MAR05-2004-001712

Abstract for an Invited Paper
for the MAR05 Meeting of
the American Physical Society

Band Anticrossing Effects in Dilute Nitrides

WLADEK WALUKIEWICZ, Lawrence Berkeley National Laboratory

Recent advances in nonequilibrium epitaxial growth techniques have led to successful synthesis of alloys of distinctly different semiconductors. An important class of such materials are Highly Mismatched Alloys (HMAs). These are compound semiconductors formed when metallic (electronegative) anions are partially replaced by isoelectronic, more electronegative (metallic) atoms. Dilute nitrides in which highly electronegative N atoms partially replace standard group V elements are the most prominent and extensively studied class of HMAs. Using $Ga_{1-y}In_yN_xAs_{1-x}$ as a prototypical HMA, experimental and theoretical studies will be presented that show how all the unusual properties of these alloys can be explained by considering the interaction between highly localized states of substitutional N atoms and the extended states of $Ga_{1-y}In_yAs$ matrix in the Band Anticrossing (BAC) model. The interaction splits the conduction band into two nonparabolic bands resulting in large changes in the electrical and optical properties of these materials. The BAC model provides a consistent and quantitative description of experimentally observed data including the large band gap bowing, splitting of the conduction band, and increase enhancement of the electron effective mass. Also, it explains the mutual passivation effect in which group IV donors form nearest neighbor pairs with substitutional N atoms, which eliminates the activity of both species. Most recently we have found that the electronic properties of N-rich $GaN_{1-x}As_x$ ($x<0.06$) HMAs are determined by an anticrossing interaction between localized donor-like As states and the valence band states of the GaN matrix. The finding provides a basis for a description of the electronic structure of these alloys in the whole composition range.