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2015

Li, D., Liu, Y., de la Mata, M., Magen, C., Arbiol, J., Feng, Y., & Xiong, Q. (2015). Strain-induced spatially indirect exciton recombination in zinc-blende/wurtzite CdS heterostructures. *Nano Research*, 8(9), 3035-3044. doi:10.1007/s12274-015-0809-8

<https://hdl.handle.net/10356/141389>

<https://doi.org/10.1007/s12274-015-0809-8>

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Strain induced spatially indirect exciton recombination in zinc-blende/wurtzite CdS heterostructures

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The spatially indirect exciton recombination has been observed in zinc-blende/wurtzite CdS heterostructures induced by the applied strain, which can lead to the application in the field of laser cooling and ultrasensitive strain sensors.

Strain induced spatially indirect exciton recombination in zinc-blende/wurtzite CdS heterostructures

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KEYWORDS

Strain, CdS Nanobelts, Photoluminescence, Spatially Indirect Exciton Recombination, Inter-Crystalline Phase Transition

ABSTRACT

Strain engineering provides an effective route to tune the fundamental properties of semiconductors for electric and optoelectronic applications. Here we report on how the applied strain changes the emission properties of the heterostructures consisting of different crystalline phases in the same CdS nanobelts. The strained portion gives an extra emission peak at the low energy side, which shows a blueshift with increasing strain. Furthermore, the extra emission peak follows Varshni equation with temperature and exhibits band filling effect at high excitation power. This extra emission peak is tentatively attributed to the spatially indirect exciton recombination between different crystalline phases of CdS. The first principle calculations based on the spatially indirect exciton recombination have been carried out, which agrees with the experimental results. Strain is proved to be able to enhance the anti-Stokes emission, suggesting that the efficiency of the laser cooling might be improved by strain engineering.

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1 Introduction

Strain offers an effective route to modulate the band gap and tune the optical and electric properties of semiconductors other than electric and magnetic fields [1-6]. With the high crystalline quality and large surface-to-volume ratio, the nanostructures can bear much larger strain than that in their bulk counterparts [2]. As a result, strain in nanostructures can introduce some unique phenomena that cannot occur in their bulk counterparts. Recently, a number of works have been carried out to address how the strain influences the optical and electric properties of nanostructures in order to provide the insight for the next generation flexible electric and photonic devices with new functionalities [1, 3, 4, 7-15]. The conductance of ZnO nanowires decreases with the increasing strain [16] while an enhanced electron mobility has been achieved in strained silicon [17]. An extreme large redshift of exciton emission has been observed in buckled CdS nanowires [2] and strained GaAs nanowires [12] due to the increase of the lattice constant under the applied strain. In addition, strain is responsible of the exciton fine splitting in ZnO nanowires, as demonstrated recently [5]. With proper strain engineering, pseudo-heterostructures can be realized in homogeneous nanowires which will work like traditional heterostructures [18]. In addition, strain can induce a crossover from indirect band gap to direct band gap resulting in greatly enhanced emission [10, 19, 20].

Cadmium sulphide (CdS) is an important II-IV group direct band gap semiconductor with a band gap of 2.5 eV at room temperature [21]. Owing to their excellent optical properties and visible band gap, CdS nanostructures are considered not only to be very promising candidates for electrical and optoelectronic applications including field-effect transistors, waveguides, lasers, solar cells and field emitters, but also offer good platforms for fundamental research [22-26]. CdS in nanobelt morphology has recently been identified as the groundbreaking choice of

semiconductors for laser cooling suggesting considerable promise in all solid state optical refrigeration [25, 27, 28]. There are two crystalline structures in CdS, namely, zinc blende (ZB) and wurtzite (WZ) structures [29]. Under ambient condition, CdS nanobelts and nanowires exhibit WZ structure since WZ phase is more stable in atmosphere [30]. The applied strain dependence of the optical properties of WZ CdS nanobelts and nanowires has already been investigated [2, 31]. However, it remains elusive how the applied strain changes the optical properties of heterostructures consisting of WZ and ZB CdS nanobelts. Such investigations would provide a full picture of CdS nanobelts under strain, giving meaningful knowledge for flexible device applications.

Here we report on the strain dependent photoluminescence (PL) spectroscopy of heterostructures consisting of WZ and ZB crystalline domains present in CdS nanobelts. We carried out temperature and excitation power dependent emission under different applied strain strength. Under the applied strain, an extra emission peak has been observed at the low energy side of band-edge emission which shows a blue shift when increasing strain and excitation power. The extra emission peak follows Varshni equation with temperature as well. To understand the origin of this extra peak, we propose a spatially indirect exciton recombination model which takes into account the inter-crystalline phase transition of the heterostructures. The simulation based on the inter-crystalline phase transition agrees with the experimental results. Finally, we found that the existence of the ZB phase would enhance the anti-Stokes emission, which is beneficial for laser cooling of semiconductors.

2 Experimental

Figure 1. (a) Low magnification HAADF image of one CdS nanobelt. (b) Atomic-resolution HAADF image of the green squared region in (a), highlighting the presence of twin boundaries along the growth direction. (c) FFT of (b). (d) FFT of (e). (e) Atomic resolution HAADF image of the CdS WZ structure. (f,e) Magnified detail of the area yellow squared in (e) displayed in grey scale (f) and temperature color (g).

The CdS nanobelts were synthesized in a home-built vapor transport chemical vapor deposition system [22]. In Figure 1a we show one of the CdS nanobelts studied under aberration-corrected high angle annular dark field (HAADF) conditions, allowing to distinguish the atomic position within Cd-S dumbbells and thus obtaining a direct image of their polarity [32]. The nanobelts have rectangular shape and grow along the $[1-100]$ direction. The lateral facets of these belts belong to the $\{0001\}$ family, while the front and back ones are $\{11-20\}$ planes. The nanobelts crystallize mainly in the hexagonal WZ structure. However, the appearance of longitudinal twin boundaries parallel to the $[1-100]$ growth direction nanobelt and R is the local radius of the curvature [3].

(Figure 1b,c), and extending along the entire length of the nanobelts, creates different polytypic domains, similar to those twinning superlattices observed in III-V nanowires [33, 34]. As the twins are randomly distributed, among the polytypic domains we also find some ZB regions, despite the fact that the CdS mainly crystallizes as pure WZ (Figure 1d,e). In Figure 1e-g are also included some atomic resolution images of the CdS WZ structure where the atomic columns of the material are clearly distinguished. Notice that the material grows along a non-polar direction, being the lateral facets of the nanobelts oppositely polarized while the front and back ones are also non-polar.

To investigate the strain dependent emission in the polytypic domains of CdS nanobelts, we introduced strain by dispersing CdS nanobelts across the pillars on a silicon-on-insulator (SOI) substrate etched using a reactive ion etching (RIE) (Figure 2a). The pillars are 1 μm in height and around 1 μm in length for the top surface. The samples were mounted in a microscopy continuous flow cryostat (Cryo Industry of America, USA) to change the surrounding temperature from 77 K to 340 K. The PL measurements were carried out using a Micro-Raman spectrometer (Horiba-JY T64000) in the backscattering configuration excited by an Ar ion laser (457 nm). For the anti-Stokes emission measurements, we used a 532 nm solid state laser to excite the nanobelts.

3 Results and discussion

Figure 2a shows a 60° tilt view SEM image of a CdS nanobelt supported by a silicon pillar on SOI substrate. The thickness of the nanobelt used here is around 50 nm, which was measured by atomic force microscopy (AFM, Veeco Instrument, Nanoscope III). The strain ϵ starts to increase from the bottom part and reaches a maximum value, around 0.29 %, at the top of the pillar which was evaluated based on the equation $\epsilon = \frac{t}{2R}$ where t is the thickness of

Then, we carried out the PL measurements along the

nanobelt, as indicated by red arrow, excited by a 457 nm laser with a power of 50 μ W at 77 K. The detailed PL peak assignment of CdS nanobelts can be found elsewhere [23]. The PL spectra show several important features: (i) the presence of strain gives rise to an extra emission peak at the low energy side indicated by the red dashed curve; (ii) with the increase of the strain, the peak position of the extra emission peak blue shifts

and the intensity of the extra emission peak increases; (iii) the position of extra emission peak is very sensitive to the applied strain; (iv) The free exciton (both free exciton A or FXA and B or FXB) and bound exciton emission peaks maintain the same energies with the change of strain which indicates that the applied strain here is quite small.

Figure 2. (a) An SEM image of a CdS nanobelt suspended across a pre-patterned silicon pillar on silicon above insulating substrate. The scale bar is 1 μ m. (b) The PL spectra at 77 K scanning along the nanobelt as indicated by the red arrow in (a). All spectra are normalized and shifted vertically for clarity. (c) PL spectra extracted from (b) for three positions at 77 K as indicated in (a): without strain (position 1), medium strain (position 2) and maximum strain (position 3) in our investigation. The spectra were fitted and decomposed into individual components based on Gaussian function.

To clearly observe those features, in Figure 2c we pick up the PL spectra from three typical positions at Figure 2b: position 1 without strain, position 2 with medium strain and position 3 with the maximum strain in our investigation as indicated in Figure 2a. The experimental spectra were fitted and decomposed into individual components as shown in a series of traces. Without strain (position 1), the PL spectrum is dominated by the exciton emission with relative weak donor-acceptor pair (DAP) emission at low energy side [23]. When strain applied (position 2), an extra emission peak appears at the tail of phonon replica of DAP emission, while the exciton emission and DAP emission are present, too. Nevertheless, the intensity of the extra emission peak is comparable to that of

exciton emission. As the strain increases to the maximum value investigated (position 3), the position of the extra emission peak blue shifts and the intensity surpasses that of the exciton emission.

To find out the origin of the extra emission peak, we carried out temperature and excitation power dependent PL measurements at those three positions excited by a 457 nm laser with a power of 50 μ W, as shown in Figure 3a-c. As the temperature decreases, the exciton emission peaks show a monotonous blueshift and the DAP emission appears below 150 K. With strain, the extra emission peak also shows a blueshift and the intensity of the extra emission peak increases as the temperature decreases. For the portion with the maximum strain (position 3), the intensity of the extra emission peak can become even

stronger than that of exciton emission below 150 K.

Figure 3. The temperature dependence of PL spectra for position 1 (a), position 2 (b) and position 3 (c) as indicated in Figure 2(a). All spectra have been normalized and shifted vertically for clarity. (d) The free exciton A peak versus temperature extracted from (a)-(c) for those three different positions. The discrete points are experimental results and the solid lines are Varshni fittings. (e) The extra emission peak versus temperature extracted from (a)-(c) for position 2 and position 3. The discrete points are experimental results and the solid lines are Varshni fittings.

Based on the Gaussian fitting, the temperature dependence of FXA and the extra emission peak are extracted as shown in Figure 3d and 3e. For all three positions, the FXA emission peak shows a blueshift as the temperature decreases following the Varshni equation due to the change of the lattice constant and electron phonon coupling strength [35]. Compared with the unstrained portion (position 1), the FXA emission of the strained areas (position 2 and 3) exhibits a small redshift at higher temperatures and the energy difference of FXA emission between strained and unstrained portions decreases with the decrease of the temperature and finally vanishes below 150 K. One possible reason for such phenomena is that the applied strain can induce a strong electric

field due to the piezoelectric effect. As a result, the free carrier recombination plays an important role at higher temperatures due to the electric field induced exciton ionization at the strained portions. Surprisingly, the extra emission peak also follows Varshni equation as the temperature changes, indicating that the extra emission peak, like free exciton emission, originates from energy bands rather than from defect levels.

In addition, we carried out excitation power dependent PL spectroscopy. For the unstrained portion, the DAP emission saturates but the peak remains at the same energy as the excitation power increases (Figure 4a). Nevertheless, as the excitation power increases, the extra emission peak shows a blueshift and finally reaches a saturation value while

the width of the extra emission peak continuously broadens for the strained portions (Figure 4b, 4c and 4d). The blueshift of the extra emission peak with the excitation power is most probably due to the band filling effect or Burstein-Moss (BM) effect. Based on the parabolic-band model, the BM shift ΔE_{BM} is proportional to the carrier density $n^{2/3}$ [36, 37]. In view of that the photogenerated carrier density is proportional to the excitation power P in the range

here investigated, the BM shift ΔE_{BM} should linearly increase with $P^{2/3}$. We also give the fitting results (solid lines in Figure 4d) based on the equation $E \propto P^{2/3} + A$, where A is fitting parameter. The trend of the experimental results is very close to that of the fitting ones, which supports that the blueshift of the extra emission peak with increasing excitation power is truly due to the BM effect.

Figure 4. Excitation power dependence of PL spectra at 77 K for position 1 (a), position 2 (b) and position 3 (c) as indicated in Figure 2(a). All spectra have been normalized and shifted vertically for clarity. (d) Excitation power dependence of the extra emission peak for positions 2 and 3 extracted from (b) and (c) in logarithm scale. The discrete points are experimental results and the solid lines are fitting results based on the BM effect.

To understand the origin of the extra emission peaks, we propose a spatially indirect exciton recombination model originated from the inter-

crystalline phase transition of the heterostructures based on the first principle calculation. The spatially indirect exciton recombination has been observed in a number of materials with ZB/WZ polytypism such as

InP, GaN and GaAs [38-43]. The schematic diagram of the ZB/WZ interface used for calculation is shown in Figure 5a. Density Function Theory (DFT) was used to study the electronic properties of CdS. The generalized gradient approximation (GGA) [44] and hybrid functional (HSE06) [45] were used to describe the exchange-correlation potential. The cell structural and ionic positions were optimized via the Vienna Ab-initio Simulations Package (VASP) code [46, 47] within the full-potential projector augmented wave (PAW)

method [48, 49]. The plane wave cutoff energy was set to 500 eV and the atomic positions were fully relaxed so that the forces acting on each atoms was less than 0.02 eV/Å. The energy convergence criterion was set to 10^{-5} eV. $8 \times 8 \times 8$ and $6 \times 10 \times 6$ Gamma-centered k-points grids were used in structural optimizations and energy calculations for ZB and WZ, respectively. The unit cell of WZ phase was chosen to be a cuboid in order to compare with ZB regarding the shear applied.

Figure 5. (a) Schematic of WZ/ZB interface labelled with green line (left WZ, right ZB). (b) The approximate band alignment for the WZ/ZB CdS nanobelt. The band alignment and all possible optical transitions for one WZ/ZB CdS heterostructure unit without strain (c) and with strain (d). With strain, the conduction band of ZB phase moves far away from the valence band of WZ phase, resulting in the blueshift of the extra emission peak. (e) The energy diagram and band alignment for one WZ/ZB CdS heterostructure unit under strain with high excitation power. The bottom of conduction band of the ZB phase has been occupied and the quasi-Fermi level moves into the conduction band, leading to the blueshift of the extra emission peak with the increase of the excitation power.

The superlattice of WZ-CdS/ZB-CdS was constructed based on experimental configuration to analyze the valence-band offsets (VBOs) of the

interfaces under strain. The dangling bonds were saturated by hydrogen atoms and a 15 Å vacuum layer was inserted. The VBO can be calculated by the following formula:

$$\Delta E_V = \Delta E_{CL} + (E_{ZB}^{Ad} - E_{ZB}^{VBM}) + (E_{WZ}^{Ad} - E_{WZ}^{VBM})$$

where $(E_{ZB}^{4d} - E_{ZB}^{VBM})$ is the energy difference between 4d electron level and valence band maximum (VBM) in the ZB-CdS thin film, and the $(E_{WZ}^{4d} - E_{WZ}^{VBM})$ is the energy difference between 4d electron level and VBM in the WZ-CdS thin film. While $\Delta E_{CL} = E_{ZB}^{ZB/WZ} - E_{WZ}^{ZB/WZ}$ is the energy difference between ZB phase and WZ phase CdS core levels (CL) in the superlattice junction. The core level (CL) was used as the average electrostatic potential (AEP) to align the valence band [50].

The bulk WZ-CdS and ZB-CdS were calculated to determine the VB with respect to the corresponding AEP in the bulk using HSE hybrid functional under 0.5% strain. Figure 5b shows the schematic of the energy diagram in real space with different width for both, WZ and ZB regions, which results in the variation of the lowest energy level of conduction band of the ZB region due to the quantum confinement effect. The conduction band offset was determined based on the valence band offset and the band gap of respective region. Without strain, both the valence and conduction bands of the ZB phase are below those of WZ phase, forming type-II band alignment as shown in Figure 5c [51]. In this case, the emission is dominated by WZ phase while the emission from ZB phase and spatially indirect exciton emission from the inter-crystalline phase (red arrows in Figure 5c) are too weak to be observed. With hydrostatic and uniaxial strain, the difference between CL and VBM in WZ phase is larger than that in ZB phase, which is also the case without strain. However, with shear strain, both the valence band and conduction band of ZB phase are lifted up compared with those of WZ phase, as shown in Figure 5d. The calculation indicates that the valence band discontinuity between those two phases is 44 meV and the bandgap difference is 87 meV. The conduction band offsets can be obtained as 131 meV, indicating that photogenerated electrons are mainly distributed in ZB phase while photogenerated holes are confined in the WZ phase near the interfaces. The presence of strain would increase the electron-hole overlap for the

spatially indirect exciton transition (Figure 5d), which has been observed in Ge/Si quantum dots [52]. As a result, the spatially indirect exciton recombination is greatly enhanced and strong enough to be observed in the PL spectra. Far away from the interfaces, the emission is still from the WZ phase. The increase of the extra emission intensity with decreasing temperature suggests that the extra emission peak comes, indeed, from the lowest excitonic states (spatially indirect exciton emission due to the inter-crystalline phase transitions here). In addition, the spatially indirect band gap recombination of the extra emission peak is much broader, which can be attributed to the width variations of the ZB regions. Due to the quantum confinement effect, such variations can change the bottom of the conduction band from ZB domains (Figure 5b), resulting in a broader emission peak.

The calculation indicates that the energy difference between the conduction band of ZB phase and the valence band of the WZ phase increases with the increase of the applied strain within the investigated range. As a consequence, the extra emission peak would show a blueshift as the applied strain increases. Indeed, we observed a blueshift of the extra emission peak with increasing strain (scanning from position 1 to position 3 in Figure 2b), which provides a strong evidence for our proposed spatially indirect exciton recombination model. As the extra emission peak moves to the higher energy side with the increasing strain, the superposition of the extra emission peak with DAP ones gives rise to the stronger emission of the extra peak compared with that of the exciton emission (Figure 2b). Furthermore, the stronger electric field induced by the larger strain may also contribute to the intensity increase of the extra emission peak. As the temperature changes, both the valence band of WZ and the conduction band of the ZB follow Varshni equation, indicating that the temperature dependence of the extra emission peak can be described by Varshni equation as well (Figure 3e).

Under the shear strain, the photogenerated electrons near the interfaces flow to the ZB phase regions due to the band alignment (Figure 5e). As the excitation power increases, more and more electrons concentrate inside the ZB phase regions and start to take up the higher energy levels due to the smaller density of states for two dimensional ZB strips (only 3-5 nm in width). As a result, the quasi-Fermi level of electrons moves into the conduction band promoting the extra emission peak movement to the higher energy side with the increase of the excitation power, suggesting that BM effect occurs (Figure 5e and Figure 4d).

Figure 6. The anti-Stokes PL spectra from those three positions indicated in Figure 2(a) excited by a 4.5 mW 532 nm laser at 77 K. The left panel shows the low energy part and right panel shows the high energy part. To compare, the spectra at the high energy part have been magnified. The very narrow peak around 2.26 eV can be attributed to the Si Raman scattering.

Finally, we have carried out the anti-Stokes PL measurement on the strained CdS nanobelt, the basis of the laser cooling of semiconductors which has been recently demonstrated in CdS nanobelts [25, 27, 28]. Figure 6 displays the anti-Stokes PL from both strained and unstrained CdS nanobelt excited by a 532 nm laser with a power of 4.5 mW. Compared with the unstrained portion, both the exciton emission and DAP emission of anti-Stokes PL from the strained CdS nanobelt are greatly enhanced, suggesting that the applied strain may improve the laser cooling efficiency. The enhancement of the anti-Stokes

emission by applied strain may be attributed to the enhanced absorption at the low energy side due to the presence of the inter-crystalline phase absorption.

4 Conclusions

We have successfully synthesized heterostructures consisting of ZB and WZ crystalline phases in the same CdS nanobelts. The temperature and excitation power dependent PL spectroscopy under applied strain has been carried out to investigate how applied strain affects emission of the heterostructures. An extra emission peak is identified at the low energy side with applied strain and is observed to exhibit a blueshift with increasing strain. This extra peak is proposed to originate from the spatially indirect exciton recombination of the inter-crystalline phase regions, qualitatively verified by the first principle calculation. The applied strain could enhance anti-Stokes PL which might improve the laser cooling efficiency. Our findings suggest that our WZ/ZB CdS heterostructures provide a good platform to investigate optical processes between the inter-crystalline phases and can be utilized to fabricate ultrasensitive strain sensors.

Acknowledgements

This work is mainly supported by Singapore National Research Foundation through a NRF fellowship grant (NRF-RF2009-06) and NRF Investigatorship grant (NRF-NRFI2015-03), and Singapore Ministry of Education via two AcRF Tier 2 grants (MOE2011-T2-2-051 and MOE2013-T2-1-049). This work was also supported in part by AFOSR through its Asian Office of Aerospace Research and Development (FA2386-13-1-4112). D.L. acknowledges the World Future Foundation (WFF) for awarding him the WFF PhD Prize in Environmental and Sustainability Research (2014) and the financial support to this work. Y.L. acknowledges the support from High Performance Computing Center (HPCC) at NTU and Dr. Yang

Ming from NUS for meaningful discussions. J.A. acknowledges the funding from Generalitat de Catalunya 2014SGR1638 and Spanish MINECO MAT2014-51480-ERC_(e-ATOM). MdIM thanks CSIC Jae-Predoc program.

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