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Band Structures and Bandgap Bowing Parameters of Wurtzite and Zincblende III-nitrides

Lin, Wen-Wei; Kuo, Yen-Kuang

Abstract

The III-nitride semiconductor materials attract much attention in the past few years owing to their important application in light-emitting diodes and semiconductor lasers. Since the III-nitride semiconductor devices are usually grown on the sapphire substrate, they all have wurtzite crystal structures. The energy bandgaps of the wurtzite III-nitrides are usually obtained experimentally. Several researchers have investigated the energy bandgaps and the bandgap bowing parameters of the wurtzite InGaN, AlGaN, and AlInN alloys; however, the results are quite diverging. In this work we investigate the band structures of the wurtzite InGaN, AlGaN, and AlInN alloys with a CASTEP simulation program. The simulation results suggest that the wurtzite InGaN, AlGaN, and AlInN have a bandgap bowing parameter of 1.21 eV, 0.35 eV, and 3.33 eV respectively. Our simulation results also indicate that the widths of the top valance bands of the wurtzite InGaN and AlGaN alloys decrease when the indium and aluminum compositions increase while the width of the AlInN top valence band has a maximum value of about 6.57 eV when the aluminum composition is near 0.53. In this paper, the investigation of the band structures and bandgap bowing parameters for the zincblende InGaN, AlGaN, and AlInN alloys is also reported.