EXECUTIVE SUMMARY OF THE REPORT OF MINOR PROJECT ENTITLED " SYNTHESIS AND CHARACTERIZATION OF NANOCRYSTALLINE LEAD TUNGSTATE AND STRONTIUM MOLYBDATE" UNDER FINANCIAL ASSISTANCE FROM UNIVERSITY GRANTS COMMISSION, SWRO, BANGALORE, MRP(S)-367/08-09/KLKE027/UGC-SWRO

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The world of material science is undergoing vast changes especially in the realm of nanostructured materials. Nanotechnology is an enabling technology which will influence the way we live. Nanoscience and nanotechnology will revolutionize many scientific fileds especially microelectronics, superconductors, automotive and aircraft engines, prosthetic implants, medical diagnostics and drug delivery, computers and peripherals etc. One of the significant aspects of nanomaterials is the size dependent tailoring of physical properties. As the grain size reduces to nanometers, the number of atoms on the grain boundaries increases and the contribution from these surface or boundary atoms will play a decisive role in determining the properties of nanomaterials. Nanostructured materials offer excellent opportunities to study how new properties emerge and how its physics can be modelled. Materials belonging to the tungstate and molybdate family have a long tradition of practical applications and have been the subject of intense research over the past century. Lead tungstate (PbWO4) and strontium tungstate (SrWO4) crystals belong to the tungstate family. It is to be noted that these materials has high density, short radiation length, small Moliere radius, and excellent radiation intensity, and thus it is known to be one of the best materials for high energy physics detectors.

Nanocrystalline lead tungstate samples were synthesized using chemical precipitation technique. The crystal structure and grain size of the samples were determined from X-ray diffraction pattern of the samples. The X-ray diffraction pattern showed typical peaks corresponding to scheelite phase $PbWO_4$. The crystallite size was found to be 29 and 22 nm. In order to check the purity of the sample, infrared spectrum was recorded in the range 600 – 1000 cm^{-1}. The specimen showed an intense peak at 788 cm^{-1} which is a typical peak reported for bulk lead tungstate. The presence of such a peak clearly showed that the sample synthesized belonged to lead tungstate. UV-Visible spectra of nanoparticles of two different grain sizes were recorded. Analysis of the spectra showed that the samples have direct band gap. The band gaps of the sample have been determined from absorption spectra. The increase in band gap with decrease in particle size indicated quantum confinement effect. In summary the UV-Visible absorption spectra of PbWO4 nanoparticles of present study clearly showed the significant changes that occur in the electronic properties during transition from bulk to nanoregime. Further more the experimental evidence for blue shift of absorption edge and optical band gap widening can be helpful in understanding the quantum size effect and can throw light into the band structure of scheelite type tungtates. The Raman spectrum of the sample was recorded at room temperature from the range 50 – 1200 cm^{-1}. The peaks found in the range 250 – 1200 cm^{-1} were found to be sharp and intense. These correspond to internal modes of vibration of $PbWO_4$. All these peaks are identified and are assigned to stretching and bending vibrations of $WO_4{}^{2-}$ tetrahedron. The peaks found in the region 50 – 250 cm^{-1} were found to be broad and they correspond to lattice modes. The broadness of Raman peaks compared to that of bulk crystals of lead tungstate is due to the nanostructuring of the sample.

Nanocrystalline sample of strontium tungstate was prepared using chemical precipitation technique. The crystal structure and phase was analysed using X-ray diffraction studies. The crystallite size was estimated using Hall-Williamson analysis of XRD data by eliminating strain. The size determined using Hall-Williamson analysis was found to be 26 nm. The sample was further characterized using UV-Visible absorption spectrum. The band gap was found to be 5.51 eV which is blue shifted from that reported for bulk SrWO4. The absorption spectra also showed a peak at 3.8 eV. The mid IR spectrum showed peaks which are characteristics of strontium tungstate. This illustrates that our sample was chemically pure. The Raman spectrum of nanocrystalline strontium tungstate showed several peaks corresponding to internal and external modes of vibrations. All peaks can be indexed to the scheelite phase of $SrWO_4$. The Raman spectrum showed high frequency internal modes and low frequency external modes of vibration. The lattice modes are found to be broad and is due to nanostructuring of the sample.