

# Local Structure Investigation of Rapidly Synthesized $W_xV_{1-x}O_2$

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Vanadium dioxide ( $VO_2$ ) has been widely studied, in part, due to its near room temperature phase transition<sup>[1][2]</sup>. Below the transition temperature, 68°C,  $VO_2$  is a semiconducting monoclinic phase,  $P2_1/c$ ; whereas, above 68°C, it is a metallic tetragonal phase,  $P4_2/mnm$ . Substituting vanadium with 3d and 4d transition metals allows tunability of the phase transition temperature<sup>[3][5][4]</sup>. Conventional furnace synthesis requires multiple days to achieve phase purity. A microwave-assisted synthesis is presented which decreases synthesis time by four orders of magnitude, from days to minutes. Tungsten substitution amount has been verified through inductively coupled plasma mass spectrometry. Differential scanning calorimetry and superconducting quantum interference device measurements confirms that the transition temperature decreases with increasing tungsten amount. Synchrotron powder x-ray diffraction and Rietveld analysis verifies phase purity. The Rietveld analysis uncovered the phase fraction of un-substituted vanadium dioxide. Boxcar fitting of in-situ heating total scattering data analyzed with the pair distribution function determined whether there is a time difference between the change in the local and average structure during phase transformation.

## References

- [1] Serena A. Corr, Daniel P. Shoemaker, Brent C. Melot, and Ram Seshadri. Real-space investigation of structural changes at the metal-insulator transition in  $VO_2$ . *Phys. Rev. Lett.*, 105(5):1–4, 2010.
- [2] Zenji Hiroi. Structural instability of the rutile compounds and its relevance to the metal-insulator transition of  $VO_2$ . *Prog. Solid State Chem.*, 43(1-2):47–69, 2015.
- [3] K. L. Holman, T. M. McQueen, A. J. Williams, T. Klimczuk, P. W. Stephens, H. W. Zandbergen, Q. Xu, F. Ronning, and R. J. Cava. Insulator to correlated metal transition in  $V_{1-x}MoxO_2$ . *Phys. Rev. B - Condens. Matter Mater. Phys.*, 79(24):1–8, 2009.
- [4] Xiaogang Tan, Wei Liu, Ran Long, Xiaodong Zhang, Tao Yao, Qinghua Liu, Zhihu Sun, Yuanjie Cao, and Shiqiang Wei. Symmetry-controlled structural phase transition temperature in chromium-doped vanadium dioxide. *J. Phys. Chem. C*, 120(49):28163–28168, 2016.
- [5] Xiaogang Tan, Tao Yao, Ran Long, Zhihu Sun, Yajuan Feng, Hao Cheng, Xun Yuan, Wenqing Zhang, Qinghua Liu, Changzheng Wu, Yi Xie, and Shiqiang Wei. Unraveling metal-insulator transition mechanism of  $VO_2$  triggered by tungsten doping. *Sci. Rep.*, 2:1–6, 2012.