

Supplementary Materials

Novel InGaSb/AlP quantum dots for non-volatile memories

Demid S. Abramkin^{1,2}, Victor V. Atuchin^{3,4,5,6*}

¹Laboratory of Molecular Beam Epitaxy of III-V Semiconductor Compounds, Institute of Semiconductor Physics, SB RAS, Novosibirsk 630090, Russia

²Department of Physics, Novosibirsk State University, Novosibirsk 630090, Russia

³Laboratory of Optical Materials and Structures, Institute of Semiconductor Physics, SB RAS, Novosibirsk 630090, Russia

⁴Research and Development Department, Kemerovo State University, Kemerovo 650000, Russia

⁵Department of Industrial Machinery Design, Novosibirsk State Technical University, Novosibirsk 630073, Russia

⁶R&D Center “Advanced Electronic Technologies”, Tomsk State University, Tomsk 634034, Russia

Corresponding author: atuchin@isp.nsc.ru

Table S1. Materials parameters for AlP, GaP, InP, AlSb, GaSb and InSb at 300 K, which were used for the calculations. a_0 – lattice constant, C_{11} , C_{12} , C_{44} – elastic constants, $E_g^{\Gamma,X,L}$ – bandgaps for Γ , X and L valleys, $a_{\Gamma,X,L,v}$ – hydrostatic deformation potentials for the conduction band edge in Γ , X and L points of the Brillouin zone and valence band, $b_{X,v}$ – shear deformation potential for the conduction band at X point of the Brillouin zone and valence band, Δ_0 – energy of spin-orbital splitting in the valence band, VBO – valence band offsets, m_Γ – electron effective mass in the Γ point of the Brillouin zone, m_X^t and m_X^l – transversal and longitudinal electron effective mass in the X point of the Brillouin zone, m_L^t and m_L^l – transversal and longitudinal electron effective mass in the L point of the Brillouin zone, m_{hh} , m_{lh} , m_{SO} – effective masses for the heavy, light and spin-orbital splitting holes, F – Kane’s parameter, E_P – Kane’s matrix element, $\gamma_{1,2,3}$ – Luttinger parameters for the valence band.

Parameter	AlP	GaP	InP	AlSb	GaSb	InSb
a_0 , Å	5.4672 ^a	5.4505 ^a	5.8697 ^a	6.1355 ^a	6.0959 ^a	6.4794 ^a
C_{11} , GPa	1330 ^a	1405 ^a	1011 ^a	876.9 ^a	884.2 ^a	684.7 ^a
C_{12} , GPa	630 ^a	620.3 ^a	561 ^a	434.1 ^a	402.6 ^a	373.5 ^a
C_{44} , GPa	615 ^a	703.3 ^a	456 ^a	407.6 ^a	432.2 ^a	311.1 ^a
E_g^Γ , eV	3.552 ^a	2.808 ^a	1.352 ^a	2.300 ^a	0.7267 ^a	0.173 ^a
E_g^X , eV	2.487 ^a	2.272 ^a	2.313 ^a	1.616 ^a	1.032 ^a	0.568 ^a
E_g^L , eV	3.537 ^a	2.642 ^a	1.943 ^a	1.895 ^a	0.752 ^a	0.868 ^a
a_Γ , eV	-6.88 ^b	-9.41 ^b	-6.34 ^b	-8.12 ^b	-9.33 ^b	-6.84 ^b
a_X , eV	3.98 ^b	0.63 ^b	0.59 ^b	1.91 ^b	-0.20 ^b	1.41 ^b
a_L , eV	-1.74 ^b	-4.41 ^b	-3.41 ^b	-2.91 ^b	-4.38 ^b	-2.20 ^b
a_v , eV	2.64 ^b	-0.58 ^b	-0.41 ^b	0.73 ^b	-1.32 ^b	0.31 ^b
b_X , eV	6.75 ^c	6.5 ^c	3.3 ^c	6.0 ^c	6.46 ^c	4.53 ^c
b_v , eV	-1.5 ^a	-1.6 ^a	-2.0 ^a	-1.35 ^a	-2.0 ^a	-2.0 ^a
Δ_0 , eV	0.07 ^a	0.08 ^a	0.108 ^a	0.676 ^a	0.76 ^a	0.81 ^a
VBO , eV	-1.74 ^a	-1.27 ^a	-0.94 ^a	-0.41 ^a	-0.03 ^a	0 ^a
m_Γ	0.22 ^a	0.13 ^a	0.0795 ^a	0.14 ^a	0.039 ^a	0.0135 ^a
m_X^t	0.155 ^a	0.253 ^a	0.88 ^a	0.123 ^a	0.22 ^a	0.22 ^c
m_X^l	2.68 ^a	2.0 ^a	0.88 ^a	1.357 ^a	1.51 ^a	1.51 ^c
m_L^t	0.15 ^d	0.15 ^a	0.47 ^a	0.23 ^a	0.10 ^a	0.25 ^a
m_L^l	1.2 ^d	1.2 ^a	0.47 ^a	1.64 ^a	1.3 ^a	0.25 ^a
m_{hh}	0.63 ^f	0.32 ^a	0.85 ^f	0.8 ^f	0.34 ^f	0.26 ^f
m_{lh}	0.20 ^f	0.14 ^f	0.089 ^f	0.13 ^f	0.0447 ^f	0.0162 ^f
m_{SO}	0.30 ^a	0.25 ^a	0.21 ^a	0.22 ^a	0.12 ^a	0.11 ^a

F	-0.65 ^a	-	-	-	-1.63 ^a	-
E_P , eV	17.7 ^a	-	-	-	27.0 ^a	-
γ_1	3.35 ^a	-	-	-	13.4 ^a	-
γ_2	0.71 ^a	-	-	-	4.7 ^a	-
γ_3	1.23 ^a	-	-	-	6.0 ^a	-

^a[33], ^b[80], ^c[79], ^d GaP value, ^e GaSb value, ^f [81].

Table S2. Bowing parameters for GaAlP, InGaP, AlInP, GaAlSb, InGaSb, AlInSb, AlSbP, GaSbP and InSbP [33].

Bowing parameter	GaAlP	InGaP	AlInP	GaAlSb	InGaSb	AlInSb	AlSbP	GaSbP	InSbP
$a_0, \text{\AA}$	0	0	0	0	0	0	0	0	0
C_{11}, GPa	0	0	0	0	0	0	0	0	0
C_{12}, GPa	0	0	0	0	0	0	0	0	0
C_{44}, GPa	0	0	0	0	0	0	0	0	0
E_g^Γ, eV	0	0.65	-0.48	-0.044 +1.22x	0.415	0.43	2.7	2.7	1.9
E_g^X, eV	0.13	0.20	0.38	0	0.33	0	2.7	2.7	1.9
E_g^L, eV	0	1.03	0	0	0.4	0	2.7	2.7	1.9
a_Γ, eV	0	0	0	0	0	0	0	0	0
a_X, eV	0	0	0	0	0	0	0	0	0
a_L, eV	0	0	0	0	0	0	0	0	0
a_v, eV	0	0	0	0	0	0	0	0	0
b_X, eV	0	0	0	0	0	0	0	0	0
b_v, eV	0	0	0	0	0	0	0	0	0
Δ_0, eV	0	0	-0.19	0.3	0.1	0.25	0	0	0.75
VBO, eV	0	0	0	0	0	0	0	0	0
m_Γ	0	0.051	0.22	0	0.0092	0	0	0	0
m_X^t	0	0	0	0	0	0	0	0	0
m_X^l	0	0	0	0	0	0	0	0	0
m_L^t	0	0	0	0	0	0	0	0	0
m_L^l	0	0	0	0	0	0	0	0	0
m_{hh}	0	0	0	0	0	0	0	0	0
m_{lh}	0	0	0	0	0.011	0	0	0	0
m_{SO}	0	0	0	0	0	0	0	0	0

The critical sizes of SAQDs were obtained by solving of equation (1). It is can be presented in the following form:

$$h_c = \frac{b \cos(\lambda)}{f} \left(1 + \frac{(1-\nu/4) \ln\left(\frac{h_c}{2b}\right)}{4\pi \cos^2(\lambda)(1+\nu)} \right) \quad (16).$$

In the case of the $A_xB_{1-x}C_yD_{1-y}$ quaternary alloy, lattice constant mismatch is

$$f = \frac{a_{mat}}{a_0} - 1 = \frac{a_{mat}}{xy \cdot a_{AC} + (1-x)y \cdot a_{BC} + (1-x)(1-y) \cdot a_{BD} + x(1-y) \cdot a_{AD}} - 1 \quad \text{and} \quad \text{Burgers vector}$$

$$\text{magnitude is } b = \frac{a_{0t}}{\sqrt{2}} = \frac{xy \cdot a_{AC} + (1-x)y \cdot a_{BC} + (1-x)(1-y) \cdot a_{BD} + x(1-y) \cdot a_{AD}}{\sqrt{2}}. \quad \text{We solved this}$$

equation by the graphic method, as it is illustrated in the **Figure S1**.

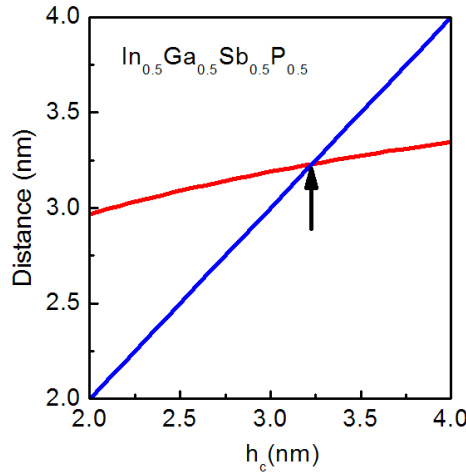


Figure S1. Solving of the equation (16) by the graphic method for the case of $\text{In}_{0.5}\text{Ga}_{0.5}\text{Sb}_{0.5}\text{P}_{0.5}/\text{AIP}$ SAQD. Linear part of the equation depicted by the blue line, the logarithmic one by the red line. The black arrow points to the obtained h_c value.