

Strain-induced localized states within the matrix continuum of self-assembled quantum dots

Voic Popescu,¹ Gabriel Becher,² and Alexander Zinger^{1,a}

¹National Renewable Energy Laboratory, Golden, Colorado 80401, USA

²Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

(Received 16 April 2009; accepted 6 June 2009; published online 14 July 2009)

Quantum dot-based infrared detectors often involve transitions from confined states of the dot to states above the minimum of the conduction band continuum of the matrix. We discuss the existence of two types of resonant states within this continuum in self-assembled dots: (i) virtual bound states, which characterize square wells even without strain and (ii) strain-induced localized states. The latter emerge due to the appearance of “potential wings” near the dot, related to the curvature of the dots. While states (i) do couple to the continuum, states (ii) are sheltered by the wings, giving rise to sharp absorption peaks. © 2009 American Institute of Physics. [DOI: 10.1063/1.3159875]

Localized states within the continuum have long been known as virtual bound states (VBS).^{1–5} They emerge in sharply varying (e.g., square well) potentials and have been discussed for quantum wells^{4,5} and quantum spheres.⁶ The interaction of the bound states with continua is relevant to the increasingly important dephasing properties of the quantum dot (QD) states⁷ as well as for bound-to-continuum intraband spectroscopy.⁸ Additionally, in nuclear physics the Breit–Wigner resonances¹ and in atomic physics the Fano effect² deal with interactions of a bound state with the continuum. The existence of bound states above the continuum threshold in *epitaxial self-assembled* QDs has been debated recently, calling⁷ for further studies and a quantitative assessment of their importance, especially in connection with the QD-based infrared photodetectors.^{9–11}

Indeed, unlike the *flat* interfaces characterizing quantum wells, QDs have *curved* shapes, leading to the strain-induced formation of local potential barriers

strain-induced localized states (SILS) in *strained* InAs/GaAs and comparing it with analogous calculations for *strain-free* InAs/GaSb we show the finger-prints of SILS. Whereas the peaks related to VBS are broad, those stemming from SILS are sharp, resembling the intradot transitions. Moreover, they are equally present for isolated and stacked dots, showing that the potential wings effectively shield the SILS from both the matrix states and those resulting from the dot-dot interaction.

The single particle states

$\psi_i(\vec{r})$ have been calculated by a multiband, multivalley, pseudopotential approach,¹⁵ using a basis set consisting of a strain-dependent linear combination of bulk bands.¹⁶

show the potential wings as pronounced maxima underneath and above the dot. This position-dependent barrier has a maximum of ≈ 120 meV and decays to the matrix (GaAs) conduction band minimum (CBM) within 6–7 nm. The wings originate from the compressive strain in the barrier material in the direct vicinity of the dot. No such wings are observed in an unstrained system such as in Fig. 1(a).

Solving for the eigenstates of the QD systems, we classify the states associated with such QDs into four categories according to: (i) the localization (L) or delocalization (D) of the corresponding wave functions in vertical $[001]$ (z) and lateral (xy) directions (arXiv:1606.03795v1 [cond-mat.str-el] 16 Jun 2016).

self-assembled QDs, isolated or stacked, act in a similar way: They shield the electronic states within the dot from *all* other states, both matrix and those arising from the effects of dot-dot interaction.

The comparison of unstrained InAs/GaSb with strained InAs/GaAs QD systems has illustrated what happens to SILS once the wings are completely absent—they are converted into VBS that are not strongly anchored into the dot. Alternatively, by alloying the InAs dot in InAs/GaAs with Ga, the dot-to-barrier strain can be reduced. This way, one can trace back the SILS evolution when the wings become gradually less shielding. As can be seen in Fig. 3(b), for an $\text{In}_{0.6}\text{Ga}_{0.4}\text{As}$ dot, the amplitude of the wing potential is also reduced by alloying. Now, the e_B state can tunnel away from its home base and explore the *interdot* space (gray shading). We see from the wave function line-plot in Fig. 3(b) that now the e_B state becomes localized in the interdot space, trapped inside the local potential minima formed between the dots by the overlapping wings of neighboring dots. Following the delocalization of e_B , the intraband transition into this state [red solid line in Fig. 3(a)] is weaker and broader than in the strong-wing case of nonalloyed InAs/GaAs system. We can imagine that, as the wing potential is further reduced, the e_B state will morph into a VBS, affording smoother interdot transport and stronger coupling with the continuum.

To conclude, we have investigated the resonant states within the matrix continuum of QD systems, providing a recipe to identify numerically the VBS. The main accomplishment of this work is the characterization of a different type of localized states above the matrix continuum. These SILS appear because of the potential wings created in the proximity of the dot in strained structures, under specific conditions of QD size and QD/matrix combination. Comparing the manifestation of SILS with that of VBS we have found that: (i) unlike VBS, the SILS are only weakly coupled

to the continuum (ii) the SILS appear as strong, sharp peaks in the intraband absorption. Note that the wings could shelter the photo-generated carrier in SILS from recombination, thus contributing positively to the photoconductivity gain.

Work at NREL was funded by the U.S. Department of Energy, Office of Basic Energy Science, Materials Science and Engineering Division, under Contract No. DE-AC36-08GO28308 to NREL.

¹G. Breit and E. Wigner, *Phys. Rev.* **49**, 519 (1936).

²U. Fano, *Phys. Rev.* **124**, 1866 (1961).

³J. von Neumann and E. Wigner, *Phys. Z.* **30**, 465 (1929).

⁴A. M. S. L. F. (on) 332.7 N. 1. (umann) 332.7 (and) 332.7 E.) 332.7 W 39.9 (gener,) 332.280 TD 59