Valence band symmetry effects on the optical properties of (Al,Ga)N and (Al,Ga)N/GaN quantum wells

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Group III nitrides are generally heteroepitaxially grown along the c axis. In GaN, depending on the substrate and on the growth process, the crystal field term in the **k** = **0** valence band Hamiltonian, related to the anisotropy of the wurtzite phase, is positive (typically on sapphire substrates) or near zero (typically on Si substrates). On the other hand, in AlN, the c/a ratio is significantly lower than the ideal value and this crystal field term turns to be strongly negative (typically ~ - 200 meV, depending on the strain state). As such, a change in the symmetry of the valence band maximum states is expected as a function of composition in $Al_xGa_{1-x}N$.

This is indeed what is concluded from a systematic study of the luminescence and reflectivity of undoped $Al_xGa_{1-x}N$ samples grown by metalorganic vapour phase epitaxy or molecular beam epitaxy with x up to 0.7. The symmetry crossover can explain some often quoted effects in $Al_xGa_{1-x}N$: discrepancies in the band gap bowing parameter, large Stokes shift, luminescence polarization and even variation of luminescence efficiency with composition. We also discuss using a simplified model the trends to be expected in (Al,Ga)N/GaN quantum wells, and the results are shown to be in qualitative agreement with experiments.

Finally, we also discuss the alloy composition measurement issue.