

Shape-controlled nanoarchitectures using nanowalls

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We report on growth of shape- and position-controlled ZnO nanowalls as building blocks for nanometer-scale architectures and devices. In order to control both the shape and the position of ZnO nanowalls, a patterned SiO₂ growth-mask layer was prepared by lithography on Si substrates with a thin GaN intermediate layer, and subsequently ZnO nanowalls were grown selectively only along the pattern edges by metal-organic vapor-phase epitaxy. We further demonstrated fabrications of nanoarchitectures, shape- and dimension-controlled ZnO nanotubes, employing the selective growth method of ZnO nanowalls. The diverse shape and all the dimensions of ZnO nanotubes were simply controlled by changing lithographic patterns and growth time. Transmission electron microscopy revealed that the ZnO nanotube consists of a nanowall with a fairly uniform wall thickness of 15 nm. The single crystallinity of ZnO nanotubes was clearly confirmed by both high-resolution TEM and electron diffraction pattern. In addition, the field-emission characterizations and the lighting device using position-controlled nanotube field emitters were demonstrated using the artificially controlled nanostructures as one application. This simple, precise, and well-controlled “bottom-up” method provides promising building blocks for the fabrication of novel nanostructures with desired arrangements and morphology as required for various nanodevice applications.

Intermediate scattering function from molecular dynamics to mimic the quasi-elastic neutron scattering spectroscopy

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Neutron scattering spectroscopy is suitable for investigating materials containing hydrogen atoms such as biomaterials, polymers, and liquids because of its characteristics. Quasi-Elastic Neutron Scattering (QENS) provides clues to reveal the dynamics of materials through its measured quantity, the Intermediate Scattering Function (ISF). This can also be obtained from the Molecular Dynamics (MD) simulation. It is useful to have simulation results to understand the collective mechanism of the individual atoms and overcome the experimental limits. This paper mainly describes the ISF calculation scheme from MD. The proposed one is applied to the supercooled confined water case. We confirm it has a liquid-liquid transition by comparing ISFs from both the experiment and the simulation.