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Carrier localization and the origin of luminescence in cubic InGaN alloys

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The electronic structure and optical properties of cubic (nonpiezoelectric) InGaN are investigated using large scale atomistic empirical pseudopotential calculations. We find that (i) strong hole localization exists even in the homogeneous random alloy, with a preferential localization along the [1,1,0] In–N–In–N–In chains, (ii) even modest sized (<50 Å) indium rich quantum dots provide substantial quantum confinement and readily reduce emission energies relative to the random alloy by 200–300 meV, depending on size and composition, consistent with current photoluminescence, microscopy, and Raman data. The dual effects of alloy hole localization and localization of electrons and hole at intrinsic quantum dots are responsible for the emission characteristics of current grown cubic InGaN alloys. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1405003]

The development and commercialization of InGaN-based optoelectronic devices has occurred despite a limited understanding of the underlying electronic structure and light emission mechanisms of this alloy.[1] Although relatively efficient emission has been achieved for the entire visible range, optimization based on an understanding of the underlying electronic structure is expected to substantially improve device performance. Current InGaN alloys exhibit numerous anomalous phenomena that have been interpreted as indicative of an unconventional electronic structure. The following have been observed experimentally: (i) highly efficient photoluminescence (PL), despite a high dislocation density,[1] (ii) discrete states of varying energy inside the band gap in both quantum wells and epilayers,[2,3] (iii) a large Stokes' shift between emission and absorption energies, in both cubic and wurtzite InGaN samples,[2] (iv) an S-like dependence of emission energy on temperature,[4] (v) persistent photoconductivity,[5] (PPC). Collectively, these phenomena are indicative of localized excitons. While many of the observed localization phenomena can be attributed to the strong electric polarization existing in the *wurtzite* alloy, measurements on *cubic* alloys,[2,3] that lack polarization by symmetry, have found that the above phenomena persist. Thus, polarization alone is insufficient to explain the localization properties of InGaN. In general, there are two classes of localization in crystalline semiconductor alloys: (a) localization occurs even in a spatially homogeneous alloy due to the microscopic difference in potentials of the alloyed atoms,[6,7] and (b) localization due to spatial inhomogeneity (e.g., clustering, dot formation).[8,9]

(b) emission from quantum confined states in intrinsic quantum dots. In order to investigate the electronic properties of InGaN alloys, we adopt a twofold strategy: First, we simulate perfectly random InGaN alloys using supercells containing random distributions of In atoms. Second, we simulate the effects of spontaneous dot formation by embedding In-rich spheres of varying In composition and diameter inside a lower In-content InGaN alloy. This approach permits us to separate the electronic36336 Å. Such random distribu-

tions create naturally

[12,13] not only single In impurity sites, but also In pairs, chains, and clusters. Strain-minimizing atomic displacements ensuing from the In–Ga atomic size mismatch are incorporated using the valence force field approach. We assume that the lattice constant of the supercell varies linearly with In composition. In order to model the *intrinsic quantum dots* we use larger, ~140 000 atom or ~120×120×120 Å, supercells to contain the larger-scale In-rich regions. The electronic structure of the relaxed supercells is then obtained via the modern version of the empirical pseudopotential method[14] (EPM). Unlike traditional EPM, this potential reproduces not only experimentally correct band gaps, but also effective masses, and interfacial band offsets. In addition, we use explicitly strain dependent pseudopotentials in order to accurately reproduce the deformation potentials for both valence and conduction band states and thus explicitly include the effect of internal strains in the material due to the large bond length mismatch. Wave functions are obtained in a plane-wave basis (thus, affording multiband coupling).

Electronic localization along [1,1,0] In chains in InGaN random alloys: We calculated the near-gap conduction and

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valence states of unstrained random alloys, averaging the results of 15 different randomly generated alloy configurations. Although no states are present within the gap at any concentration, we find a surprising localization of the valence states. Bellaiche *et al.*[12] demonstrated marked hole

287 meV. Thus, we find that the observed 240 meV reduction in gap in nominally 33% alloys[3] is consistent with ∼28 Å dots of 100% In composition, and is also consistent with larger dots of lower composition, e.g., a 76% 40 Å dots.