Comparison of continuum and atomistic methods for the analysis of InAs/GaAs quantum dots.

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***Abstract*—We present a comparison of continuum $\vec{k}\cdot\vec{p}$ and atomistic empirical Tight Binding methods for the analysis of the optoelectronic properties of InAs/GaAs quantum dots.**

I. Introduction

Self-assembled InAs/GaAs quantum-dot structures (QD) have recently received much attention due to their relevance for optoelectronic devices [1] .

Relevant aspects in this context are to accurately model the optical properties of QD and to consider the influence of the lattice mismatch induced strain field and its effects on the bandstructure and optoelectronic properties. The strain distribution in solids is usually treated with the continuum mechanical model [2], or with the valence force field model [3], or using density functional techniques [4].

For the calculation of electronic states in QD several schemes have been used with different levels of sophistication, for example the simple effective mass approximation [5], the multiband $\vec{k}\cdot\vec{p}$ theory [6], or atomistic approaches like the tight-binding (TB) [7] and the pseudopotential method [8].

Atomistic models are computationally more demanding, with a computational effort which grows with the number of the atoms, but they provide inter-atomic details which could be notable important as a nanostructure approaches a lattice-constant dimension. On the other hand, continuum models are computationally fast and accurate for nanostructures with dimensions much larger than a lattice constant, they are not restricted by a maximum size of a structure, but their accuracy is strongly reduced when the dimensions of a structure reach an atomic length scale.

The first models of the $\vec{k}\cdot\vec{p}$ theory as a perturbative theory were presented in the work of Dresselhaus et al. [9], and Kane [10], while an approach based on symmetry arguments was given by Luttinger [11]. The multiband scheme for bulk materials was extended to heterostructures by an ad hoc symmetrization procedure [12]. Successively, the so-called exact envelope function approximation (EFA) [13] was used to derive a 6-band model for the valence bands of zincblende heterostuctures [14], while an 8-band model has been provided by Pokatilov et al. [15].

Being a continuous media model, approaches based on EFA eventually break down for very small structures and an atomistic description becomes inevitable [16], [17]. The computational cost of such methods, however, limits their application to rather small structures. Empirical TB methods [17] are able to treat structures consisting of few million atoms on distributed supercomputer clusters and to about $2-3\cdot10^5$ on typical workstations.

Optoelectronic properties of InGaAs zincblende QD with varying shape and size have already been studied with $\vec{k}\cdot\vec{p}$ theory [18], and with 8-band model to investigate the effect of strain and band-mixing [19].

Recently a comparison of empirical TB and $\vec{k}\cdot\vec{p}$ models has been performed for zincblende GaN/AlN QD without including strain and piezoelectrical fields [20].

In this paper we present a systematic comparison of energy levels, wave functions and electric dipole moments given by empirical TB and $\vec{k}\cdot\vec{p}$ models including electromechanical fields for realistic InAs/GaAs self-assembled QD.

II. Theory

A. $\vec{k}\cdot\vec{p}$ method

The 8-band model includes the electron, heavy-holes, light-holes and spin-orbit split-off bands around the Γ point of the Brillouin zone, and treats all the other bands as remote. The wave function of a state n with energy E_n is given by a linear combination of the eight Bloch parts weighted by the respective envelope functions, $\psi_n=\sum_{i=1}^{8}\phi_i u_i$, where ϕ_i are the envelope function and u_i are the Bloch states [15].

B. Tight binding method

The empirical TB is based on a linear combination of atomic orbital ansatz for the wavefunctions. The matrix elements are treated as parameters and fitted to accurate bandstructure calculations or experimental data. In this work we use a $sp^3s^*d^5$ parameterization [21] that includes strain effects via deformation potentials and fitted Harrison scaling rules.

C. Dipole moments

Within the $\vec{k}\cdot\vec{p}$ model the dipole matrix elements $\vec{\mu}_{nm}$ are ill-defined in crystals involving extended Bloch states [22], so we instead calculate the momentum matrix element $\vec{p}_{nm}\equiv\vec{p}^{(\phi)}_{nm}+\vec{p}^{(u)}_{nm}$, where $\vec{p}^{(\phi)}$ and $\vec{p}^{(u)}$ are the envelope and the Bloch parts of the momentum matrix element, respectively, and it is usual to neglect the envelope part [18]. Then $\vec{\mu}_{nm}$ are

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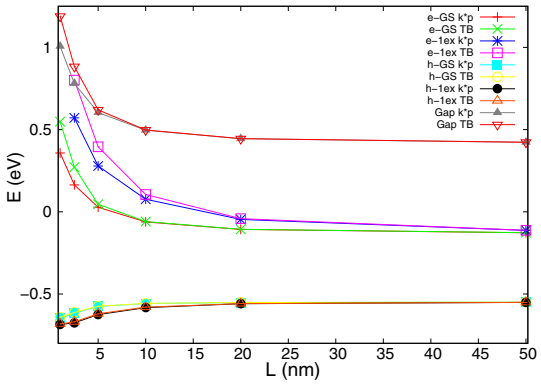

Fig. 1: Optical gap (Gap) and electronic (e) and holes (h) ground states (GS) and first excited states (1ex) as a function of the well length L.

afterwards calculated by $\vec{p}_{nm} = \frac{im_0}{e}\omega_{nm}\vec{\mu}_{nm}$, with $\hbar\omega_{nm} = E_n - E_m$, m_0 free electron mass and e electronic charge.

In the framework of TB model optical transitions are computed using a simple dipole approximation and the Hellmann-Feynman theorem to represent the position operator in terms of known TB parameters [24]. Our approach neglects intra-atomic matrix elements [25], [26] that generally give a small correction. Excitonic effects are also not considered in this work.

III. Results

In order to compare the results of the two methods, we need to use an equivalent set of physical parameters, i.e., the TB parameters have to be deduced in terms of $\vec{k}\cdot\vec{p}$ [21]. To verify the consistency of our choice, in the first part of our contribution we compare results of InAs/GaAs quantum wells with different size L. In Figure 1 we plot the optical gap and the electronic and holes ground and first excited states as a function of the well length L given by the two models.

As we can see, the curves of the optical gap already converge for $L = 5$nm. So in the main part of our contribution we can compare results given by the two models for realistic truncated-pyramid $In_cGa_{1-c}As$/GaAs QD with different size. We present results for the energy levels and we compare systematically the confined wave functions given by the two methods. As is well known the shape and the spacial distribution of the wave functions strongly influence the optical properties of a nanostructure, e.g., because of a different overlap of the states [19], hence we also analyze and compare some of the most relevant interband dipole moments.

As an example of our work, in Figure 2 we show the electronic and holes ground state calculated using the $\vec{k}\cdot\vec{p}$ model, while in Figure 3 is plotted the holes ground state given by TB method together with the atoms of the different chemical species building the heterostructure.

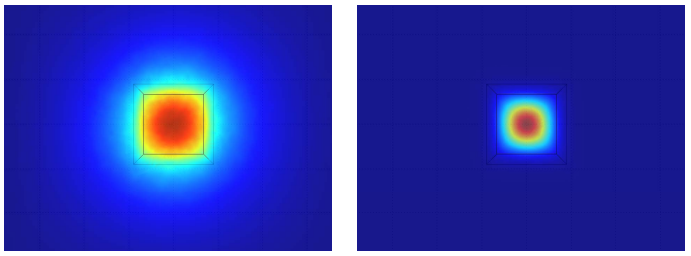

Fig. 2: Electronic (left) and holes (right) GS as given by the $\vec{k}\cdot\vec{p}$ model in the xy plane.

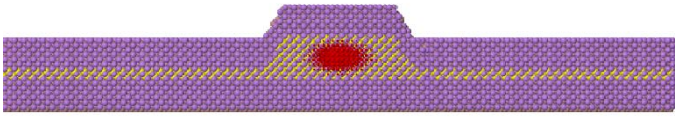

Fig. 3: Holes ground state given by TB method plotted with the atoms of the different chemical species in the xz plane.

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