

# Structure Study on $V_2O_5$ Nanotubes

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## Introduction

Many materials of technological importance, particularly nanophase materials, do not possess the long-range order of conventional crystals. Often, it is this deviation from perfect order that makes them technologically and/or scientifically important. An important example is vanadium pentoxide. Crystalline vanadium pentoxide,  $V_2O_5$ , is a key technological material widely used in applications such as optical switches, chemical sensors, catalysts, and solid-state batteries [1-3]. The material possesses outstanding structural versatility and can be manufactured into nanotubes (Fig. 1) that have many of the same useful physicochemical properties as those of the parent  $V_2O_5$  crystal, but they are significantly enhanced. For example, the high specific surface area of the nanotubes renders them even more attractive as positive electrodes in secondary Li batteries [4]. In addition, the nanostructured material has a good potential for use in completely novel applications, such as nanoactuators [5] and nonlinear optical limiters [6].

A detailed knowledge of the atomic-scale structure of vanadium oxide nanotubes is needed to understand their important properties. Unfortunately, the diffraction pattern of a material with such a complex morphology and limited structural coherence shows a pronounced diffuse component and only a few Bragg

peaks [Fig. 2(a)]. This limits the applicability of conventional techniques for determining structure from powder data, such as Rietveld refinement.

## Methods and Materials

To determine the structure of  $V_2O_5$  nanotubes, we employed a nontraditional experimental approach that goes beyond Bragg scattering in the diffraction data. The approach is the atomic pair distribution function (PDF) technique [7, 8].

It takes both the diffuse and Bragg components of the diffraction data into account and yields the atomic ordering in terms of quantitative parameters such as a unit cell and symmetry, even when the material is ordered only on the nanometer length scale. The experiments were carried out at XOR beamline 1-ID at the APS by using x-rays with an energy of 80.6 keV. The use of x-rays with such a high energy allowed us to access higher wave vectors, which is essential for obtaining PDFs with good real space resolution. Also, it helped reduce several unwanted experimental effects, such as absorption and multiple scattering.

## Results and Discussion

Diffraction spectra of nanostructured and crystalline  $V_2O_5$  are shown in Fig. 2. As can be seen in Fig. 2, the lack of perfect long-range order due to the curvature of

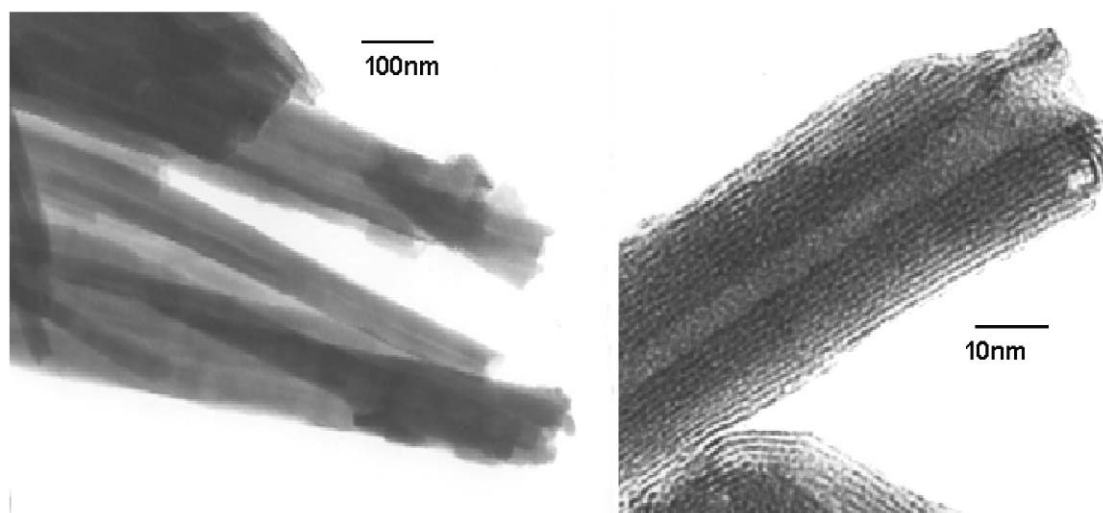


FIG. 1. Transmission electron microscopy (TEM) images of vanadium oxide nanotubes used in the present study; wrapping layers can be seen at higher magnification (right).

the tube walls has a profound effect on the diffraction pattern of nanophase  $V_2O_5$ . While the diffraction pattern of crystalline vanadium pentoxide shows sharp Bragg peaks up to wave vectors as high as  $Q \sim 15 \text{ \AA}^{-1}$ , the pattern of the nanotube counterpart shows only a few Bragg-like features that merge into a slowly oscillating diffuse component already at  $Q$  values of  $\sim 6$  to  $8 \text{ \AA}^{-1}$ . The diffraction patterns in Fig. 2 were reduced to atomic PDFs and used to test and refine structure models for  $V_2O_5$  nanotubes. The outcomes of this modeling effort will be reported on elsewhere.

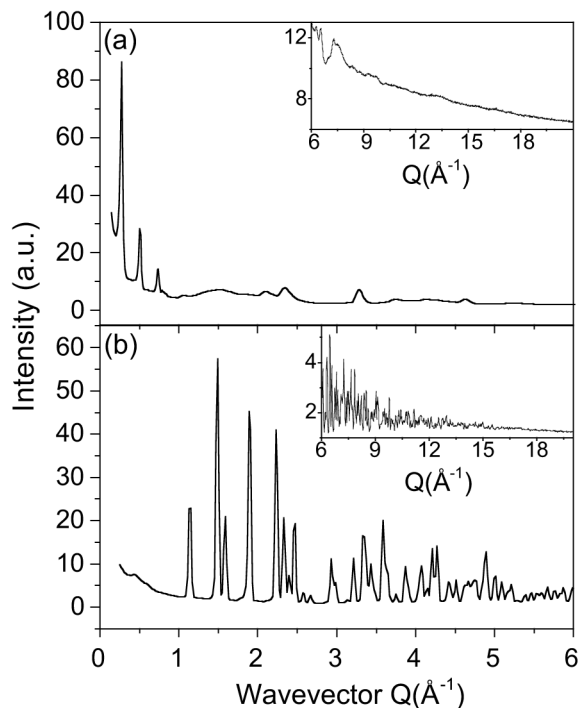


FIG. 2. Experimental powder diffraction patterns for  $V_2O_5$  nanotubes (a) and crystalline  $V_2O_5$  (b). The high- $Q$  portion of the patterns is shown in the insets on an enlarged scale.

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