Investigating the Effect of Non Linear Piezoelectricity on the Excitonic Properties of III-N Semiconductor Quantum Dots

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***Abstract*- We investigate the effects of linear and non linear piezoelectricity in wurtzite III-N semiconductors and their influence on the electronic properties of low dimensional quantum dots. By studying the dependence of the biexciton on structural and geometrical parameters of the nanostructure, we show second order to be important particularly when the strain in the nanostructure is reduced**

I. INTRODUCTION

It is well known that the piezoelectric effect in bulk III-V semiconductors arises from lack of inversion symmetry along particular crystallographic directions[1-2] and is found in devices as diverse as light-emitting diodes (LEDs), lasers, power electronics, transducers and micropositioners.[3-9] In III-N semiconductors and their nanostructures piezoelectricity is a key factor and influences optical and electrical properties, by virtue of both a magnitude of the field typically a factor of 10 larger than e.g. GaAs[10] and a polarization vector in most cases parallel to the growth direction.[11]

Conventionally piezoelectric effects have mainly been considered to the first order in strain.[12-15] The widely used piezoelectric coefficients formalism suffers from the intrinsic problem of experimentally determining such coefficients and in the case of wurtzite the additional problem of determining the spontaneous polarization component.[10]

Second order effects of the same magnitude of the first order have also been reported in the InGaAs system[16-17] and in III-N semiconductors.[18-22] However for III-N semiconductors a comprehensive set of second order piezoelectric coefficients has not yet been presented, preventing a true test of the effect of second order piezoelectricity in nanostructures to be explored.

II. NUMERICAL RESULTS AND DISCUSSION

In the framework of Harrison's theory and the scheme previously established by Migliorato *et al* [16] we use ab initio density functional theory in the local density approximation to extract the elastic and dielectric properties of single crystals under various degrees of pressure in the 3 main crystallographic directions. The results, properly combined in a formulation that takes into account the dipole formation between cations and anions, together with the modification of the dipoles along all bonds in the tetrahedron of the wurtzite structure, leads self consistently to the combined identification of both spontaneous and strain induced polarization coefficients. Furthermore we were also able to produce the second order piezoelectric coefficients, an essential step needed in calculating the total polarization in the widely used calculation schemes based on solving the discretized Poisson equation. Our results indicate that most of the previous literature on the subject agrees with our more complete model only for very large strains, while in the limit of small strain deviation of up to 100% are present. Furthermore the spontaneous polarization component is found to be always reduced by 25%-80% compared to previous estimates.

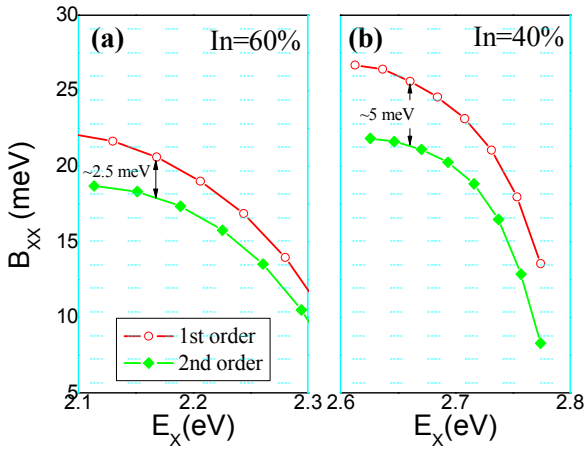

Fig 1: Biexciton binding energies for InGaN/GaN quantum Dots with 60% and 40% In content and a variety of sizes/shapes. The difference between the 1st and second order piezoelectric fields is shown (red and green circles).

We tested our model on InGaN/GaN and AlGaN/AlN quantum dot nanostructures. The presence of 3D confinement on a very small scale makes electrons and holes (and consequently excitons) highly localized and hence particularly sensitive to local properties of the material such as shape, composition and piezoelectric polarization. Because of the

particular sensitivity towards the symmetry of the confinement potential we concentrated on calculating, in the framework of multiband k.p theory and configuration interaction (CI), the emission and binding energy of the biexciton complex. For this complex we investigated (Fig. 1) a variety of combinations of structural parameters of the nanostructure and in particular we tested our model for piezoelectricity against the standard linear model and the classic parameters given in the literature.

We conclude as expected that when strain is reduced in the nanostructures due to either a lower lattice mismatch of the alloy comprising the island compared to the substrate (a condition typically obtained by considering a lower In content in the alloy) or larger sizes of the quantum dot, the difference between our second order model and linear theory is ranging between 2 and 5meV for the set of sizes and composition investigated.

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