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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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