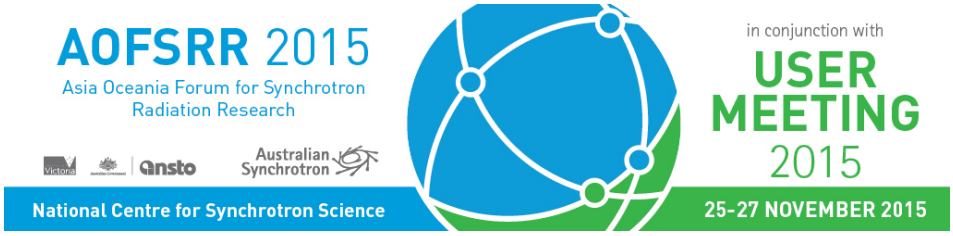

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The Thermal Expansion of Li and Na intercalated ZrW2O8

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Thermal expansion has been associated with many factors limiting the functionality and lifetime of various devices. Zirconium Tungsten Oxide, ZrW2O8, is known for its isotropic Negative Thermal Expansion (NTE) from 0.3 to 1050 K. In this study we report a novel approach to controlling the thermal expansion of this material. Li- and Na-ion batteries were constructed with ZrW2O8 used as an anode into which Li and Na intercalates. The main advantage of using batteries is the ability to precisely control the amount of Li and Na that is inserted. Electrochemical analysis shows that ZrW2O8 exhibits higher first discharge capacity of 463 mAh/g as an anode for Li-ion batteries compared to 114 mAh/g in Na-ion batteries. In principle, this suggests that more Li can intercalate into ZrW2O8 than Na. In situ synchrotron powder X-ray diffraction (XRD) data shows that Li and Na intercalates into ZrW2O8 as the batteries are discharged. While ZrW2O8 maintains its stability as Na was inserted to the maximum capacity, it breaks down into an amorphous phase as Li is inserted. Interestingly, in both cases no shifts were observed in the ZrW2O8 reflection positions as Li and Na are inserted which may suggest that ZrW2O8 is a zero-strain material for Li and Na insertion.

Synchrotron VT-XRD will be used to quantify the effect of the amount of intercalated Li and Na into ZrW2O8 on its thermal expansion and whether that may result in zero thermal expansion.

Keywords

Negative Thermal Expansion - Batteries - Synchrotron - ceramic - Zero Thermal expansion

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