

Electronic Supplementary Information

for

Multi-band luminescent ZnO/ZnSe core/shell nanorods and their temperature-dependent photoluminescence

Xu Yang,^a Qin Yang,^b Zhigao Hu,^c Wu Zhang,^a Hui Li,^a Lequn Li,^a Yining Qiu,^a Ning Xu,^a Jiada Wu*^a and Jian Sun*^a

^aDepartment of Optical Science and Engineering and Shanghai Engineering Research Center of Ultra-Precision Optical Manufacturing, Fudan University, Shanghai 200433, China

^bCollege of Science, Guizhou Minzu University, Guiyang 550025, China

^cSchool of Information Science & Technology, East China Normal University, Shanghai 200241, China

S1. XRD characterization

Figure S1 shows the XRD patterns of the annealed bare ZnO NRs, as-fabricated ZnO/ZnSe core/shell NRs and annealed ZnO/ZnSe core/shell NRs fabricated on Si substrates. Besides weak peaks indexed to the (101), (102) and (103) diffractions of hexagonal wurtzite ZnO, the (002) diffraction (peaking at $2\theta = 34.38^\circ$ with a full width at half-maximum (FWHM) of 0.17°) of hexagonal wurtzite ZnO (JCPDS: 36-1451) dominates the XRD pattern of the bare ZnO NRs, revealing that the ZnO nanorods have a good hexagonal wurtzite structure and grew with the preference of (002) orientation along the *c*-axis perpendicular to the substrate. After the coverage of ZnSe outside the ZnO NRs, a prominent peak appears at about 27.20° together with two additional weak peaks. The peak near 27.20° is attributed to the diffraction by the (111) plane of cubic zinc blende ZnSe (JCPDS: 37-1463), revealing that the ZnSe shells are featured with cubic zinc blende structure and grow with the preference of (111) orientation. The broadening of the diffraction peaks indicates the small crystallite size of the ZnSe shells. After annealing at 800°C in N_2 for 60 min, both the (002) wurtzite ZnO and (111) zinc blende ZnSe diffraction peaks exhibit increased intensities and narrowed widths, revealing the growth of ZnO and ZnSe crystallites during the annealing process and an improvement in the crystallinity of both the ZnO cores and the ZnSe shells due to annealing.

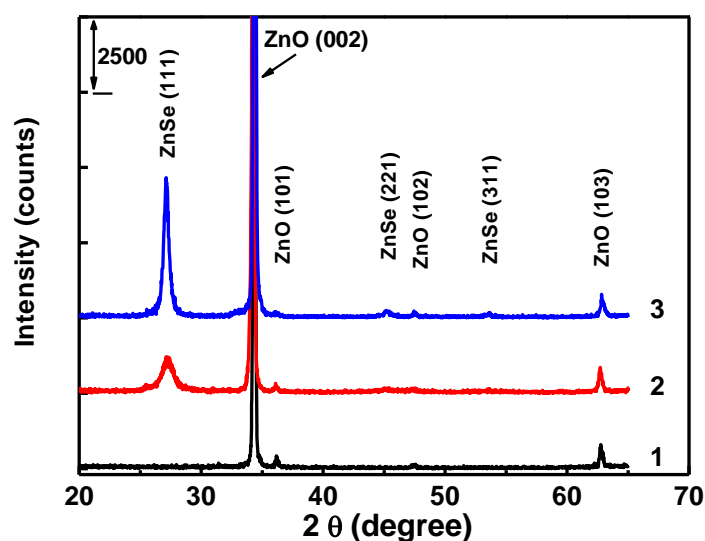


Figure S1 XRD patterns of annealed bare ZnO NRs (1), as-fabricated ZnO/ZnSe core/shell NRs (2) and annealed ZnO/ZnSe core/shell NRs (3).

S2. FTIR measurements

The ZnO cores exhibit IR features of characteristic hexagonal wurtzite ZnO, while the ZnSe shells present IR features of cubic zinc blende ZnSe, as shown by spectra 1 and 2 in figure S2 which were taken from the annealed bare ZnO NRs and the as-fabricated ZnO/ZnSe core/shell NRs, respectively. In addition to the IR absorptions from the substrate (marked by * in figure S2), the principal absorptions ranging from 335 to 470 cm^{-1} in spectra 1 and 2 can be attributed to the stretching mode of Zn–O–Zn [1]. Coverage of ZnO cores with ZnSe shells results in a strong and narrow absorption at 205 cm^{-1} . This absorption corresponds to the transverse optical (TO) mode of zinc blende ZnSe [2]. For the annealed ZnO/ZnSe NRs, the absorptions ascribed to ZnO and ZnSe have a small blue shift, confirming the improvement in the crystal structures of the ZnO cores and the ZnSe shells due to annealing. In particular, the absorptions attributed to ZnO become strong and well resolved, peaking at 378 and 409 cm^{-1} , respectively, much closer to the $\omega_{T//}$ and $\omega_{T\perp}$ frequencies of the TO modes of wurtzite ZnO [1].

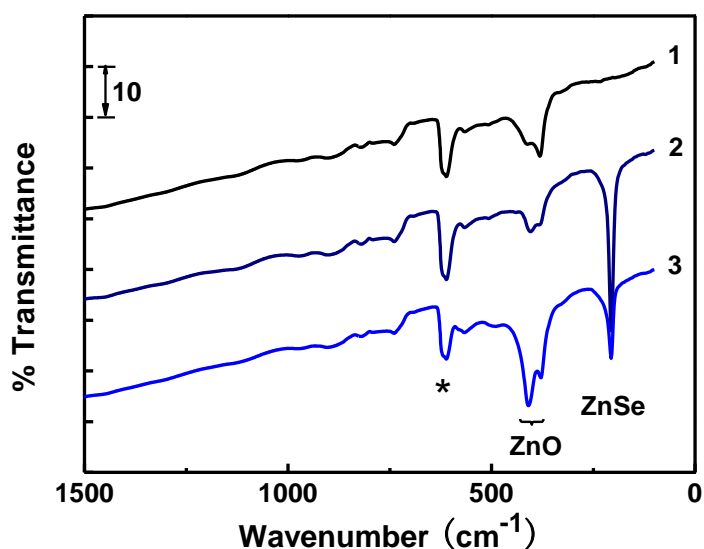


Figure S2 FTIR spectra of annealed ZnO NRs (1), as-fabricated ZnO/ZnSe core/shell NRs (2) and annealed ZnO/ZnSe core/shell NRs (3).

S3. Raman backscattering measurements

Raman backscattering measurements provide another evidence for the wurtzite

structure of the ZnO cores and the zinc blende structure of the ZnSe shells as well as the improvement in the crystallinity due to post-fabrication annealing. Figure S3 illustrates the Raman spectra taken from the annealed bare ZnO, as-fabricated and annealed ZnO/ZnSe core/shell NRs. Besides the scattering band centered around 465 cm^{-1} which corresponds to the high-frequency branch of the ZnO non-polar optical phonon mode [E_2 (high)], the Raman spectrum of the bare ZnO NRs is dominated by a Raman peak at 572 cm^{-1} attributed to the longitudinal optical (LO) modes with the A_1 and E_1 symmetries [A_1 (LO)/ E_1 (LO)] of ZnO and their overtones 2LO and 3LO modes peaking at 1145 and 1720 cm^{-1} , respectively. They are all characteristic Raman features relating to the wurtzite phase of ZnO [3,4]. An additional Raman peak appears at 248 cm^{-1} for the ZnO/ZnSe core/shell NRs whether annealed or not. This peak is attributed to the ZnSe LO mode [5] and scattered from the ZnSe shells. Compared with the as-fabricated sample, the annealed ZnO/ZnSe core/shell NRs present stronger Raman signals scattered from both the ZnO cores and ZnSe shells, indicating the improved structures relative to the sample before annealing.

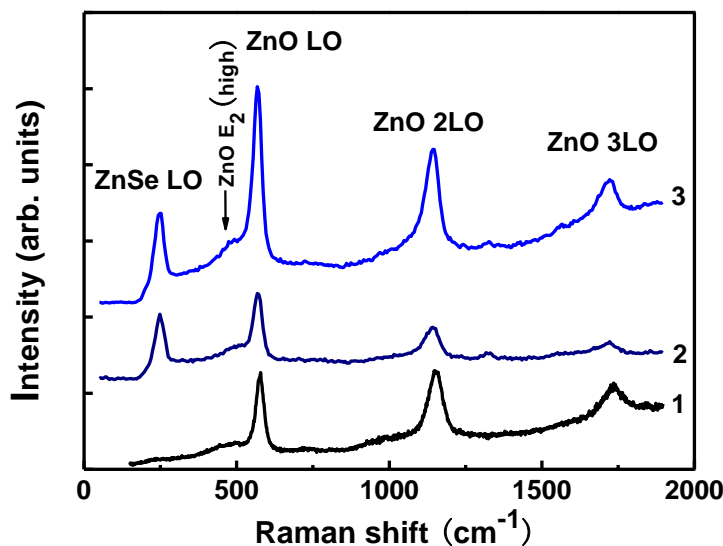


Figure S3. Raman backscattering spectra of annealed ZnO NRs (1), as-fabricated ZnO/ZnSe core/shell NRs (2) and annealed ZnO/ZnSe core/shell NRs (3).

References

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