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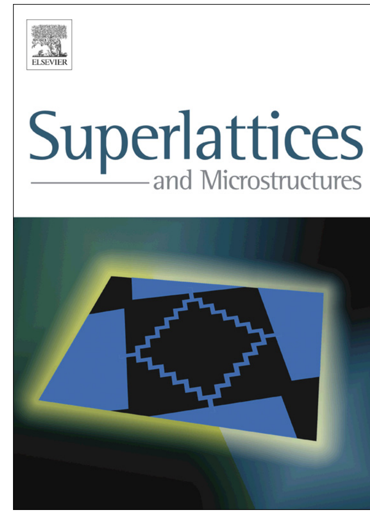

Enhanced Optical Properties of $W_{1-X}Mo_x O_3 \bullet 0.33H_2O$ Solid Solutions with Tunable Band Gaps

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Enhanced Optical Properties of $W_{1-X}Mo_xO_3$ • $0.33H_2O$ Solid Solutions with Tunable Band Gaps

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Abstract

A series of W1-xMoxO30.33H2O (x = 0, 0.25, 0.50, 0.75) nano/microstructures and MoO3 •0.55H2O with elongated morphology were prepared by using hydrothermal technique. Aqueous acidified solutions of ammonium metatungstate hydrate ((NH4)6H2W12O40X H2O) and ammonium heptamolybdate tetrahydrate ((NH4)6Mo7O24•4H2O) were hydrothermally reacted to yield the desired nano/microstructures. In the WO3 •0.33H2O crystal lattice can be substituted with up to 75 % Mo without structural alterations. When the Mo atoms increase, from 0 to 75 at. %, the band gap of the, as-prepared, W1-x MoxO30.33H2O material decreases from 2.55 to 2.15 eV. In order to corroborate experimental data, first-principle calculations using DFT and DFT+U framework were employed which revealed indirect semiconductors up to x=0.75. We suggest that the increase in the Mo fraction (25, 50 and 75%) by hydrothermal synthesis (pressure and temperature) is responsible for the narrowing of the band gap.

Keywords: oxide semiconductors, electron microscopy (STEM, TEM and SEM), visible and ultraviolet spectrometers, band-structure, crystallography, optical properties, band gap tunable.

1. Introduction

Hydrated transition metal oxides such as WO3nH2O and MoO3nH2O (n = 0, 0.33, 1 or 2) have been studied extensively due to their special electronic and optoelectronic properties. These materials have enormous potential applications in the fields ranging from condensed-matter physics to solid-state chemistry [1], such as photo-electrochemical energy conversion [2], gas sensors [3], photo-catalysts [4], lithium-ion batteries [5], solar cells [6], electron emitters [7] and optical storage media [8]. Hydrated oxides, compared with their single metal oxide constituents (WO3 and MoO3), have potential application in electrochemical devices. In the case of solid solutions, molybdenum-tungsten oxide (W1-xMoxO30.33H2O) materials show more promise due to the ability to control the components, structural characteristics tailoring, physical/chemical properties modulation. Furthermore, an improvement in the performance in the above-mentioned applications is expected due to the “synergistic effect” in the composites, when Mo is included in the lattice. Recently, tremendous effort has been dedicated to the preparation [9, 10, 11], formation, mechanism study [12, 13, 14], and property investigation [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29] of $W_{1-x}Mo_xO_3.3H_2O$. The $W_{1-x}Mo_xO_3$.3H2O showed