

EXAFS Studies of Wadsley-Roth Phase $(W_{0.2}V_{0.8})_3O_7$ as a Battery Anode

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ABSTRACT

Recent years have shown a demand for a more ecological and efficient alternative to alkaline batteries. Lithium batteries are a prime candidate, prompting research into electrode materials with the potential to store energy effectively and withstand numerous uses. Our anode of interest, $(W_{0.2}V_{0.8})_3O_7$, would be an economical alternative to established niobium-based lithium-ion batteries due to the increased abundance of the primary component, vanadium. Additionally, Wadsley-Roth Phase crystallographic structures, of which our anode is an example, have been a promising material due to their unique properties of crystallographic shearing. Such structures allow for extraordinary lithium-ion diffusion while simultaneously maintaining structural integrity. After synthesizing our anode material and assembling coin cells, we utilized the Advanced Photon Source (APS) at Argonne National Laboratory in order to conduct EXAFS (Extended X-ray Absorption Fine Structure) spectroscopy on our material, as well as carried out cycling tests at the Illinois Institute of Technology. Analysis of the data shows that $(W_{0.2}V_{0.8})_3O_7$ maintains an efficient charge/discharge ratio while simultaneously withstanding any significant structural alterations over the course of one hundred cycles. This indicates that our anode is structurally sound and is a promising candidate for future research.

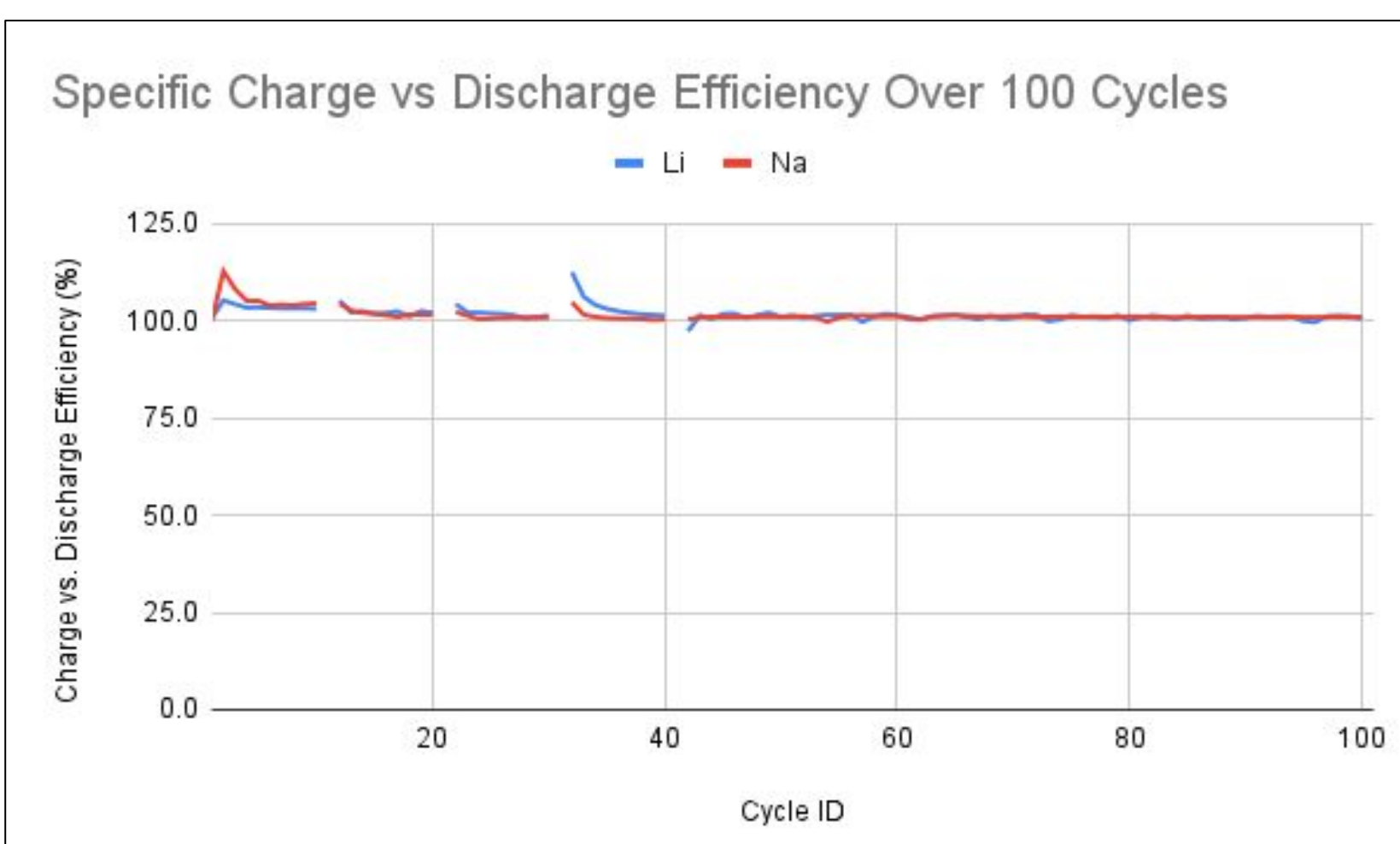
MOTIVATION

A growing preference for non-carbon-dependent energy sources has led to heightened demand for reusable energy. Explorations have pivoted towards lithium-ion batteries, which are considered an eco-friendly alternative compared to traditional battery systems due to their longer lifespan and increased energy density. These advantages could place the Wadsley-Roth phase $(W_{0.2}V_{0.8})_3O_7$ as a chief lithium-ion battery anode candidate.

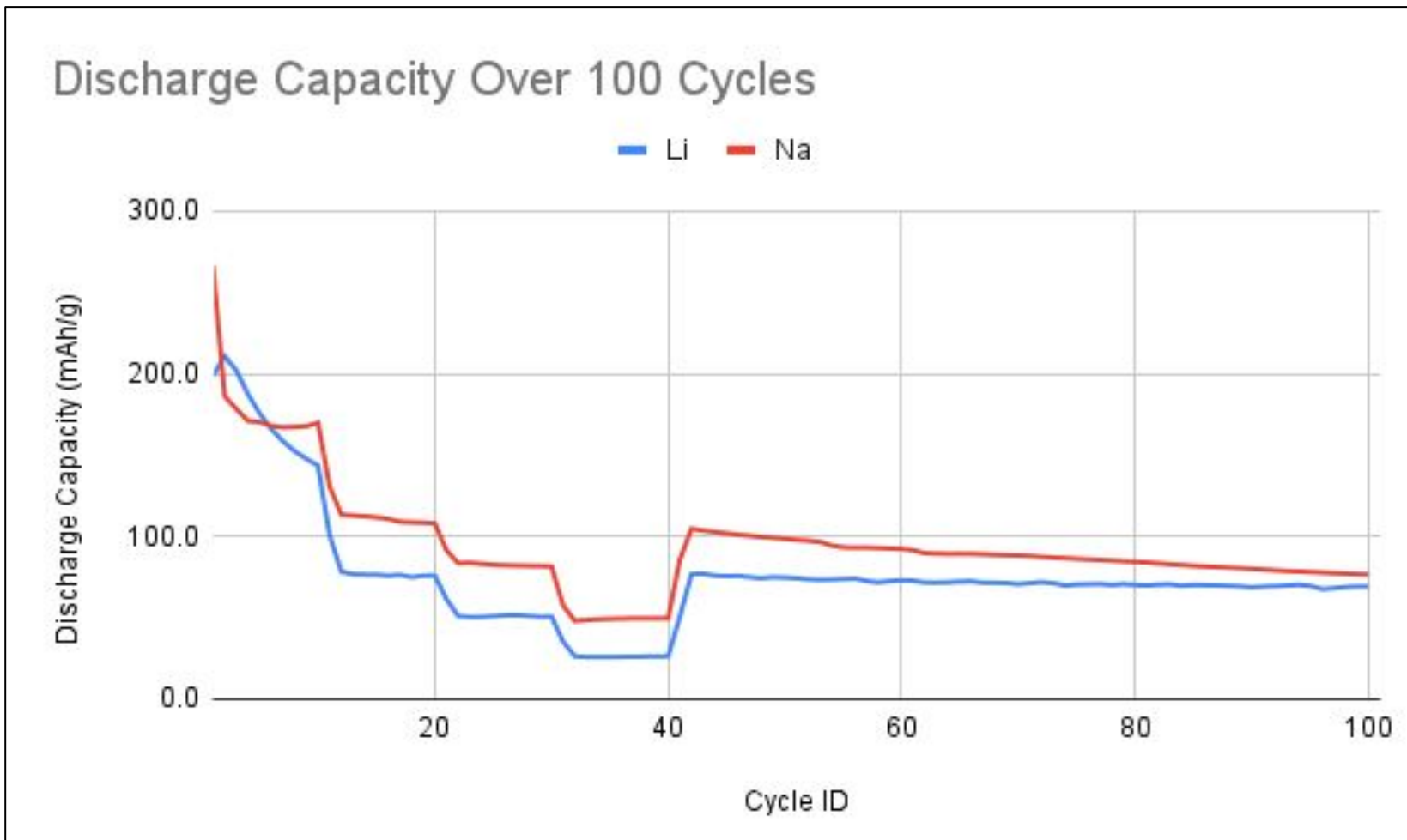
METHODS

The anode material was synthesized by mixing, ball-milling, and annealing WO_3 , V_2O_3 and V_2O_5 . The material was then pressed into pellets and tested by continuous cycling. Additionally, the same material was spread thinly and evenly on thin copper foil with the assistance of an alcohol component. These samples underwent EXAFS testing using the APS beamline. The gathered data was analyzed using Athena software.

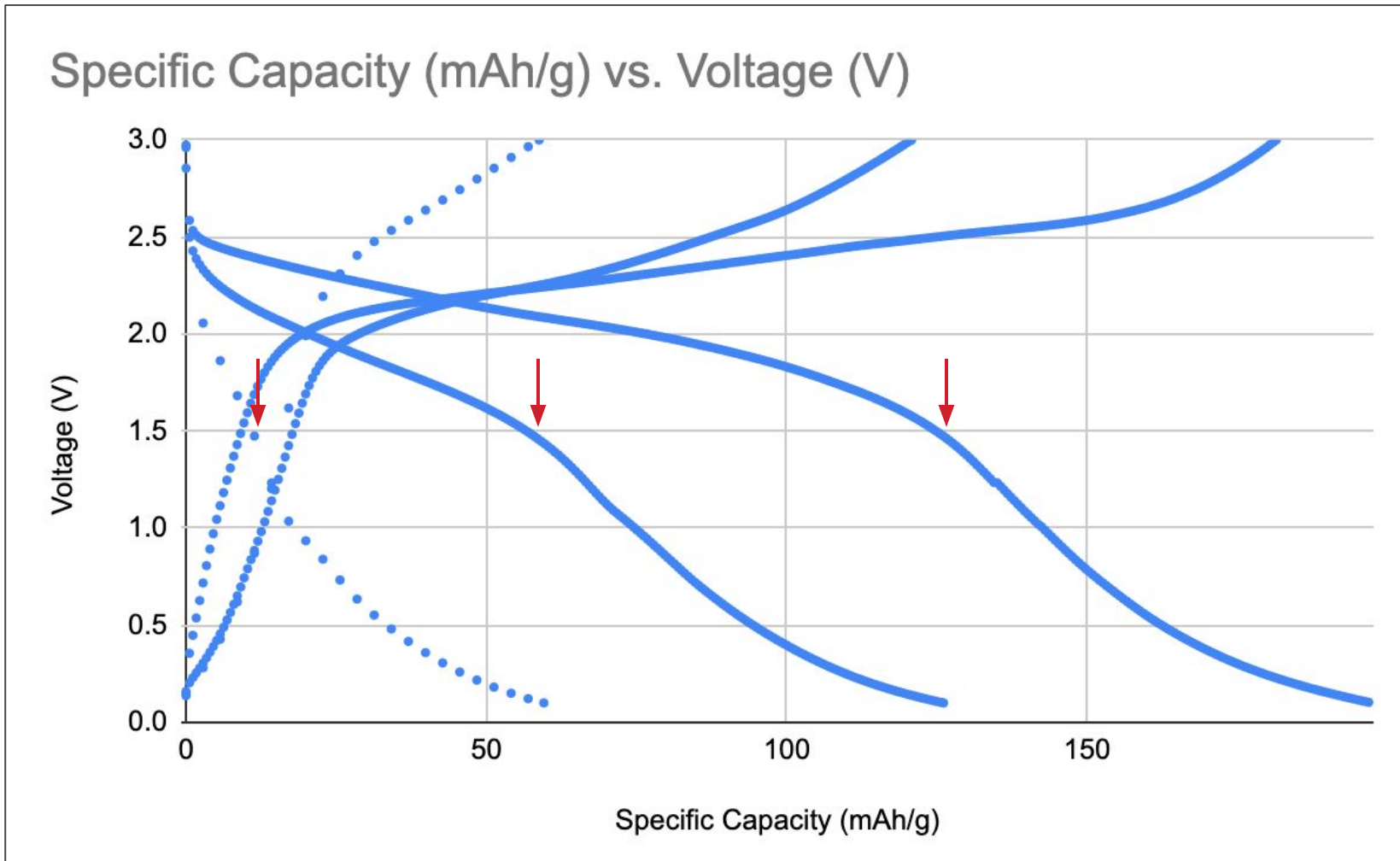
RESULTS



The charge/discharge efficiency of our cell remained approximately at 100% over 100 cycles.

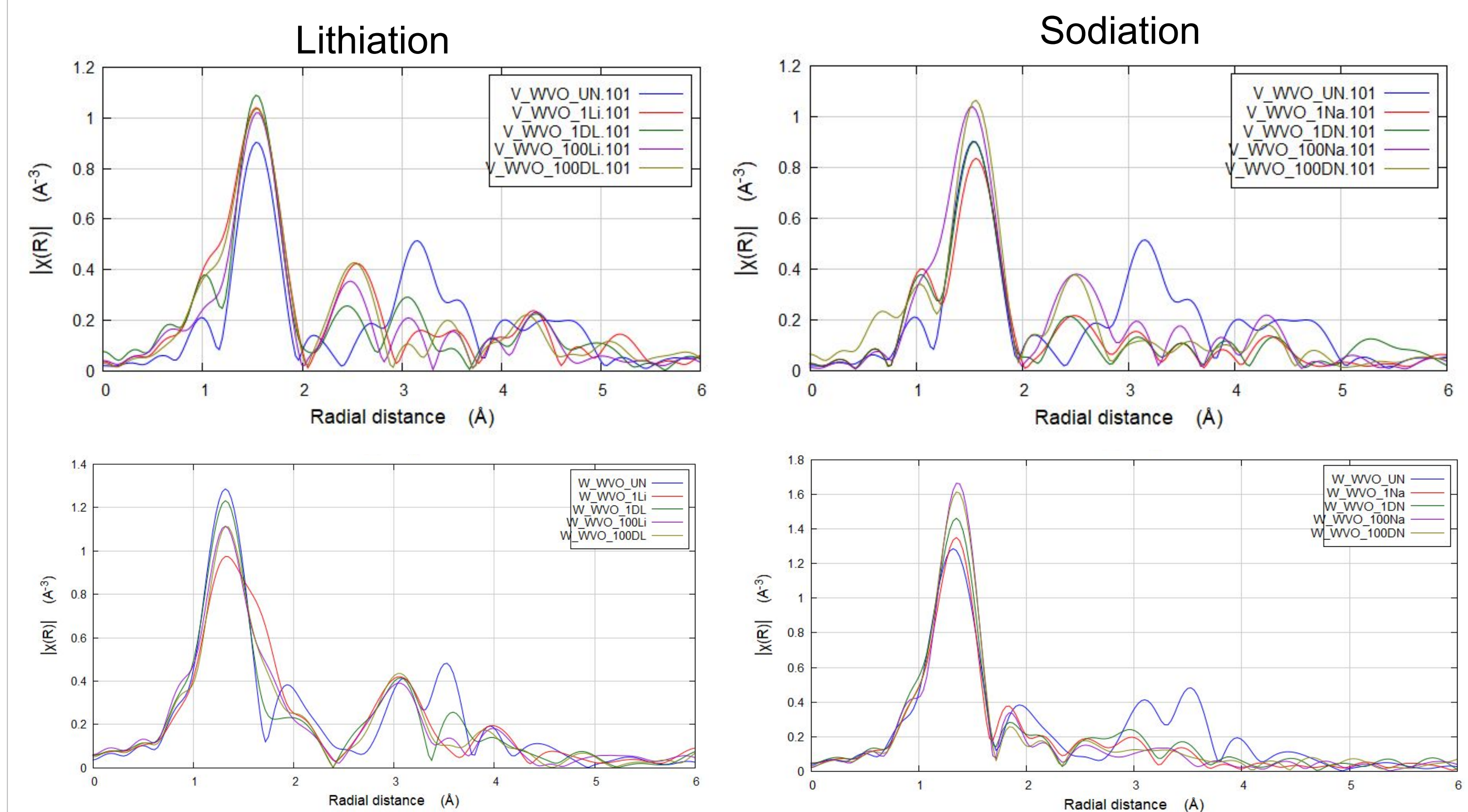


Our cell maintained a stable, proportionate discharge capacity even after the initial charge was altered.



The reduction potential of our cell is consistently at 1.5 V across all cycles, suggesting that its structure remains stable.

Extended X-Ray Absorption Fine Structure (EXAFS) Data



Battery cycling data demonstrates the lithiated/delithiated and sodiated/desodiated states and the magnitude of oxidation over radial distance.

The peaks of the first charge and discharge for both lithiation and sodiation show dramatic vertical shifts, meaning the structure of our anode is altered significantly during the first cycle. However, by 100 cycles, very little change can be seen between the charge and discharge peaks, which suggests that the structure stabilizes after continuous lithiation or sodiation.

DISCUSSION

After 100 cycles, both lithiated and sodiated elements maintained a charge-discharge efficiency around 100%, suggesting that a $(W_{0.2}V_{0.8})_3O_7$ battery anode works as a viable battery. The maintained steady-state of both vanadium and tungsten proves their structural stability capabilities.

LIMITATIONS

The cell was left exposed to the atmosphere while waiting to be measured, and we believe it self-oxidized because there was a minimal amount of change in the local structure between the lithiated/delithiated and sodiated/desodiated states as seen in the EXAFS data. Therefore, we cannot determine if there are structural changes during lithiation and sodiation, given the current EXAFS data.

NEXT STEPS

We recommend a repeated experiment to accurately gauge the structural changes during the lithiation and delithiation cycles. We suggest performing in-situ measurements of the anode to get a better picture of how the battery changes before and after lithiation and sodiation.

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