Electronic Supplementary Information

Improved sensitization efficiency in Er^{3+} ions and SnO_2 nanocrystals co-doped silica thin films

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1. An estimation on the average sizes of SnO_2 NCs with the increasing annealing temperature according to the excitation peaks' position.

As shown in Fig.4, the redshifts of the excitation from band-to-band transition of SnO_2 nanocrystals (NCs) can be explained as the enlargement of the average sizes with the increasing annealing temperatures. Based on these excitation peaks, we also estimated the average size of SnO_2 NCs using the effective mass theory [1].

$$E_g(R) = E_g(R\to\infty) + \frac{h^2}{8R^2}\times\left(\frac{1}{m_e^*}+\frac{1}{m_h^*}\right) - \frac{1.8e^2}{4\pi\varepsilon\varepsilon_0 R} + smaller\ terms ,$$

where $E_g(R)$ is the band gap energy of SnO_2 NCs, R is the average radius of SnO_2 NCs, $E_g(R\to\infty)$ is the band gap energy of SnO_2 bulk materials and ε is the relative dielectric constant. m_e^* and m_h^* stand for the effective mass of an electron and a hole, respectively. For SnO_2 NCs,

$$E_g(R\to\infty) = 3.60\ eV,\ \varepsilon = 14,\ \varepsilon_0 = 8.85\times10^{-12} F/m,$$

$$m_e^* = 0.35\, m_0,\ m_h^* \gg m_e^*,$$

where m_0 stands for the free electron mass. Meanwhile, $E_g(R)$ can be calculated as follows,

$$E_g(R) = \frac{1240}{\lambda_{exc}}$$

where λ_{exc} stands for the excitation peak from band-to-band transition of SnO_2 NCs.

As shown in Table 1, it is found that the average sizes of SnO_2 NCs with different annealing temperatures are consistent with the TEM observations.

Table 1S. Band gaps and average sizes of SnO_2 NCs after annealing at different temperatures.

Annealing temperature / °C	800	900	1000	Bulk materials
λ_{exc} / nm	293	300	322	—
Band gap / eV	4.23	4.13	3.85	3.60
Average size / nm	2.92	4.22	5.12	—

2. XRD patterns of samples after annealing at 1000°C.

In order to characterize further the formation of SnO_2 NCs, the aged gels were annealed at 1000 °C and then milled into powers for the X-ray diffraction (XRD, using 0.1540562 nm Cu Kα radiation) test.

XRD pattern for corresponding sol-gel powers containing with 20% Sn after annealing at 1000°C is demonstrated in Fig. 1S(a). The pattern shows all the diffraction peaks assigned to tetragonal rutile crystalline phase of the SnO_2 NCs (JCPDS No. 41-1445), which is consistent with the TEM observation results. As shown in Fig. 1S(b), the related XRD spectra express a slight shifting, revealing the fact that Er^{3+} ions should be very likely incorporated in the D_{2h} lattice site of Sn^{4+}.

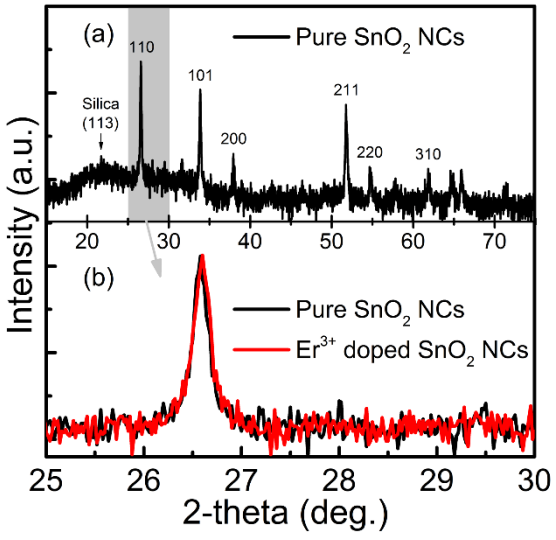

Fig.1S (a) XRD pattern of the 20% Sn doped SiO_2 powder samples after annealing 1000 ^oC. (b) Comparison of XRD spectra of pure and Er^{3+}-doped SnO_2 NCs silica thin films.

Reference

[1] L. Brus, *J. Phys. Chem.*, 1986, **90**, 2555.