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Kadantsev, Eugene S.; Hawrylak, Pawel

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Absolute deformation potentials and robust *ab initio* model for band shifts induced by (001) biaxial strain in group IIIA-VA semiconductors

Eugene S. Kadantsev[a)] and Pawel Hawrylak
Quantum Theory Group, Institute for Microstructural Sciences, National Research Council, Ottawa, Canada K1A 0R6

A model for the evolution of conduction and valence bands of IIIA-VA (InAs, GaAs, and InP) semiconductors under (001) biaxial strain is developed. The model is based on the *ab initio* calculations which take into account finite strain dependent relaxation of the reference levels. The results of *ab initio* full potential calculations of absolute deformation potentials (ADPs) and (001) biaxial strain-modified band edges are reported. It is shown that in type I heterostructures subjected to (001) compressive biaxial strain, the corrections due to nonzero ADP of the core reference levels reduce the strained band offset for holes. © *2011 American Institute of Physics*. [doi:10.1063/1.3537815]

Energies of the band edges as a function of strain, absolute deformation potentials (ADPs), and natural band offsets (NBOs) are parameters of major interest in connection with the modeling of the semiconductor heterostructures such as self-assembled quantum dots[1]—the building blocks of photonic devices.[2,3] Some progress has been achieved in the calculation of deformation potentials,[4–8] natural band offsets,[5,6,9–11] and strain-induced band edges[12,13] from first-principles. The electronic band structure calculations are usually carried out using the Kohn–Sham form of density functional theory[14–16] (KS DFT) and should be further verified when implementations based on KS DFT+many-body perturbation theory become more widely available.

It is to be emphasized, however, that even within the framework of KS DFT, different computational schemes result in different predictions for the NBOs and ADPs. For example, the ADP of the valence band maximum (VBM) in IIIA-VA semiconductors was obtained to have negative[7] (VBM energy goes down as volume increases) or positive (VBM energy goes up as volume increases) sign.[4,5,8] Very often, the inconsistencies between the results reported by different authors can be traced back to the difficulty surrounding the definition of the absolute energy scale[17] in calculations employing Born–von Karman periodic boundary conditions.

Our present work is motivated by the desire to enable parametrization of the empirical tight-binding Hamiltonian to account for the effects of hydrostatic and biaxial strains in semiconductor heterostructures. Previous *ab initio* models of biaxial strain[12,13] were obtained by neglecting the relaxation of the reference energy levels due to strain. In this work, we explicitly calculate the uniaxial and hydrostatic ADPs of the reference core levels and find that they are of order 1–2 eV and are *not negligible*. We then develop robust *ab initio* model for band shifts due to (001) biaxial strain which takes into account the strain relaxation of the core energy levels.

To compute the band energies, we use KS DFT (Refs. 14 and 15) in the local spin density approximation,[16,18] variational treatment of spin-orbit coupling, and the augmented plane wave plus local orbitals (APW+lo) representation.[19,20]

EXC!TING APW+LO program[21] is used in all the calculations. The calculations are performed using "primitive" unit cell and superlattices where applicable. Convergence with respect to the energy cutoffs, reciprocal space sampling, and the size of the superlattice was ensured.

To calculate the ADP of the reference core level $E_{ref} = 1/2(E_{1s}^{anion} + E_{1s}^{cation})$ (average of the 1s core level energies of anion and cation), we construct superlattices along (100), (110), and (111) crystallographic directions. Half of the supercell is then subjected to the tensile or compressive uniaxial strain along the "direction of growth." Typically, the lattices are strained by 1%–2%. The uniaxial absolute deformation potentials of the reference level a_V^{1s} are determined from the finite energy difference between the "core" levels located in the strained/unstrained part of the supercell. Once the uniaxial potentials are determined, we perform the angular average[8] to obtain the hydrostatic core deformation potential a_V^{1s}.

The supercell calculations are illustrated in Fig. 1 for GaAs subjected to tensile uniaxial strain. Figure 1 shows E_{ref} along the *z*-direction for the (001) superlattice. The left side of the superlattice corresponds to the region exposed to ten-

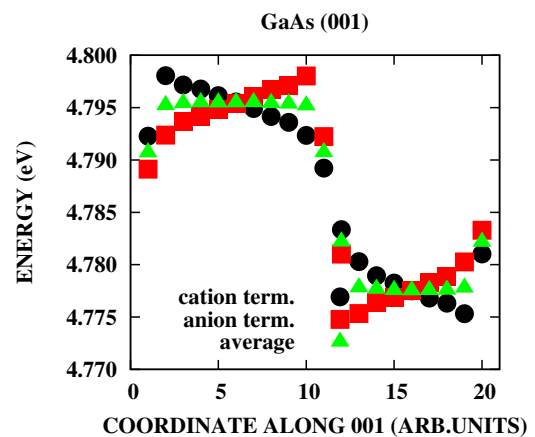FIG. 1. (Color online) Superlattice calculation of the core ADP in GaAs. The energy reference is arbitrary. The (001) superlattice is subjected to 1% uniaxial tensile strain. The "strained part" of the supercell is on the left. The calculations have to be performed for anion- and cation-terminated superlattices and the effects of the built-in electric field are averaged out.

a)Electronic mail: ekadants@babylon.phy.nrc.ca.

TABLE I. Deformation potentials (eV) $a_V^{VBM/1s}$ of VBM with respect to $1s$ core levels and the deformation potentials of the direct band gap $a_V^{CBM} - a_V^{VBM}$ for InAs, InP, and GaAs.

Method	$a_V^{CBM/1s}$	$a_V^{VBM/1s}$	$a_V^{CBM} - a_V^{VBM}$
	InAs		
This work	−5.86	−0.83	−5.03
Wei and Zunger[a]	−5.93	−1.00	−4.93
	InP		
This work	−5.60	−0.17	−5.43
Wei and Zunger[a]	−5.71	−0.41	−5.30
	GaAs		
This work	−8.21	−0.80	−7.41
Wei and Zunger[a]	−8.46	−1.21	−7.25

[a]Linearized augmented plane wave (LAPW) calculation from Ref. 7.

TABLE III. Coefficients obtained from the fit of biaxial strain-modified band edges to third degree polynomial in $\varepsilon_\parallel$.

Band α	C_1	C_2	C_3
	InAs		
CBM	−3554.24	203.81	97970.7
HH	−2653.54	12080	−79225.8
LH	3831.07	74578.3	32446.9
SO	1202.52	−83656.8	−46808.1
	InP		
CBM	−3447.64	925.234	62295.4
HH	−2122.07	11680.7	−30662.1
LH	3806.34	107858	−676415
SO	1993.34	−119070	693622
	GaAs		
CBM	−7345.78	−501.231	163604
HH	−2117.63	20146	−65765.3
LH	4357.87	52925.9	−287271
SO	2370.2	−52556	301211

TABLE II. ADPs (eV) for conduction band minimum a_V^{CBM}, valence band maximum a_V^{VBM}, and the deformation potentials of the direct band gap $a_V^{CBM} - a_V^{VBM}$ for InAs, InP, and GaAs.

Method	a_V^{CBM}	a_V^{VBM}	$a_V^{CBM} - a_V^{VBM}$
	InAs		
This work	−4.31	0.72	−5.03
Van de Walle[a]	−5.08	1.00	−6.08
Li et al.[b]	−3.87	1.79	−5.66
	InP		
This work	−4.45	0.98	−5.43
Van de Walle[a]	−5.04	1.27	−6.31
Li et al.[b]	−4.10	1.83	−5.93
	GaAs		
This work	−6.24	1.17	−7.41
Van de Walle[a]	−7.17	1.16	−8.33
Li et al.[b]	−5.91	2.24	−8.15

[a]"Model solid" theory of Ref. 5.
[b]LAPW calculations of Ref. 8.

sile uniaxial strain. Note that E_{ref} is larger in the strained part of the superlattice which corresponds to *positive deformation potential*.

The absolute volume deformation potential for band α at volume V is defined as $a_V^\alpha = dE_\alpha/d\ln(V)$, where E_α is the "absolute" band energy. We calculate ADPs for VBM as $a_V^{VBM} = a_V^{VBM/1s} + a_V^{1s}$, where $a_V^{VBMax/1s}$ is the deformation potential with respect to E_{ref} and a_V^{1s} was determined from the supercell calculations. The ADP of the conduction band minimum (CBM) is given by $a_V^{CBM} = a_V^{VBM} + (a_V^{CBM} - a_V^{VBM})$, where $(a_V^{CBM} - a_V^{VBM})$ is a well-defined deformation potential of the gap. The results of our calculations and results from Refs. 8 and 5 are summarized in Tables I and II. We find that all the ADPs for VBM of InAs, InP, and GaAs are positive.

The existing *ab initio* models of biaxial strain[12,13] were obtained assuming zero ADP of the core reference levels. Therefore, there is a need to develop a revised model for the biaxial strain. The (001) biaxial strain can be presented as a linear combination of hydrostatic and (001) uniaxial strains. The movement of E_{ref} with respect to some "absolute reference point" under the (001) biaxial strain is described by $dE_{ref} = [(1+\varepsilon_\parallel)^3 - 1]a_V^{1s} + (\varepsilon_\perp - \varepsilon_\parallel)a_V^{1s/001}$, where $\varepsilon_\parallel$ and $\varepsilon_\perp$ are the in-plane and out-of-plane strain tensor elements and the first and second terms in dE_{ref} stem from the hydrostatic and (001) uniaxial strains, respectively.
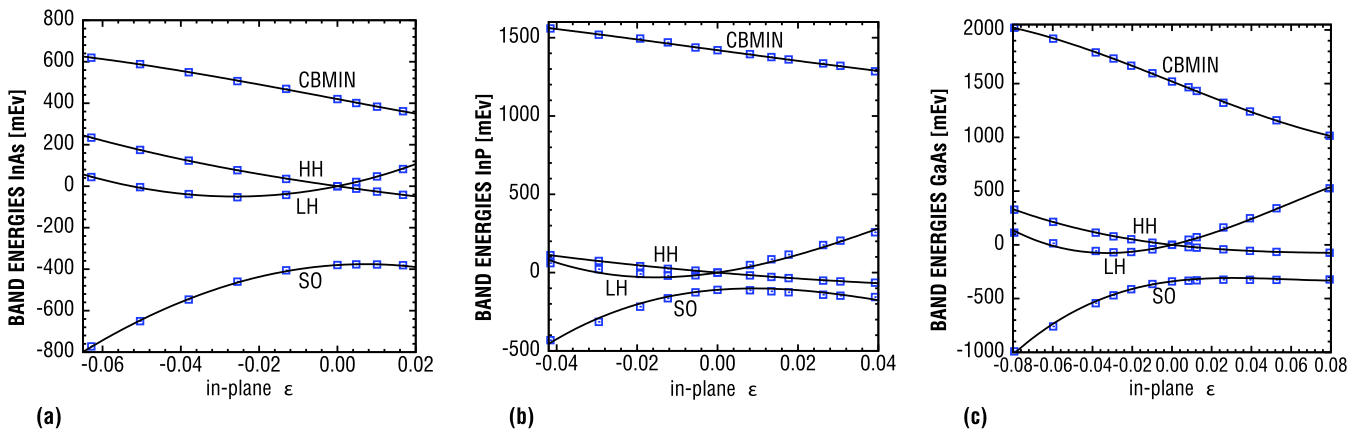

FIG. 2. (Color online) The (001) BBEs as a function of the "in-plane" strain $\varepsilon_\parallel$. The solid lines are fit to the polynomial of third degree in $\varepsilon_\parallel$.

FIG. 3. (Color online) Energy of InAs VBM as a function of compressive biaxial strain $E_{BIAXIAL}^{VBM} = NBO + C_{1VBM}\varepsilon_{\parallel} + C_{2VBM}\varepsilon_{\parallel}^2 + C_{3VBM}\varepsilon_{\parallel}^3$ for two difference choices.

The biaxial strain-modified band edges (BBEs) which include the effects of the "relaxation" of the core levels are illustrated in Fig. 2 for InAs, InP, and GaAs, respectively. The *ab initio* BBEs for band α are fitted to the polynomial of third degree $E_{BIAXIAL}^{\alpha} = C_{1\alpha}\varepsilon_{\parallel} + C_{2\alpha}\varepsilon_{\parallel}^2 + C_{3\alpha}\varepsilon_{\parallel}^3$. The expansion coefficients are summarized in Table III. The nonzero positive ADPs of the core levels affect the evolution of band edges under biaxial strain by moving *all bands* up or down in energy. This shift depends on the magnitude of strain. For example, in the case of InAs subjected to the compressive biaxial strain ($\varepsilon_{\parallel} < 0$), a situation encountered for InAs quantum dot grown on GaAs substrate, the position of the reference level E_{ref} with respect to the "absolute energy reference" shifts down due to the overall negative change in the volume. For InAs subjected to compressive strain, the shift is illustrated in Fig. 3 for two values of natural band offsets (210 and 460 meV). For a given value of the natural band

offset, the strained band offset is lower in the model which explicitly takes into account the finite ADP of the reference core levels. The strained band offsets can be thought of as a depth of the quasiparticle confinement. Therefore, combination of the "uncorrected" BBEs with large NBOs will result in the localization of holes that is too strong which will influence the theoretical predictions with regard to (multi)exciton complexes.

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