

Atomic Resolution Studies of W Dopants Effect on the Phase Transformation of VO₂

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Metal-Insulator Transition (MIT) in VO₂ has attracted attention of many theorists and experimentalists for more than fifty years since the discovery of the phenomena by Morin [1]. The distinctive aspects of this material are structural phase transition, sharp resistivity and optical transparency changes by several order of magnitudes at ~ 340 K [2]. These distinctive properties have inspired many applications such as thermo/electrochromics, Mott transistors, thermal actuators, gas sensors, strain sensors and temperature sensors. Recent efforts focus on controlling of phase transition and adjusting of slight opening around the transition temperature. These efforts mostly concentrate on using different dopants, which result in different material properties and play a critical role in device applications.

In this work, we have focused on the effect of tungsten (W) dopant in the VO₂ matrix by use of aberration corrected scanning transmission electron microscopy. The high-resolution Z-contrast imaging of individual single-crystalline W_xV_{1-x}O₂ nanowires indicates W atoms in the structure as shown in Figure 1a. Nanowires with different W concentrations (0.2, 0.5, and 0.8 atom %) that correspond to different transition temperatures (330, 314, and 295 K respectively) were studied. The comparison between the strain map analyses of high-resolution images of different nanowires reveals the effect of dopants on phase transition of VO₂ (Figure 1b-c). The dopants create anisotropic stress in the monoclinic VO₂ structure. This stress, which is either caused by the physical or electronic mismatch between W and V atoms, could facilitate the phase transition from monoclinic structure to tetragonal structure. Electron Energy loss spectroscopy was also used to investigate the valence change due to the addition of the W atoms in the VO₂ structure. We also verified the experimental observation by Density Functional Theory (DFT) calculations. [3][4]

References:

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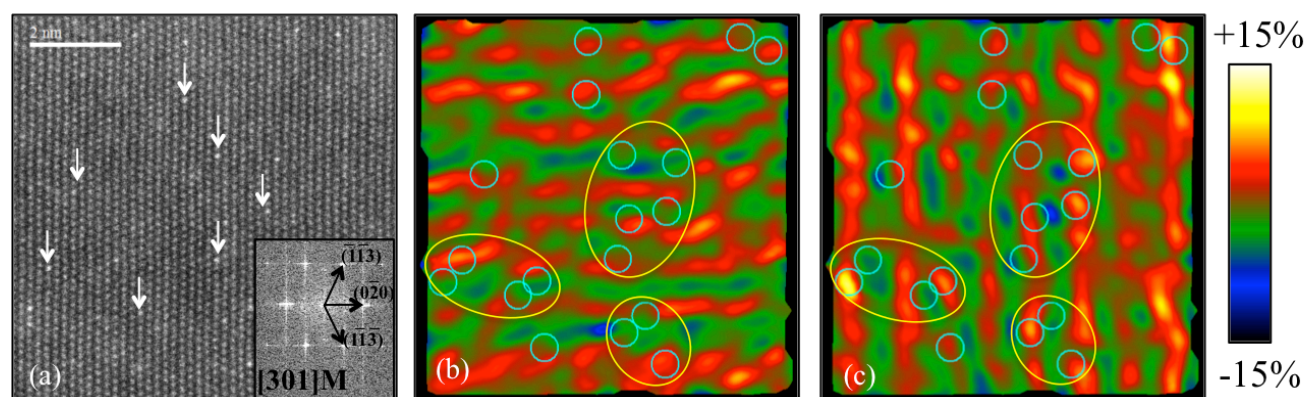


Figure 1. (a) Atomic resolution HAADF image of $W_xV_{1-x}O_2$ nanowires ($x=0.5$ atom%). Insets correspond to the FFT of (a) which indicates that (a) has been acquired along the $[301]$ zone axis of the monoclinic structure. The spots with higher intensity imply the existence of W in each column as compared to other spots. (b-c) strain maps are along to and perpendicular to $(\bar{1}\bar{1}3)$ lattice planes.