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Surface defect states of $CdTe_xS_{1-x}$ quantum dots

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ABSTRACT

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Recently, semiconductor quantum dots (QDs) have attracted great attention due to their important applications in the fields of nonlinear optics, spin electronics, and integrated photonic devices [1-3]. Semiconductor QDs possess strong quantum confinement effect because their size is close to the Bohr radius of excitons [4,5]. The outstanding advantage of ternary semiconductor QDs over binary semiconductor QDs lies in that the energy band structure of ternary semiconductor QDs can be tuned by adjusting the stoichiometric ratio [6]. More flexible and important applications are expected for ternary semiconductor QDs [7]. In 1996, Paiva et al. reported an electrical switching in borosilicate glasses doped with $CdTe_xS_{1-x}$ QDs [7]. Subsequently, Liu et al. reported the optical absorption and photoluminescence properties of shell-core CdTeS ODs dispersed in glasses [8]. Recently, Mao et al. synthesized nearinfrared-emitting CdTeS alloyed QDs, which have great potential in biological and medical applications [9]. Surface defect states have important influences on carrier relaxation dynamics of semiconductor QDs [10]. However, up to now, little attention has been paid to surface defect states of ternary semiconductor QDs.

The aim of this Letter is to study the properties of surface defect states of $CdTe_xS_{1-x}$ QDs. The stoichiometric ratio was determined by use of the energy dispersive analysis of x-ray (EDAX). The photoluminescence (PL) spectrum, the photoluminescence excitation (PLE) spectrum, and the surface passivation were adopted

* Corresponding author. E-mail address: qhgong@pku.edu.cn (Q. Gong). Properties of surface defect states of $CdTe_xS_{1-x}$ quantum dots with an average diameter of 7 nm are investigated experimentally. The stoichiometric ratio is found to be 0.13:0.87 for Te:S by use of the energy dispersive analysis of x-ray. The photoluminescence spectrum, the photoluminescence excitation spectrum, and the surface passivation are adopted to characterize the properties of surface defect states. The energy levels of surface defect states of CdTe_xS_{1-x} quantum dots are also determined.

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to characterize the properties of surface defect states. The energy of the bandgap and the energy level of surface defect states were obtained.

The chloroform solution of $CdTe_xS_{1-x}$ QDs used in our experiment was obtained from URA Company, China. The shape and the size of $CdTe_xS_{1-x}$ QDs were measured by use of the scanning electron microscopy (SEM) (Model DB235, FEI Company, USA) and the high-resolution transmission electron microscopy (HR-TEM) (Model H-9000NAR, Hitachi Company, Japan), respectively. The measured results of the SEM and HR-TEM images are shown in Fig. 1. The SEM image indicates that $CdTe_xS_{1-x}$ QDs took on the surface topography of irregular spherical nanoparticles. Based on the HR-TEM image it could be determined that the average diameter of $CdTe_xS_{1-x}$ QDs was 7 nm, and the size deviation was less than 10%. To investigate the stoichiometric ratio, we performed the EDAX experiment and the measured results are shown in Fig. 2. The stoichiometric ratio was found to be 0.13:0.87 for Te:S. The strong dispersion peak of Cu originates from the Cu substrate. The dispersion peak of Si may results from Si impurities on the substrate surface.

The linear absorption spectrum of CdTe_{0.13}S_{0.87} QDs was measured by a UV-visible spectrophotometer (Model Agilent 8453, Agilent Technologies, USA) and the result is shown in Fig. 3(a). The linear absorption spectrum exhibits discrete features due to transitions coupling electron and hole quantized states [11]. The three lowest electron states in the order of increasing energy are 1S, 1P, and 1D states. While the three lowest hole states in the order of increasing energy are $1S_{3/2}$, $1P_{3/2}$, and $2S_{3/2}$ states [12,13]. The

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Fig. 1. SEM image (a) and HR-TEM image (b) of $CdTe_xS_{1-x}$ QDs.

(b) **Fig. 3.** Linear absorption spectrum (a) and PL spectrum (b) of CdTe_{0.13}S_{0.87} QDs.

Wavelength (nm)

absorption peak in the long-wavelength shoulder of the linear absorption spectrum, centered around 467 nm, can be assigned to the transition coupling the 1S electron state to the $1S_{3/2}$ hole state, which is also called 1S–1S transition [11]. The energy bandgap E_{gap} of CdTe_{0.13}S_{0.87} QDs can be extracted from the absorption peak of 1S–1S transition, $E_{gap} = 2.67$ ev. This is the usual method to determine the energy bandgap of semiconductor QDs [9].

In order to study the properties of surface defect states of $CdTe_{0.13}S_{0.87}$ QDs, we measured the PL spectrum at room temperature by using a fluorescence spectrophotometer (Model F-2500, Hitachi High Technologies America, USA) and the results are shown in Fig. 3(b). The Excitation photon energy is 2.8 eV. The PL spectrum shows a dominant emission peak centered at 505 nm. The shoulder of the PL spectrum could be decomposed into two weak Gaussian peaks, the center wavelength of which was located at 555 nm and 623 nm, respectively. Nanda et al. and Chaure et al. pointed out that the dominant emission peak at the high energy originated from the band edge luminescence whereas the other two weak peaks at the low energy could be assigned to trap states arising from surface defects, such as vacancies and impurities [14,15]. To confirm the origination of the emission peaks, we measured the PLE spectrum of $CdTe_{0.13}S_{0.87}$ QDs and the measured results are plotted in Fig. 4. The changes of the intensity of 505 nm emission peak as a function of the energy of the pump light are shown in Fig. 4(a). The 505 nm emission peak can be generated under excitation of a 2.67 eV pump photon. From Fig. 4(b) it can be obtained that the 555 nm emission peak can be generated under excitation of a pump light with photon energy of 2.67 or 2.45 eV.

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