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ChemTech

International Journal of ChemTech Research
CODEN (USA): IJCRGG ISSN : 0974-4290
Vol.6, No.3, pp 1746-1748, May-June 2014

ICMCT-2014 [10th – 12th March 2014]
International Conference on Materials and Characterization Techniques

Structural, Raman and Infrared properties of V_2O_5 and $(MoO_3)_x$- $(V_2O_5)_{1-x}$ composites

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Abstract: In this study we demonstrate the physical properties of $(MoO_3)_x$- $(V_2O_5)_{1-x}$ composites for x = 0, 0.2, 0.4, 0.6 and 0.8. The composites were characterized by studying their structure, Raman and IR properties. The structure of $(MoO_3)_x$-$(V_2O_5)_{1-x}$ is orthorhombic and the grain size is decreases with increasing MoO_3 composition in $(MoO_3)_x$-$(V_2O_5)_{1-x}$.The Raman vibrational modes were not observed for x=0.2.The enhancement of Raman intensity was observed for x = 0.8 indicates the improvement in the structural property of MoO_3 due to V_2O_5 doping. From the FTIR spectra it was observed that the band at 1009 cm^{-1} is attributed to V=O stretching mode of V_2O_5. The band shifts to 1014 cm^{-1} indicating shortening of V-O_1band after incorporation of MoO_3 in V_2O_5.

Keywords: V_2O_5, MoO_3, mixed oxide, characterization.

Introduction and Experimental

V_2O_5 is widely used in elctrochromic, photochromic and thermo chromic devices. MoO_3 also exhibit photo chromic, thermo chromic and gasochromic properties. The interaction between V_2O_5 and MoO_3 is unique due to their similar ionic radii and nearly- identical structures in their higher oxidation state [1]. The present investigations are undertaken to study the properties of V_2O_5 and $(MoO_3)_x – (V_2O_5)_{1-x}$ composites.

Pure V_2O_5 powder (purity of 99.96 %) and MoO_3 powder (purity of 99.99 %) is used to prepare different composites of $(MoO_3)_x$- $(V_2O_5)_{1-x}$ for $0 < x < 1$. Various compositions of MoO_3, V_2O_5 powders have been taken in the mortar and grind well to get fine powders of the mixed oxide and they were sintered at 450 ^{0}C. The structure of the composites was performed by X-ray diffractometer (Philips PW1830) in the 2θ range from 10º to 70º. Raman spectra were recorded in the region of 0 to 1200 cm^{-1}. IR transmission spectra of composites were performed by FT-IR Spectrophotometer (JASCO FTIR-6300) in the range 600 to 4000 cm^{-1}.

Results and Discussion

The X-ray diffraction spectra for pure V_2O_5 and $(MoO_3)_x$ - $(V_2O_5)_{1-x}$ for $0 < x < 1$ were shown in Fig.1. The observed crystallographic orientations for pure V_2O_5 were (2 0 0), (0 1 0), (1 1 0), (1 0 1), (3 1 0), (1 1 1), (0 2 0), (4 1 1), (6 0 0). The data is good agreement with the JCPDS data (file no. 89-2483) of V_2O_5 and the phase is orthorhombic [2]. The grain sizes were evaluated from Scherrer's relation. At x=0.2 the intensities of (2 0 0), (1 0 1) peaks were decreased with increasing MoO_3 concentration. The grain sizes of these

crystallographic orientations are also decreasing which indicates the MoO_3 confining crystallinity of V_2O_5 to small regions. At x=0.8 we observed (0 2 0), (1 1 0), (0 4 0), (0 2 1), (1 1 1), (0 6 0), (2 0 0), (1 1 2), (0 8 1) orientations which corresponds to orthorhombic phase of MoO_3 [3].

The Raman spectra of $(MoO_3)_x$- $(V_2O_5)_{1-x}$ for $0 < x < 1$ were shown in Fig.2. For x=0 the Raman band at 145 cm^{-1} is a rigid layer-like mode and corresponds to the vibrations of –O–V–O–V–O– atoms. Band at 190 cm^{-1} is assigned to the stretching mode of $(V_2O_2)_n$. The two peaks located at 281 and 403 cm^{-1} are assigned to the bending vibration of the V=O bonds. The peaks at 690, 992 cm^{-1} were assigned to the doubly coordinated oxygen (V_2–O) stretching mode and terminal oxygen (V=O) stretching mode [4]. x=0.2 is completely amorphous which indicate the presence of small quantity of MoO_3 destruct the layered structure of V_2O_5. The growth of broad bands observed for x = 0.4 at 276 cm^{-1} indicates wagging mode, 814 cm^{-1} and a sharp but weak band at 988 cm^{-1} indicates stretching modes[5]. With further increasing the MoO_3 composition in $(MoO_3)_{0.6}$ -$(V_2O_5)_{0.8}$ the predominant peaks observed were corresponding to MoO_3 with a weak single peak at 189 cm^{-1} due to V_2O_5 and the remaining peaks were shifted. The result indicates that for x = 0.8 is the best composition which enhances the layered structure of MoO_3 due to V_2O_5 doping.The Infrared spectra recorded in the wavenumber range 600-4000 cm^{-1} for $(MoO_3)_x$ - $(V_2O_5)_{1-x}$ for $0 < x < 1$ are shown in Fig.3. For x=0 the absorption bands at 1647 cm^{-1} is attributed to bending mode of O-H vibrations [4], 1009 cm^{-1} is attributed to stretching mode (V=O), 826 cm^{-1} is attributed to V-O stretching vibration, 622 cm^{-1} arises due to different V-O bonds. At x = 0.2 band positions are shifted and few peaks are disappeared by increasing MoO_3 composition in V_2O_5. Here the band shifts to 1014 cm^{-1} indicating shortening of $V\text{-}O_1$ band after incorporation of MoO_3. The splitting and sharpening of bands in lower frequency range shows better order in mixed oxide films compared to their counter parts. The bands at 3744, 3612 cm^{-1} is due to O-H stretching in water [6], 1697 cm^{-1} is the bending mode of O-H vibration and shifted to higher frequency due to MoO_3 doping, mixed modes of V_2O_5 and MoO_3 is represented by the bands 1517 cm^{-1} and 832 cm^{-1} which corresponds to V-O stretching mode and shifted to higher frequency due to MoO_3 doping, 653 cm^{-1} is due to different V-O bonds and shifted to higher frequency due to MoO_3 doping. Further increasing MoO_3 composition for x = 0.4 the peaks at 2861, 1794 cm^{-1} is consisting of small amount of water [7]. The band at 1513cm^{-1} shows no change in the mixed mode of vibration. The V-O vibrational frequency mode observed for pure V_2O_5 at 622 cm^{-1} is shifting towards higher frequency for lower concentration of molybdenum oxide and is equal to anti-symmetric stretching mode of the Mo-O-Mo bridge. For x = 0.8 the two strong modes of vibrations observed at 987, 849 cm^{-1} and these were attributed to the Mo = O bond stretching [8] and terminal Mo = O bond of Mo^{5+} [9].

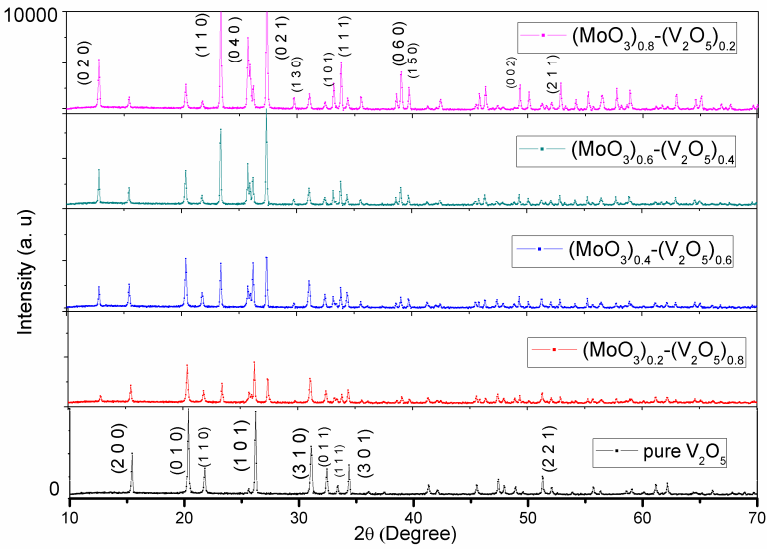

Fig 1: XRD Spectra of $(MoO_3)_x$-$(V_2O_5)_{1-x}$ for 0<x<1.

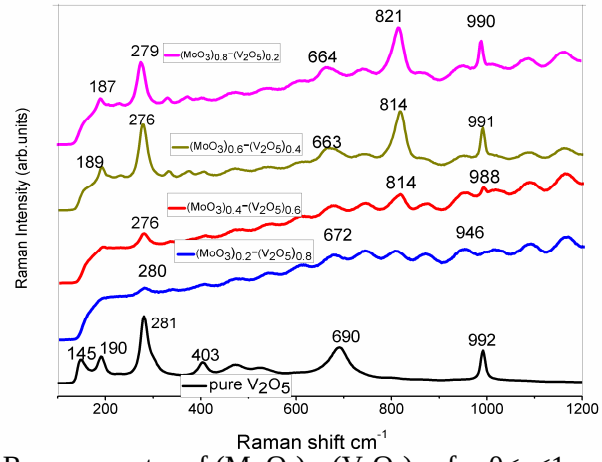

Fig 2: Raman spectra of $(MoO_3)_x$- $(V_2O_5)_{1-x}$ for 0<x<1.

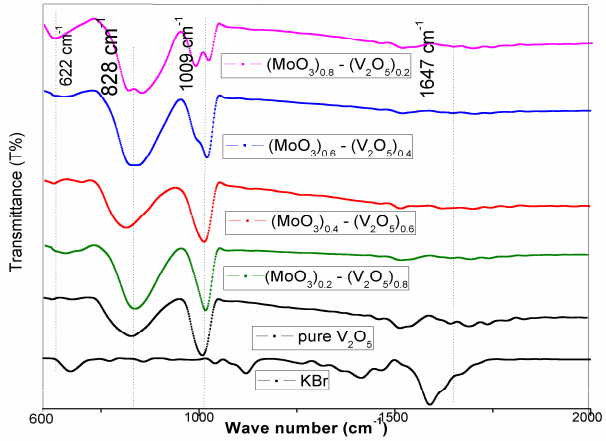

Fig 3: IR spectra of $(MoO_3)_x$- $(V_2O_5)_{1-x}$ for 0<x<1 from 600- 2000 cm^{-1}.

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