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Optical and phonon spectra of wurtzite ZnO quantum dots and nanocrystals VLADIMIR A. FONOBEROV, KHAN A. ALIM, ALEXANDER A. BALANDIN, Nano-Device Laboratory (http://ndl.ee.ucr.edu), Dept. of Electrical Engineering, University of California, Riverside, CA 92521 — ZnO nanostructures have recently attracted attention due to the proposed optoelectronic and spintronic applications. Envisioned applications require accurate knowledge of exciton states and optical phonons. We report results of the investigation of wurtzite ZnO nanostructures with diameters from 2 nm to 20 nm (quantum dots to nanocrystals). The calculated size dependence of the exciton states and UV photoluminescence spectra of ZnO nanostructures is in agreement with the experimental data [1]. In addition, both interface and confined polar optical phonon modes in ZnO quantum dots and nanocrystals have been calculated and identified in the resonant and non-resonant Raman spectra [2]. It was found that the phonon confinement resulted in phonon frequency shifts of few cm^{-1} in the non-resonant Raman spectra. We also show that UV laser excitation in resonant-Raman spectroscopy leads to large red shifts of phonon peaks (up to 14 cm^{-1}) due to heating. The authors acknowledge the support of MARCO and its Functional Engineered Nano Architectonics (FENA) Focus Center. [1] V.A. Fonoberov and A.A. Balandin, Appl. Phys. Lett. 85, 5971 (2004); [2] V.A. Fonoberov and A.A. Balandin, Phys. Rev. B 70, 233205 (2004); K.A. Alim, V.A. Fonoberov, and A.A. Balandin, Appl. Phys. Lett. 86, 053103 (2004).

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