Cathodoluminescence patterns of ZnO microrods in experiment and FDTD simulation

Bogdan J. Kowalski, Agnieszka Pieniążek, Anna Reszka, Bartłomiej S. Witkowski, Marek Godlewski

Institute of Physics, Polish Academy of Sciences, Aleja Lotnikow 32/46, PL-02668 Warsaw, Poland

The semiconductor systems composed of elements with the size comparable to the visible light wavelength attract interest as microresonators, elements of light-emitting devices, lasers etc. Their optical and electronic properties are investigated in view of optimising their crucial parameters and preparation conditions. Micro- or nanorods are particularly convenient for such studies due to their relatively simple and highly symmetric (determined by the crystallographic orientation) shape, like hexagonal ZnO microrods grown on GaN templates by ultra-fast hydrothermal method. They are vertically well aligned with length, diameter, and distribution density modified in a controlled way by changes in such technological parameters as pH value or temperature.

The electron microscopy techniques and related spectroscopic methods, like cathodoluminescence (CL), allow us to study morphology and optical properties of individual nanorods with the submicron lateral resolution. Thus, the variations of near-band-edge and defect-related CL of ZnO microrods were observed as the function of growth conditions, as well as of the experimental conditions (such as excitation density, irradiated surface area, etc.). The optimized conditions leading to the luminescence intensity patterns and spectral fine structures characteristic of resonance optical excitations (like whispering gallery modes) in a hexagonal microresonator have been achieved. The resonances occurred for microrod sizes comparable with a few CL wavelengths. A model based on the ray optics can account for the structure of CL spectra, however it fails to describe the patterns acquired by monochromatic CL imaging of the individual microrods.

The Finite-Difference Time-Domain (FDTD) method [1] of numerical modeling of electromagnetic field distribution is particularly suitable for analysis of systems with size comparable with the radiation wavelength. Relatively easy adjustment of the parameters describing the studied system makes it more convenient for simulation of real experimental data than the results of more advanced calculations available in literature [2].

The simulation of a 2D hexagonal resonator enabled us to reproduce the whispering-gallery-mode-like radial pattern for the wavelength/microrod-diameter ratio corresponding to that observed in the CL experiment. The 3D simulation confirmed that result and was also used to find the system feature responsible for the lack of axial Fabry-Perot resonances. The results suggest that disconnecting the microrods from the GaN substrate would reduce the leaking of the electro-magnetic field from them. Then, the axial resonances should be more probable, at least for the wavelengths corresponding to the low absorption of ZnO.

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[1] *Understanding the Finite-Difference Time-Domain Method*, John B. Schneider, www.eecs.wsu.edu/~schneidj/ufdtd, 2010.
[2] J. Wiersig, Phys. Rev. A **67**, 023807 (2003).