

ELECTRONIC SUPPLEMENTARY INFORMATION

A three-dimensional model for artificial atoms and molecules: Influence of substrate orientation and magnetic field dependence

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In the absence of an external magnetic field, total Hamiltonian is given as: $H = H_k + H_{strain}$, where H_k denotes the kinetic part, and H_{strain} denotes strain-dependent part. For [001] grown nanostructures, in our case [001] grown QDs and QDMs, H_k , and H_{strain} are given by Eq. (9) and Eq. (A2) of Ref. 1 respectively.

When evaluating electronic structure of a QD or a QDM which are not oriented parallel to the main crystallographic axes (x, y, z) (see Fig. 1 (a)), we define a rotated coordinate system, (x', y', z') , to describe the QD or QDM (see Figs. 1 (b) and (c)). In this case, we derive the appropriate differential equations by introducing the corresponding propagation vector $k'_j \rightarrow (1/i)\partial/\partial j'$, where $j = x, y, z$; and $j' = x', y', z'$ and specifying the rotation that expresses \mathbf{k} in terms of \mathbf{k}' (see Eq. (5)). Namely, replacing \mathbf{k}' into \mathbf{k} in each matrix element of the Hamiltonian given by Eq. (9) of Ref. 1, one obtains the Hamiltonian for [hkl] grown nanostructure (e.g. see also Ref. 2). We stress here, that although the envelope wavefunctions are oriented in accordance with the heterostructure axes, [hkl], the Bloch wave functions are defined as before, [001]. For the clarity reasons, we show explicit expression for several elements of the rotated Hamiltonian.

H_{11} is given by: $H_{11} = E_c + T$, where E_c denotes the energy of the conduction-band minimum, and T is given by:

$$T = A_c \{ (k_x U_{11} + k_y U_{12} + k_z U_{13} - i(k_x U_{21} + k_y U_{22} + k_z U_{23})) (k_x U_{11} + k_y U_{12} + k_z U_{13} + i(k_x U_{21} + k_y U_{22} + k_z U_{23})) + (k_x U_{31} + k_y U_{32} + k_z U_{33})^2 + ((k_x U_{11} + k_y U_{12} + k_z U_{13}) A_c) (k_x U_{11} + k_y U_{12} + k_z U_{13} + i(k_x U_{21} + k_y U_{22} + k_z U_{23})) - ((k_x U_{21} + k_y U_{22} + k_z U_{23}) A_c) (k_x U_{21} + k_y U_{22} + k_z U_{23}) + ((k_x U_{31} + k_y U_{32} + k_z U_{33}) A_c) (k_x U_{31} + k_y U_{32} + k_z U_{33}) \} \quad (A1)$$

Where A_c is calculated from the expression $A_c = \hbar/2m_c - 2P^2/3E_g - P^2/3(E_g + \Delta)$, m_c is the electron effective mass, E_g is the fundamental band gap, and Δ is the spin-orbit split-off energy. U_{ij} , where $i, j = 1, 2, 3$ are elements of the transformation matrix U as given by Eq. (1).

H_{12} of the rotated Hamiltonian is given by $H_{12} = iV_+$, where V_+ is given by:

$$V_+ = \frac{1}{2\sqrt{2}} \{ (P_1 + P_2) (k_x (U_{11} + iU_{21}) + k_y (U_{12} + iU_{22}) + k_z (U_{13} + iU_{23})) + ((k_x U_{11} + k_y U_{12} + k_z U_{13} + i(k_x U_{21} + k_y U_{22} + k_z U_{23})) P_2) \} \quad (A2)$$

Where, it is usually assumed that $P_1 = P_2 = P$, where P is the Kane matrix element.

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H_{33} is defined as $H_{33}=E_v-(P_++Q_+)$, where E_v is the energy of the valence band maximum, and P_++Q_+ are given by:

$$\begin{aligned}
 P_++Q_+ = \frac{\hbar^2}{2m} \{ & (\gamma_1 + \gamma_2)(k_x U_{11} + k_y U_{12} + k_z U_{13} - i(k_x U_{21} + k_y U_{22} + \\ & k_z U_{23})) (k_x U_{11} + k_y U_{12} + k_z U_{13} + i(k_x U_{21} + k_y U_{22} + k_z U_{23})) + \\ & (\gamma_1 - 2\gamma_2)(k_x U_{31} + k_y U_{32} + k_z U_{33})^2 + ((k_x U_{11} + k_y U_{12} + k_z U_{13})(\gamma_1 + \\ & \gamma_2))(k_x U_{11} + k_y U_{12} + k_z U_{13}) + ((k_x U_{31} + k_y U_{32} + k_z U_{33})(\gamma_1 - \\ & 2\gamma_2))(k_x U_{31} + k_y U_{32} + k_z U_{33}) + i((k_x U_{21} + k_y U_{22} + k_z U_{23})3\chi)(k_x U_{11} + \\ & k_y U_{12} + k_z U_{13}) - i((k_x U_{11} + k_y U_{12} + k_z U_{13})3\chi)(k_x U_{21} + k_y U_{22} + k_z U_{23}) \}
 \end{aligned} \tag{A3}$$

Where γ_i , where $i=1,2,3$ are modified Luttinger parameters,³ and χ is related to the fourth Luttinger parameter κ by $\kappa=\chi-1/3$.¹

As the last example, we show H_{35} element of the rotated Hamiltonian:

$$\begin{aligned}
 R = \frac{1}{2} \sqrt{3} \frac{\hbar^2}{2m} \{ & (k_x U_{11} + k_y U_{12} + k_z U_{13} - i(k_x U_{21} + k_y U_{22} + k_z U_{23}))(\gamma_2 + \\ & \gamma_3)(k_x U_{11} + k_y U_{12} + k_z U_{13} - i(k_x U_{21} + k_y U_{22} + k_z U_{23})) + (k_x U_{11} + k_y U_{12} + \\ & k_z U_{13} + i(k_x U_{21} + k_y U_{22} + k_z U_{23}))(\gamma_2 - \gamma_3)(k_x U_{11} + k_y U_{12} + k_z U_{13} + \\ & i(k_x U_{21} + k_y U_{22} + k_z U_{23})) \}
 \end{aligned} \tag{A4}$$

Based on the similarity that exists between Eq. (9) and Eq. (A2) of Ref. 1, where γ_i 's correspond to the deformation potentials, b and d , and the product of the components, $k_i k_j$, of the crystal momentum vector, correspond to the strain tensor components ε_{ij} , one can derive the expressions for the matrix elements of strain-depend part of the Hamiltonian.^{4,5}

For the completeness, let us add that it is also possible to derive the appropriate Hamiltonian for any crystallographic orientation by rotating both, angular and crystal momenta in accordance to relationship defined by Eq. (5).

References:

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