

Supporting Information

Tetragonal $VNb_9O_{24.9}$ -based Nanorods: A Novel Form of Lithium Battery Anode with Superior Cyclability

Ge Li,^{a,b} Xiaolei Wang^{*b}, and Xueming Ma^{*a}

[a] G. Li, Prof. X. Ma
State Key Laboratory of Precision Spectroscopy, and Department of Physics,
East China Normal University
Shanghai, 200241, China
E-mail: xmma@phy.ecnu.edu.cn

[b] G. Li, X. Wang
Department of Chemical and Biomolecular Engineering,
University of California, Los Angeles
Los Angeles, CA 90095, USA
E-mail: xlwang0813@ucla.edu

Experimental

Synthesis of $VNb_9O_{24.9}$ nanorods: $VNb_9O_{24.9}$ nanorods were synthesized through an aerosol-assisted method. Briefly, ammonium niobate (V) oxalate hydrate (4.895 mmol, 1.483 g), ammonium metavanadate (0.786 mmol, 0.092 g) were dissolved in DI-water (100 mL) followed by an addition of HCl solution (2.0 M, 0.5 mL) under ultrasonication for 1 hour to form a light green and transparent solution. Then Pluronic F-127 (1.5 g) was added and the mixture was stirred for 24 hours at room temperature to form a light blue and transparent solution. The solution underwent an aerosol process at 450 °C in an aerosol synthesis instrument reported somewhere else.²³ The product was collected and then annealed at 550 °C in air for 5 hours with a ramp rate of 5 °C min⁻¹. The claybank powders were collected for structure characterizations and electrochemical measurements.

X-ray diffraction (XRD) experiments were conducted on a X'Pert Pro X-ray diffractometer (Panalytical B.V.); scanning electron microscopic (SEM) experiments were conducted on a JEOL JSM-6700 FE-SEM (JEOL); transmission electron microscopic (TEM) experiments were conducted on a Philips CM120 operated at 120 kV (Philips/FEI).

Electrode Fabrication and Electrochemical Measurements: The $VNb_9O_{24.9}$ nanorods was assembled onto nickel foil current collector. Briefly, 80% of the electrochemically active material, 10% carbon black, and 10% *poly(vinylidene fluoride)* (PVDF) were dispersed in *N-methylpyrrolidinone* (NMP) to form slurries. The homogenous slurries were coated on a nickel foil substrate and dried at 100°C for 12 h under vacuum. To make 2032 type coin cells, glass fiber (GF/D) from Whatman was used as the separator; lithium was used as the counter electrodes; 1 M $LiClO_4$ in propylene carbonate (PC) was used as the electrolyte. The cells were assembled in a glovebox under an argon atmosphere. Electrochemical measurements were carried out on a VMP3 potentiostat/galvanostat (Bio-Logic LLC, Knoxville, TN). Cyclic voltammetric (CV) measurements were carried out using cutoff voltages of 3.000 and 1.000 V versus Li^+/Li . The charge and discharge measurements were carried out on a LAND CT2000 (Wuhan Jinnuo Electronics, Ltd., Wuhan, China) at different current densities.

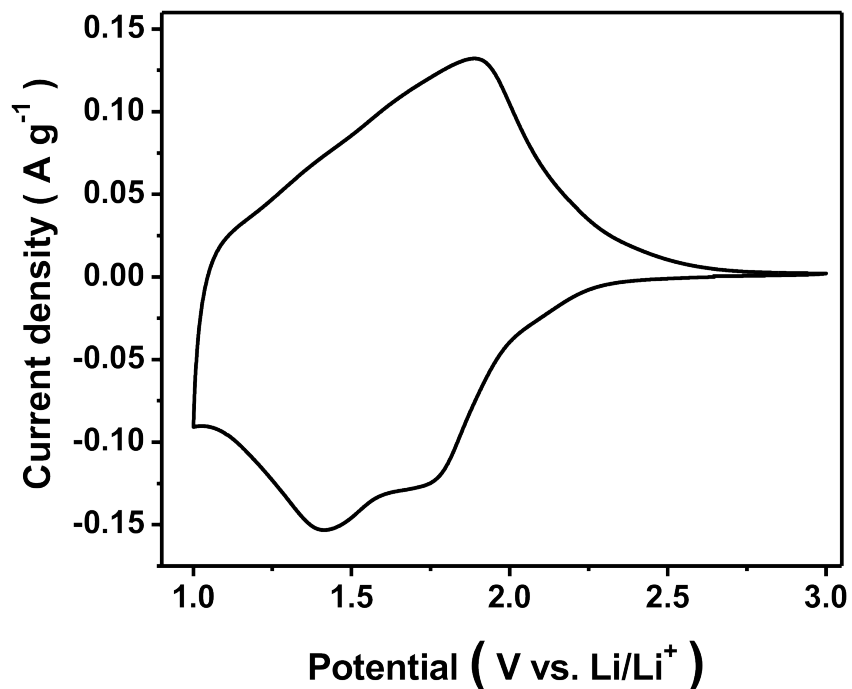


Figure S1. 1st CV curve of the electrode based on pure Nb₂O₅ at a scan rate of 0.5 mV s⁻¹ with a cutting-off voltage from 3.0 to 1.0 V.

Table 1. Atomic Parameters for VNb₉O₂₅

Atom	<i>x</i>	<i>y</i>	<i>z</i>
Nb(1)	0.0000(0)	0.0000(0)	0.0000(0)
Nb(2)	0.2189(1)	0.1052(1)	-0.0022(10)
Nb(3)	0.6749(1)	0.1179(1)	0.0001(10)
V	0.0000(0)	0.5000(0)	0.2500(0)
O(1)	0.4868(5)	0.2189(4)	0.5085(81)
O(2)	0.9503(5)	0.1160(5)	-0.0112(77)
O(3)	0.3532(5)	0.1577(4)	-0.0042(82)
O(4)	0.1763(5)	0.2170(4)	-0.0085(82)
O(5)	0.2512(5)	0.1108(4)	0.4872(62)
O(6)	0.0000(0)	0.0000(0)	0.5000(0)
O(7)	0.0743(4)	0.4470(4)	0.0231(47)