Contribution ID: **1** Type: **Poster**

Neutron Diffraction Studies of Catalytic GaN/ZnO Nanoparticles

Tuesday 19 July 2016 16:50 (2h 40m)

The search for the clean and recyclable energy sources is an ongoing effort for variety of scientific communities. One of the approaches is the hydrogen generation using solar water-splitting photocatalysis. The most promising materials for such catalysis are GaN/ZnO nanoparticles with extremely narrow energy-band gap. Their performance is significantly improved as compared to the bulk counterparts due to more efficient electron-hole pair separation, short electro-hole diffusion lengths to the interface and large interfacial surface area. However, our understanding of these materials is still very limited and it is not yet clear how the energy gap could be further reduced. It is partially related to the fact that interpretation of the x-ray scattering data of GaN/ZnO nanoparticles is difficult due to low contrast between the atoms. On the other hand, the crystal structure of nanoparticles can have size induced deviations from the average crystal structure. In this work we show how neutron diffraction and pair-distribution function (PDF) analysis successfully overcome those limitations and provide local and average structure of GaN/ZnO nanoparticles in a single neutron diffraction experiment. We used four different types of (Ga1-xZnx)(N1-xOx) nanoparticles, with size of 10-50 nm and x=0.075-0.56, which show the narrow energy-band gap (2.21-2.61 eV). The neutron diffraction experiments were carried out at the Nanoscale-Ordered Materials Diffractometer (NOMAD) at Spallation Neutron Source in Oak Ridge National Laboratory. The Rietveld analysis of the data provided the average crystal structure, while PDF analysis was used to probe the local structure of our samples. The Rietveld analysis revealed hexagonal wurtzite structure of nanoparticles, in agreement with previous reports on bulk materials with a similar composition. However, the local structure was found to be substantially disordered. The level of disorder is size-dependent. Based on our results we propose how the composition, size and nitridation temperature might be varied in order to obtain GaN/ZnO nanoparticles with energy-band gaps below 2.21 eV.

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Session Classification: Poster Session

Track Classification: Catalysis