Atomistic simulation of random alloy fluctuations in InGaN/GaN nanowires

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ABSTRACT

In this work we present a theoretical study of the effect of random alloy fluctuations in a InGaN inclusion embedded in a GaN nanowire on the electronic and optoelectronic properties. The calculations are based on an empirical tight-binding (ETB) model, while strain is calculated with a valence force field (VFF) method.

MODEL

Optoelectronic properties of GaN/InGaN devices have usually been calculated at an effective-medium level, modeling InGaN alloys within the Virtual Crystal Approximation (VCA). In this work, we use an atomistic approach both for the strain and the electronic states calculation. This approach allows to model in detail realistic indium distributions within the nanostructures including the effect of local strain, leading to more accurate electronic calculations. Tibercad multiscale simulation software [1] has been used to study optoelectronic properties of a 3D structure composed by a 400 nm high GaN nanocolumn, with a InGaN insertion in the middle of the nanocolumn (see Fig. 1). Indium concentration in the insertion varies between 5 and 20%. The nanocolumn diameter is 7 nm. The InGaN insertion is 2 nm high and has a diameter of around 5 nm. Based on a Finite Element grid, a set of atomistic structures comprising a random alloy InGaN inclusion, together with the surrounding GaN shell, has been generated within Tibercad. The atomistic structure has been then relaxed with a Keating valence force field (VFF) model generalized to treat non ideal wurtzites. Empirical tight-binding (ETB) calculations based on a reliable $sp^3s^*d^5$ parametrization have been performed on the relaxed structure. The electrostatic potential obtained by solving the driftdiffusion equations with classical particle densities, including both spontaneous and piezoelectric fields, has been projected from the finite-element grid onto the atomic positions by interpolation. The eigenstates have been found solving the ETB Hamiltonian and from these the optical matrix elements have been obtained.

RESULTS

In Fig.2 the in-plane strain tensor component ε_{xx} along z-axis, for x(In)=0.1, calculated with a continuous elasticity model results to underestimate the value obtained from the atomistic approach (VFF). For the latter, the result from a random sample is shown together with the one from VCA. ETB ground states have been calculated for a set of random samples, each showing a random alloy configuration in the InGaN region. In Fig. 3 and 4 the spatial probability densities for electron and hole ground states are shown for a single random sample of the InGaN random alloy, respectively with 10% and 20% In. The statistical distribution of the ground states transition energies E_t for 10% In concentration is shown in Fig.5, giving an average energy E_t=3.470 eV. Optical matrix elements are plotted in Fig.6 for a range of In concentrations between 5 and 15%. While there is an increasing spread in the random alloy distributions with the increase of In content, the mean values depend only slightly on the transition energy. This may indicate that, for such a thin nanocolumn, confinement effects overcome the effects of spatial separation of the states due to the increasing polarization fields.

ACKNOWLEDGMENT

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References

[1] www.tiberlab.com; M. Auf der Maur *et al.,* IEEE TED. **58**, 1425 (2011).

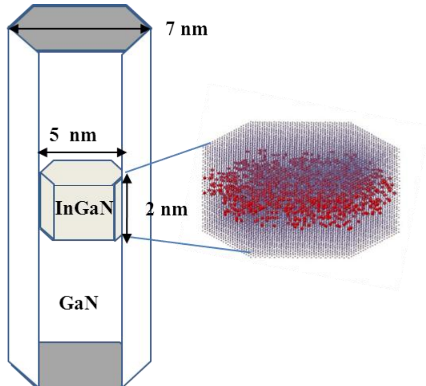

Fig.1 Model structure of the GaN nanowire with the InGaN inclusion

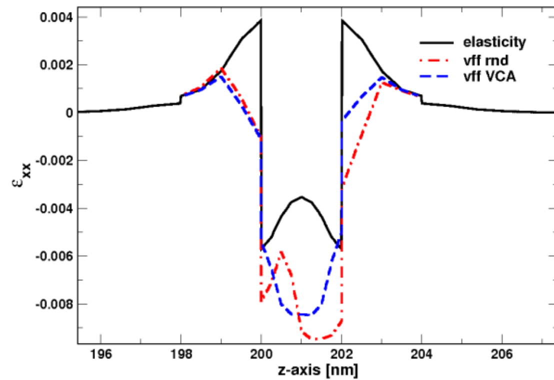

Fig.2 Strain component ε_{xx} along z-axis obtained from elasticity and vff models.

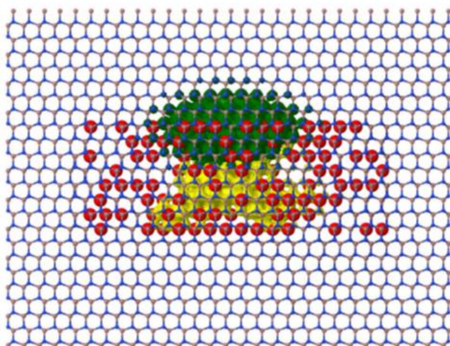

Fig. 3. Electron (yellow) and hole (green) TB ground states for a random alloy sample with x(In)= 10%

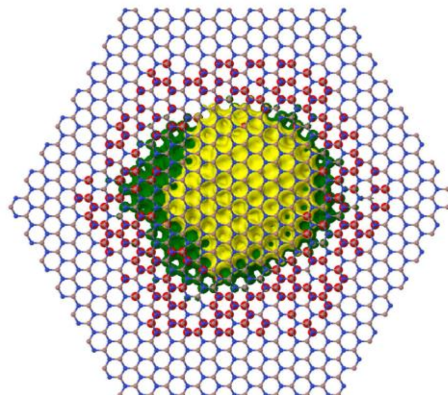

Fig. 4. Electron (yellow) and hole (green) TB ground states for a random alloy sample with x(In)= 20%

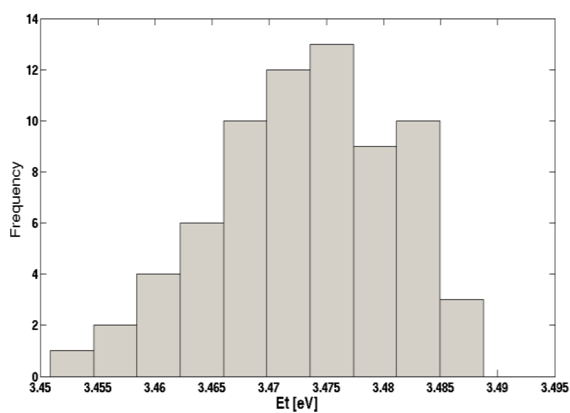

Fig. 5 Distribution of transition energies for a set of InGaN random alloy samples with In 10%

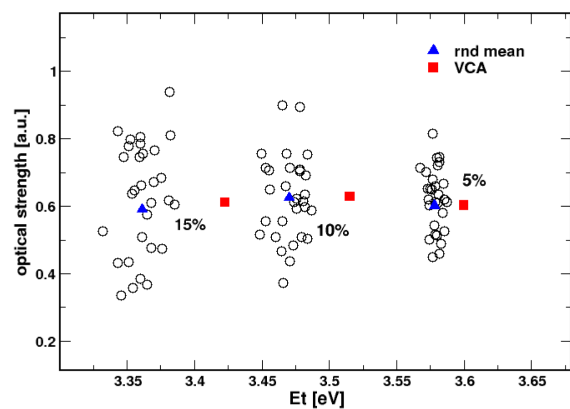

Fig.6. Optical matrix elements calculated for several In contents (results for random alloy sets and VCA).