Effect of B-In interactions on the band structure and optical properties of BGa(In)As

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The small lattice constant of boron pnictides provides a method for strain-engineering near-infrared direct-bandgap materials on silicon and GaAs. In other highly mismatched alloy systems, such as the dilute-nitrides, cluster states and nearest neighbor configurations strongly affect the optical properties.[1,2] Due to the challenging epitaxial growth of BGa(In)As beyond dilute amounts of B, the effects of B incorporation in BGa(In)As on the band structure and optical properties remain relatively unexplored both experimentally and theoretically. We have previously demonstrated high B incorporation in BGaAs, up to 20%, using molecular beam epitaxy (MBE).[3] Here we investigate the effects of B-B clusters and B-In nearest neighbor arrangement on the band structure and optical properties of BGa(In)As.

BGa(In)As films were grown on (100) semi-insulated GaAs and GaP by solid-state molecular beam epitaxy (MBE). These films were characterized with high-resolution X-ray diffraction (XRD) and room-temperature photoluminescence. Theoretical calculations of the optical properties were performed using the density function theory (DFT) package Vienna Ab initio Simulation Package (VASP) using HSE06 hybrid functionals.

Prior investigations of the BGaAs alloy suggest B cluster states near the conduction band edge may degrade optical quality as the B concentration is increased. [4,5] In our calculations, we find that the interband matrix element strength decreases only modestly with increasing B. However, the matrix element can be increased with the addition of In (3.7%). Calculations show the system energy of B cluster states (B-As-B_{n-1}-As-In) and B in nearest neighbor of In (B_n-As-In) are approximate equal, suggesting both are equally likely to form. While the addition of B in the B-In nearest neighbor configuration increases the bandgap of BGaInAs, the formation of B cluster states reduces both the energy gap and matrix element. This reduction in bandgap and optical quality is likely due to cluster states near the conduction band edge (CBE). Lindsay et al. found that the addition of 6% In to $B_{0.026}$GaAs pushed the CBE away from the B-B cluster pair levels resulting in a strong recovery in dispersion near zone center.[4] Consistent with our calculations showing an increase in matrix element with the addition of In, room temperature PL measurements of BGa(In)As films with ~3% B showed a 2x improvement in PL intensity with the addition of In. Calculations of higher In and B concentrations, towards compositions required for 1eV multi-junction solar cell junctions and telecom-range photodetectors lattice-matched to GaAs and Si are underway and will be reported at the conference.

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[1] K. Osamura et al. J. of Appl. Phys (1975)
[2] V. Lordi et al. Phys. Review B (2005)
[3] K.M. McNicholas et al. 61st Electronic Materials Conference (2019)
[4] A. Lindsay and E.P. O'Reilly, Phys. Review B (2007)
[5] R. Hamila et al. J. of Appl. Phys. (2012)
[6] V. Lordi. PhD dissertation. (2005)