Influence of ZnO nanostructure configuration on tailoring the optical bandgap: Theory and experiment

ABSTRACT

Exploiting the link between form and function of semiconductor nanostructure provides a new prospect for tailoring the features of nanoscale materials. However, achieving this remains a challenge in the fabrication of optoelectronic devices. Therefore, this research systematically presents theoretical and experimental investigations of shape dependent structural and optical properties of ZnO nanostructures (nanoparticles, vertically oriented nanorods and compact ZnO) synthesized using the electroless deposition technique to understand the principles of bandgap modification. FESEM, XRD, Photoluminescence (PL) and UV–Vis spectroscopic characterizations were employed. The characterizations show increase in lattice parameters, bandgap and density of dislocations from 0.3236 nm to 0.3258 nm, ~3.14 eV to ~3.51 eV and ~17×10^{-4} to ~39×10^{-4} , respectively as the ZnO nanostructures are transformed from compact ZnO to ZnO nanoparticles. The expansion in lattice parameter is attributed to lower compressive stress that exists in ZnO nanoparticles compared to compact ZnO. The blue shift (0.06 eV) in bandgap is ascribed to overlapping of the orbitals and energy level in ZnO nanoparticles which causes a substantial increase in energy gap between valence and conduction bands. The small size-induced hardening in ZnO nanoparticles accounts for their comparatively higher dislocation density. Theoretically, conversion from compact ZnO to ZnO nanoparticles extends the bandgap from 3.38 eV to 3.44 eV, which is consistent with the experimental results. This study confirms the shape dependency of the structure and bandgap of ZnO nanostructures, which may provide a new insight into future integrated optoelectronic device applications.