Ab Initio Studies of Aluminum Insertion into Amorphous vs Crystalline VO_2: Improvements in Voltage and Energy Density

Natl. Univ. of Singapore [1], Vadym Kulish[1], Daniel Koch[1], ◦Sergei Manzhos[1]

E-mail: mpemanzh@nus.edu.sg

Vanadium oxides (VO) are among the most promising materials that can be used as electrodes in multivalent rechargeable batteries. VO can be used as electrode materials for Al ion batteries although voltages reported to date are rather low, leading to low energy density. We explore amorphization as a strategy to increase voltage and compare Al insertion into amorphous vs crystalline VO_2. The amorphous structure is generated using a customized force field, and Al insertion is then studied by first-principles calculations. We show Al insertion in amorphous VO_2 can occur at insertion sites with well-dispersed insertion energies, with the lowest energy site much more thermodynamically favorable than any insertion site in the crystalline VO_2. We compute the voltage-composition profile for amorphous VO_2 and show that amorphization increases the average voltage of VO_2 cathode, which will lead to higher energy density. We also suggest that the stability of amorphous VO_2 cathode is improved by reducing volume expansion during Al insertion, potential leading to longer cycle life in practical applications. Overall, the demonstrated improvements suggest a significant potential of amorphous VO_2 electrodes for multivalent batteries.

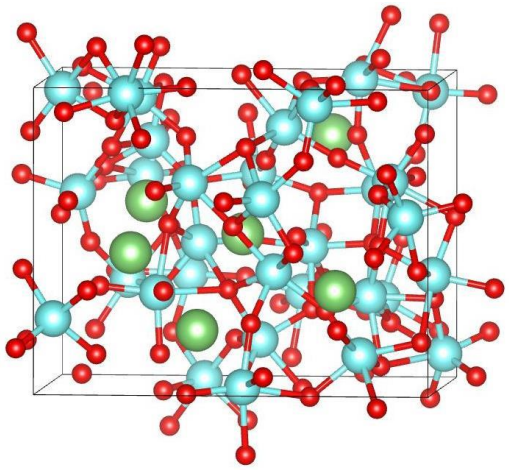

Figure 1. Left: amorphous VO2 structure with Al insertion sites. Vanadium, oxygen and aluminum atoms are shown in cyan, red and green colors, respectively.

© 2018年 応用物理学会