The origin of detection wavelength tuning in quantum dots-in-a-well infrared photodetectors

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Abstract

A theoretical investigation is performed in order to understand the origin of change of the operating wavelength of quantum dots-in-a-well photodetectors when the well width is varied. The energy levels and wave functions were found using the 8-band strain dependent $k \cdot p$ model and the intraband optical absorption spectrum was calculated in the dipole approximation within the framework of first order perturbation theory. It was found that the pure effect of changes of well width cannot be responsible for the shifts of the peaks observed in experiment [J. Appl. Phys. **96**, 1036 (2004)], which are therefore ascribed to unintentional changes in dot dimensions.

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Considerable research effort has recently been put in the development of quantum dot infrared photodetectors[1–9] (QDIPs) to overcome the limitations of quantum well based devices, leading to a recent demonstration of QDIPs operating at room temperature.[10] However, the difficulties in controlling the size and shape of self assembled quantum dots make it very hard to engineer these devices and produce a QDIP for a specified, user-defined detection wavelength.

The so called quantum dots-in-a-well (DWELL) infrared photodetectors,[11–13] where a quantum dot layer is embedded in an $In_{0.15}Ga_{0.85}As$ quantum well, have a special place among different types of QDIPs. They have been introduced with the motivation to tailor the operating wavelength by changing the well width, which would therefore lead to a recipe for producing a QDIP with the desired spectral response. Such expectations were recently confirmed experimentally[12,13] where tuning of 2–3 μm in the long wavelength atmospheric window (8–12 μm) has been achieved by varying the well width by 3–5 nm.

Current thought, based on experimental results, is therefore that it is the modification of the energy levels and the corresponding wave functions, due to the change of well width, that shifts the spectral response peak. However, it has been pointed out in Refs. 12,13 that unintentional changes in dot size may also shift the operating wavelength. Furthermore, one cannot exclude the possibility of change in the dot composition due to effects of interdiffusion and segregation. Uncertainties in the experimental determination of the dot size and composition make it very difficult to establish which of the above effects is dominant - the effect of the intentional change of well width or the effect of unintentional changes in dot size or composition. Clearly, it would be highly desirable that the effect of intentional control of well width prevails. In this letter we therefore perform a theoretical study quantifying the above effects with the aim of understanding the origin of the experimentally observed wavelength tuning in DWELLs.

The electronic structure of DWELLs was modeled using the 8-band $k \cdot p$ Hamiltonian,[14] with the strain distribution taken into account in the framework of the continuum mechanical model.[15] The components of the strain tensor were found using the finite element method.[16] It was assumed that the dot shape is cylindrically symmetric as most dots in experimentally realized QDIPs exhibit such shape. The axial approximation[17] allows us to reduce the problem from three dimensional to two dimensional. Consequently, the Hamiltonian eigenvalue problem was solved using the orthonormal function expansion method where

the basis was formed from the product of Bessel functions in the radial direction and the plane waves in the growth direction. The cylindrical symmetry of the dots introduces a good quantum number of total angular momentum m_f.[17] In typical QDIP operating conditions, only the ground state is significantly occupied, therefore the spectrum of optical absorption was calculated by adding the contribution from transitions from the ground state to each of the excited states. The optical absorption cross section was calculated in the dipole approximation using first order perturbation theory, as in Ref. 18. The inhomogeneity of the quantum dot ensemble was taken into account assuming a Gaussian lineshape on each of the transitions with a standard deviation equal to 10% of the transition energy, which is approximately equal to the experimental values for the dominant transitions in Refs. 12,13. The optical transition selection rules allow only the contributions of transitions with $\Delta m_f = 0$ in the case of $z-$polarized light and $\Delta m_f = \pm 1$ in the case of in-plane polarized light. In agreement with previous theoretical and experimental results,[19–21] our calculation shows that significant absorption of the in-plane polarized radiation from the ground state may occur only on transitions to the pair of nearly degenerate first excited states and is located in the far infrared region. The transitions in the long wavelength atmospheric window may therefore be only due to $z-$polarized radiation and we further only address the transitions due to this polarization.

The optical absorption spectrum was first calculated for a quantum dot of the shape of a truncated cone with a diameter of 15 nm, height 7 nm, base angle 60^0, and a 6 nm wide $In_{0.15}Ga_{0.85}As$ layer positioned above the dot layer, which are approximately the dimensions of the DWELL structures reported in Ref. 12. The width of the $In_{0.15}Ga_{0.85}As$ layer under the dot was varied from 1 nm to 6 nm, as in the experiment.[12] In all calculations a 0.5 nm wide wetting layer was also assumed. The results of these calculations are shown in Fig. 1. The peak of the spectrum is in both cases positioned around 8.5 μm with a relative difference between the positions of the two peaks of only 2%, while in the experiment the spectral response peak wavelength is red-shifted from 7 μm to 9.5 μm (i.e. by about 30%) when the layer width is increased in the above interval (Fig. 2 in Ref. 12). This gives us the first indication that the shift in the operating wavelength cannot be explained in terms of the effect of the well width. The transition from the ground state (having $|m_f| = 1/2$) to the third $|m_f| = 1/2$ state dominates the spectrum. Both states are bound (270 meV and 125 meV below the continuum respectively), and the influence of the well width on

their positions and separation is very weak. It is generally expected that the effect of well width should be more pronounced when the level to which the absorption is maximal has its energy within the range of the quantum well confinement potential (roughly within 15% of the conduction band offset below the continuum in the case of $In_{0.15}Ga_{0.85}As$ well). The same type of calculation was therefore performed for quantum dots of different height and In composition in the dot, in order to investigate the effect for different positions of that level. These calculations also allow quantification of the sensitivity of the peak absorption wavelength on the changes in dot size or composition.

The change in the detector operating wavelength when the height of the quantum dot is varied from 3 nm to 9 nm is shown in Fig. 2. One can see that throughout the whole investigated interval of dot heights the change in the peak absorption wavelength is less than 3% when the bottom layer width is changed from 1 nm to 6 nm. For small values of dot height ($h \lesssim 4$nm), the absorption to the state which is within the range of the quantum well confinement potential is dominant. Nevertheless, as seen from the right inset in Fig. 2, the influence of the well on the position of this state is weak. When the bottom layer width is 1 nm the wave function of the state is largely confined to the dot volume, which provides a large overlap with the ground state and strong absorption. An increase in the bottom layer width induces a change proportional to the probability that the wave function is located in the interval from 1 to 6 nm beneath the wetting layer, and since this is small (see the left inset in Fig. 2), the change in the state energy is small, too. The change of well width has a much stronger influence on states that are less confined to the dot. However, such states have a poor overlap with the ground state and do not significantly contribute to the absorption. Consequently, the influence of the well width on the absorption spectrum is weak.

The dependence of the detection wavelength on the In content in the dot is given in Fig. 3. For smaller values of In content in the dot (for example $x = 0.65$) the absorption in the case of 1 nm bottom layer is maximal towards a resonant state in the continuum (see the right inset in Fig. 3), which is less confined to the dot than the corresponding state when In content is larger. The increase in well width then has a larger impact on that state, shifting it down and correspondingly red-shifting the absorption peak (see the left inset in Fig. 3), and therefore the difference between the operating wavelengths in the case of 1 and 6 nm bottom layer increases as In molar content in the dot decreases. However, even

in the extreme case of $x = 0.5$ the relative difference between the operating wavelengths is just 10%, which is well below the experimentally observed value of 30%.

From the results obtained, a conclusion can be drawn that tuning of the detection wavelength in DWELL structures cannot be explained if one assumes that the dot remains of the same size and with the same composition. In fact, the pure effect of well width plays only a minor role in shifting the detection peaks. The observed changes in the operating wavelength can then be explained only in terms of unintentional modification of the quantum dot size because of changed growth conditions or composition due to the effects of interdiffusion or segregation. From Fig. 3 one can see that in the range of In content around $x = 1$ the changes in wavelength with the composition are only slight and that only extremely large changes in x, which are highly unlikely in the experiment, would be sufficient to explain the experimental shifts. On the other hand, variations in the size of the dot can induce more pronounced changes in the position of the peak of the spectrum, as is evident from Fig. 2. For example, a slight decrease in the size of the dots from 5 nm to 4 nm changes the wavelength by 26%, which is the value comparable to the experimentally observed ones. Bearing in mind that the shifts originating from the pure effect of well width and the changes in dot composition are significantly smaller, the dot size variations can be safely identified as the main source of wavelength tuning. All the calculations reported have also been performed for a fixed value of bottom layer width, while varying the top layer from 1 nm to 6 nm. The magnitude of the observed shifts was similar, indicating that the conclusions drawn are valid in this case too.

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Figure captions

FIG. 1: Absorption spectrum of a DWELL structure with a quantum dot of the shape of a truncated cone with a diameter of 15 nm, height 7 nm, base angle 60^0, a 6 nm wide $In_{0.15}Ga_{0.85}As$ layer positioned above the dot layer and 1 nm (full line) or 6 nm (dashed line) wide layer under the dot. The inset: Effective potential profile along the z-axis and the first three $|m_f| = 1/2$ energy levels for the same structure.

FIG. 2: Operating wavelength of a DWELL structure from Fig. 1 for different quantum dot heights, for the case of 1 nm thick bottom layer (full line) and 6 nm thick bottom layer (dashed line). The right inset: Effective potential profile along the z-axis, the ground state and the state to which absorption is maximal when the dot height is h=3.5 nm. The left inset: The wave functions of the two states in the case of 1 nm bottom layer.

FIG. 3: Dependence of the operating wavelength λ of a DWELL structure from Fig. 1 on In composition in the dot x. The absorption spectrum when the In molar content in the dot is $x = 0.65$ is given in the left inset, while the right inset shows the effective potential profile along the z-axis, the ground state and the state to which the absorption is maximal. The results are given for the case of 1 nm (full line) and 6 nm thick bottom layer (dashed line).

Figures

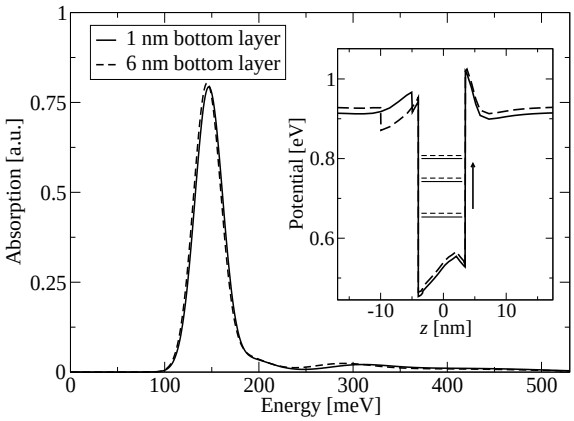
1 nm bottom layer
6 nm bottom layer
Absorption [a.u.]
Energy [meV]
Potential [eV]
z [nm]
0
0.25
0.5
0.75
1
100
200
300
400
500
0.6
0.8
-10
0
10

FIG. 1:

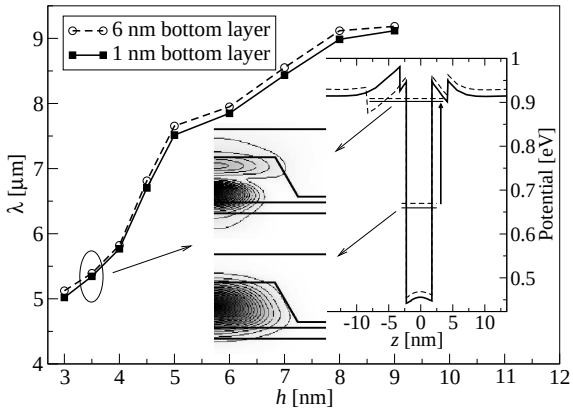

FIG. 2:

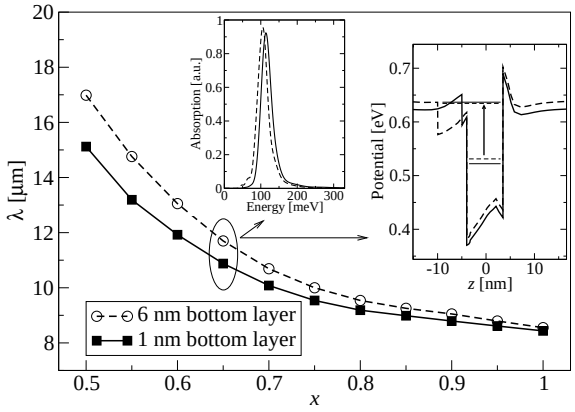
λ [μm]
x
6 nm bottom layer
1 nm bottom layer
Absorption [a.u.]
Energy [meV]
Potential [eV]
z [nm]

FIG. 3: