Type I to type II transition at the interface between random and ordered domains of $Al_xGa_{1-x}N$ alloys

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We analyze the optical and transport consequences of the existence of ordered and random domains in partially ordered samples of $Al_xGa_{1-x}N$ alloys. Using atomistic empirical pseudopotential simulations, we find that the band alignment between random and ordered domains changes from

sponds to a ''type II'' offset with holes on the random alloy domain and electrons on the ordered domain. This is demonstrated by the wave function plot in Fig. 2(b), showing localization on different domains.

Consequences of the type I to type II transition: Figure 1(c) shows as crosses the dipole matrix element versus composition, for transitions between the top five valence band states and the CBM. A Boltzmann average of those transitions at temperature $T=300$ K is shown as a solid line. While in the type I regime of $x\lesssim 0.4$ (and $x\gtrsim 0.9$) we see strong optical transitions, as expected, in the type II regime of $0.4\lesssim x\lesssim 0.8$ the transition dipoles are two to three orders of magnitude weaker. Based on the Fermi golden rule in the dipole approximation, the radiative lifetime τ for VBM $\rightarrow$CBM transition (electron–hole recombination) is inversely proportional to the amplitude squared of the dipole matrix element for the same transitions [Fig. 1(c)]. Thus, the experimental behavior of the mobility-lifetime product ($\mu\tau$)

cal factors that control the energy of the VBM of the ordered domain.

(a) *Depth of quantum wells*: The effective band offset between the Al-rich monolayers x_2 and Al-poor (Ga-rich) monolayers x_1 within the ordered domain can be modeled as the potential offset between two random alloys with composition x_1 and x_2, and is shown in Fig. 3(b). The Al layer has a deeper VBM than the Ga-rich layers (much like in pure AlN/GaN heterointerfaces[16]). We see that in the ''type I'' region the offset is below 0.5 eV, whereas in the ''type II'' region the offset is larger than 0.5 eV.

(b) *Quantum confinement*: The offset between the monolayers of the ordered domains causes quantum confinement whereby the holes localized on the Ga-rich layers will be pushed to *deeper* energies, below the VBM of the random alloy.

(c) *Band folding*: Ordering causes the VBM $\overline{\Gamma}_{3v}(\Gamma_{5v})$ to be displaced to *higher* energies by repulsion from the lower-energy folded-in $\overline{\Gamma}_{3v}(\Gamma_{6v})$ state. If effect (a) is weak, i.e., small ($\lesssim 0.5$ eV) offset, then the quantum confinement effect (b) is also weak and effect (c) of band folding and repulsion wins, leading to the VBM of the ordered domain being *above* that of the random alloy. This is the case (Fig. 1) for $x \lesssim 0.4$ and $x \gtrsim 0.9$. If, on the other hand, effect (a) is strong, i.e., large ($\gtrsim 0.5$ eV) offset between the monolayers, then quantum confinement effect (b) is also strong, leading to the VBM of the ordered alloy being pushed *below* the VBM of the random alloy. This is the case (Fig. 1) for $0.4 \lesssim x \lesssim 0.9$.

In summary, we have predicted that domains of ordered and random $Al_xGa_{1-x}N$ alloys lead to localization of both electrons and holes on the ordered domains if x is below 40% or above 90%, but in the intermediate composition range the electrons are localized on the ordered alloy, whereas the holes are localized on the random alloy. This causes a sharp drop in the absorption intensity and electron–hole recombination rate. The transition to type II is caused by a large effective band offset between the Ga-rich and Al-rich layers of the ordered structure, so that quantum confinement (pushing the VBM of the ordered material below the VBM of the random alloy) dominates over the band folding effects.

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