Influence of Manganese ions in the band gap of tin oxide nanoparticles: Structure, microstructure and optical studies

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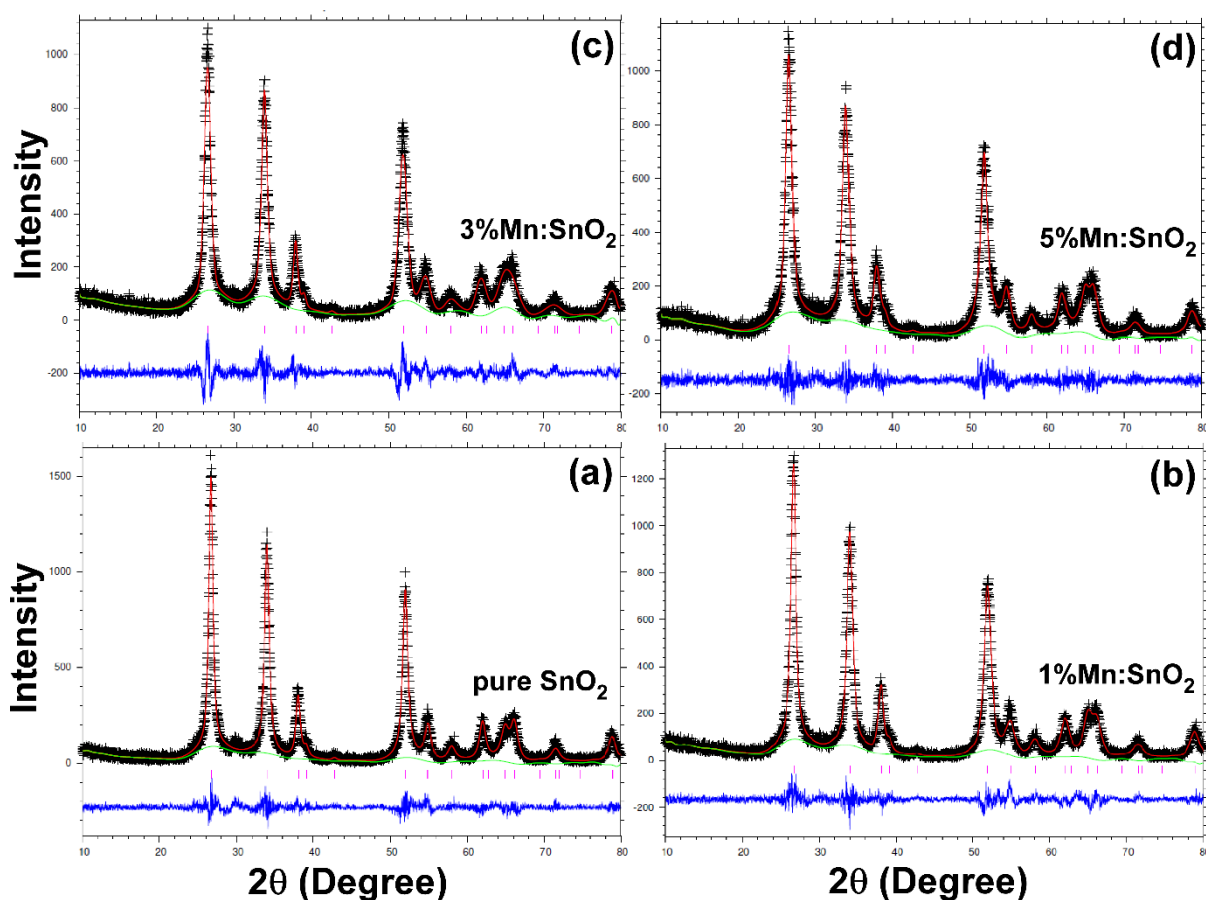
Figure 1. The Rietveld refined XRD patterns of pure, 1 mol% and 3 mol% Mn ion doped SnO$_2$ nanoparticles. The tick marks represents the calculated peak positions of tetragonal phase.

Table 1: Lattice parameters and the unit cell volume of the pure and Mn ion doped SnO_2 nanoparticles obtained from the Rietveld Analysis of the XRD patterns. Number in the bracket is the standard deviation in the calculated data. The refinement parameters are also provided.

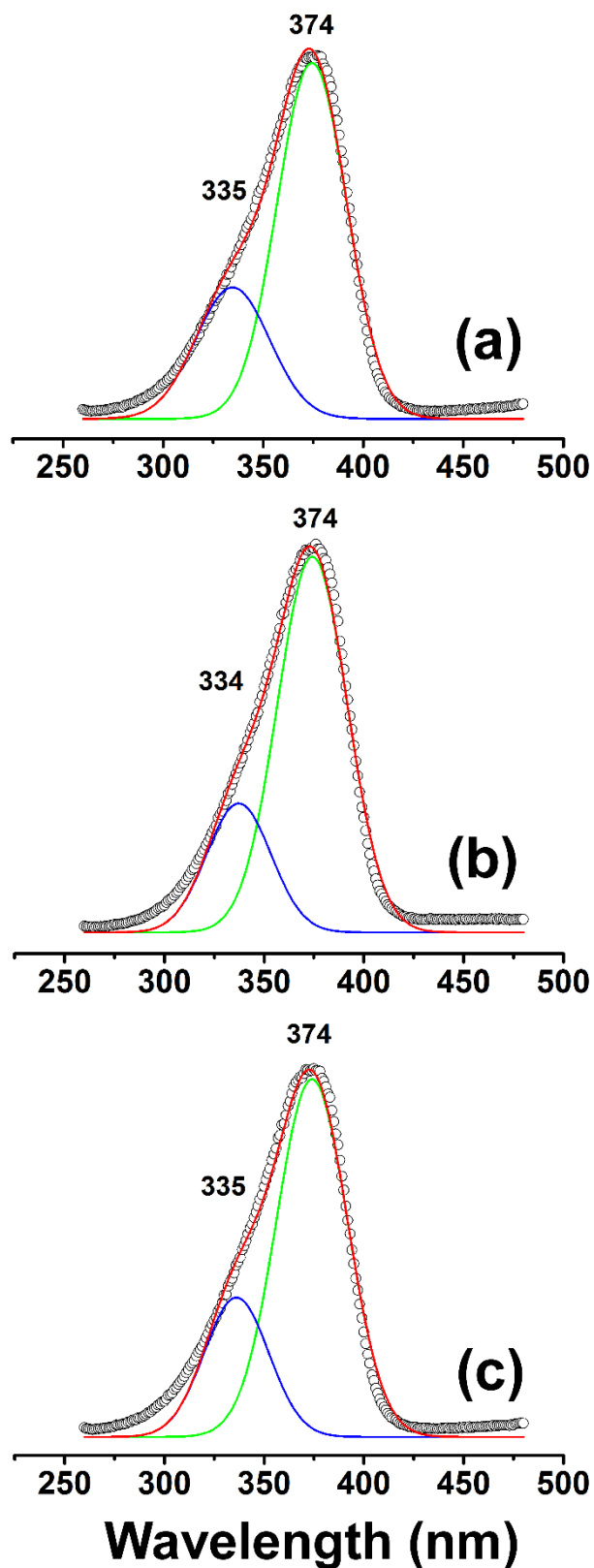|	$a = b$ (Å)	c (Å)	c/a	Unit cell volume (Å^3)	χ^2	R_{wp}	R_p	$R_F{}^2$	R_{exp}
Pure	4.7391 (±0.0007)	3.1849 (±0.0005)	0.6720	71.5300 (±0.0300)	2.948	0.167	0.114	0.066	0.098
1 % Mn	4.7392 (±0.0008)	3.1824 (±0.0006)	0.6715	71.4750 (±0.0340)	2.278	0.144	0.101	0.045	0.096
3 % Mn	4.7397 (±0.0011)	3.1802 (±0.0009)	0.6709	71.4430 (±0.0480)	2.987	0.165	0.126	0.074	0.096
5 % Mn	4.7370 (±0.0010)	3.1794 (±0.0007)	0.6712	71.3440 (±0.0420)	2.53	0.147	0.106	0.042	0.093`

Figure 2. Deconvoluted room temperature PL spectra of (a) pure SnO_2 (b) 1 mol% and (c) 3 mol% Mn ions doped SnO_2 nanoparticles. Two components corresponding to the near band edge emission (335 nm) and due to defects/surface state (375 nm) are observed. The excitation wavelength $\lambda_{ex} = 250$ nm.