Atomistic and k.p models to simulate spectral properties of InGaAs/GaAs quantum dots

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The modeling of spectral properties of quantum dots (QDs) was the subject of many theoretical studies. The methods commonly used in such calculations can be divided into two distinct classes. The first one contains multiband k · p models based on the continuous media approximation, and the second one involves various atomistic models.

We discuss the theoretical approaches for modeling of InAs/GaAs self-assembled quantum dots. We compare the results obtained from the 8-band k · p and the sp3d5s* tight-binding models, and show that discrepancies are primarily related to different treatment of strain in both methods. While the tight-binding Hamiltonian inherently accounts for strain nonlinearity via exponential factors, the standard k · p Bir-Pikus Hamiltonian is linear in strain tensor elements. Although the second-order scheme [1] was proposed, no parameters have been provided so far. In the present work, we find the values of the second-order deformation potentials [2], and calculate energy levels for electron and hole confined in a QD [2, 3]. We show that in the case of the electron, the accuracy of the continuous k · p model can be greatly improved with the second-order strain model. Finally, the model is utilized in the modeling of InGaAs/GaAs emitting at the telecom wavelengths [3].

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