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Effects of ordering on the electron effective mass and strain deformation potential in $GaInP_2$: Deficiencies of the $\mathbf{k}\cdot\mathbf{p}$ model

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The conventional eight-band $\mathbf{k}\cdot\mathbf{p}$ model predicts a *decrease* of the electron effective mass and *no dependence* of the (001) strain band-gap deformation potential with the degree η of long-range order in $Ga_{0.5}In_{0.5}P$ alloys. We show that a complete band-structure approach predicts instead that (i) the electron effective mass in the ordering direction *increases* from $0.092m_0$ for $\eta=0$ (random alloy) to $0.133m_0$ for $\eta=1$ (ordered alloy), and (ii) the strain deformation potential *decreases* in magnitude from 8.26 eV for $\eta=0$ to 6.34 eV for $\eta=1$. These two effects are caused by the mixing of the conduction-band minimum with the L-derived conduction band, neglected in the standard eight-band model.

I. INTRODUCTION

The conventional eight-band Kane model,[1] together with the envelope-function approximation,[2] has been very successful in describing the properties of the band-edge states in bulk semiconductors. When dealing with semiconductor heterostructures, however, the standard eight-band Kane model usually neglects the coupling of the band-edge states with folded states. Yet, there are important cases where band folding plays a decisive role in determining the properties of the conduction-band minimum (CBM). Such is the case when the CBM is coupled to an energetically close, folded-in state belonging to the same irreducible representation. Then the two states will mix, causing mutual repulsion. For example, in short-period $(GaAs)_n/(AlAs)_n$ (001) superlattices the direct band gap at very small n is an *increasing* function[3] of n, while any effective-mass-based approach predicts an ever-decreasing band gap as a function of n. Here we discuss similar anomalies in spontaneously ordered alloys.[4,5]

Spontaneous ordering of semiconductor alloys into short-period superlattices has been observed during vapor-phase growth in many III-V common-anion and common-cation alloys.[4] In the well-known case of the $GaInP_2$ alloy lattice matched to a (001) GaAs substrate, long-range order associated with the CuPt structure (a monolayer superlattice oriented in the $\langle 111\rangle$ direction) has been widely observed.[5] The effects of ordering on the band-gap energy[6-11] and the valence-band splitting,[7,8,10,11] have been the subject of extensive experimental[6-9] and theoretical[10,11] work. Furthermore, the spin polarization of photoemitted electrons,[11,12] the strain[11,13] and pressure[14] dependence of the band gap, and the changes in higher-energy optical transitions due to ordering[15] have been recently addressed. In this work we investigate the consequences of CuPt ordering for (i) the zone-center electron effective mass, and (ii) the band-gap deformation potential for (001) epitaxial strain. We find that band folding leads to anomalous dependence of these quantities on the degree of ordering.

Upon ordering, the zinc-blende Brillouin zone of the $Ga_{0.5}In_{0.5}P$ random alloy is folded into the Brillouin zone of the CuPt superlattice; in particular, the zinc-blende Γ and L points fold into the superlattice $\bar{\Gamma}$ point (we use an overbar to denote superlattice states). The two lowest conduction states at the $\bar{\Gamma}$ point, originating from the folded zinc-blende states Γ_{1c} and L_{1c}, are coupled through the ordering potential of the CuPt superlattice. Since in the disordered alloy these two states are rather close in energy, the coupling produces a relatively strong mixing, which is expected to have a sizable effect on the conduction-band effective mass and the band-gap deformation potential of the ordered structure.

The eight-band Kane model for the disordered alloy can be modified to include the effects of CuPt ordering on the band-edge states,[13,16] by recognizing that CuPt ordering enters the problem in a way analogous to $\langle 111\rangle$ strain.[17] Since the eight-band model does not take into account band mixing, however, the conduction-band effective mass and the band-gap deformation potential are not expected to be accurately described. Through a comparison with *ab initio* multiband calculations, we will show that the effective mass of the ordered structure is *underestimated* by the eight-band model, while the magnitude of the band-gap deformation potential is *overestimated*. These results are explained by the fact that the Γ-L mixing, which is neglected by the eight-band model, tends to *increase* the electron effective mass and to *decrease* the band-gap deformation potential.

II. METHODS

The effective mass of the band n at the Γ point of the Brillouin zone is given by

$$m^n_{\alpha\beta}=\frac{1}{\hbar^2}\left[\frac{\partial^2E_n}{\partial k_\alpha\partial k_\beta}\right]^{-1}_{\mathbf{k}=0}, \tag{1}$$

where E_n is the single-particle energy of the band n. The band-gap deformation potential is given by

$$a_{\alpha\beta}=\left[\frac{\partial E_g}{\partial\epsilon_{\alpha\beta}}\right]_{\epsilon=0}, \tag{2}$$

where E_g is the band-gap energy and $\epsilon_{\alpha\beta}$ is the (α,β) component of the strain tensor $\boldsymbol{\epsilon}$. Effective masses and deformation potentials can be obtained as a function of the ordering parameter η, describing the degree of order of the alloy, once the band energies $E_n(\mathbf{k},\boldsymbol{\epsilon},\eta)$ are known. We will calculate $E_n(\mathbf{k},\boldsymbol{\epsilon},\eta)$ using two different methods: the eight-band Kane model, which neglects mixing between folded bands, and a direct multiband approach, which fully includes band mixing.

A. Eight-band k·p calculations

In the standard eight-band Kane model for bulk semiconductors the **k** dependence of the band-edge energies is described through second order in perturbation theory; the parameters of the second-order expansion are fitted to reproduce the exact experimental effective masses of the pure bulk semiconductors. The effect of strain on the band-edge energies can also be included in the Kane model to linear order using deformation potentials.[18] The extension of the Kane model to superlattices and heterostructures is usually based on the envelope function approximation.[2,19] For short-period superlattices, however, this approach is not appropriate, because the envelope function varies over a length scale comparable with the lattice constant.

The problems introduced by the envelope-function approximation can be bypassed by starting with a conventional strain-dependent eight-band **k·p** Hamiltonian for the *disordered* alloy, and including the effects of CuPt ordering through an ordering Hamiltonian,[11,13,16,20] without any appeal to the envelope-function approximation. This method is able to predict the energies of the band-edge states[11,13] as a function of the strain tensor $\boldsymbol{\epsilon}$ and of the ordering parameter η. The strain-dependent **k·p** Hamiltonian for the disordered alloy, $H_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k},\boldsymbol{\epsilon})$, is identical to the one used in Ref. 18 for zinc-blende crystals, although the terms arising from the lack of inversion symmetry are neglected. The ordering Hamiltonian $H_{\text{ord}}(\eta)$ has the same form as the strain Hamiltonian for (111) epitaxial strain.[17] Assuming that the spin-orbit splitting is η independent,[11] $H_{\text{ord}}(\eta)$ depends only on two parameters: the crystal-field splitting $\Delta_{\text{CF}}(\eta)$ and the ratio r between the band-gap reduction and the crystal-field splitting. In the Cartesian representation[17] $\{|s\rangle,|x\rangle,|y\rangle,|z\rangle\}$ the ordering Hamiltonian in each spin subspace is given by

$$H_{\text{ord}}(\eta)=\frac{1}{3}\Delta_{\text{CF}}(\eta)\begin{bmatrix}3r+1 & 0 & 0 & 0\\ 0 & 0 & -1 & -1\\ 0 & -1 & 0 & -1\\ 0 & -1 & -1 & 0\end{bmatrix}. \qquad (3)$$

Wei, Laks, and Zunger[10] have shown that the crystal-field splitting has a quadratic dependence on the degree of ordering: $\Delta_{\text{CF}}(\eta)=\eta^2\Delta_{\text{CF}}(1)$, where $\Delta_{\text{CF}}(1)$ is the crystal-field splitting of the perfectly ordered CuPt structure. Furthermore, both experimental and theoretical results show that the band-gap reduction has a quadratic dependence on η: $\Delta E_g(\eta)=\eta^2\Delta E_g(0)$, where $\Delta E_g(1)$ is the band-gap reduction for the perfectly ordered CuPt structure. Thus, the ratio $r=\Delta E_g(\eta)/\Delta_{\text{CF}}(\eta)$ is η independent to a good approximation. The parameters we use in our **k·p** calculations[8,10,21–23] are given in Table I. The total 8×8 Hamiltonian $H=H_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k},\boldsymbol{\epsilon})+H_{\text{ord}}(\eta)$ is diagonalized numerically to get the band-edge energies as a function of **k**, $\boldsymbol{\epsilon}$, and η. Effective masses and deformation potentials are then obtained from Eqs. (1) and (2).

B. Band-structure calculations

Effective masses and deformation potentials can also be obtained from *ab initio* band-structure calculations. The equilibrium (zero strain) atomic geometry of the ordered CuPt structure is determined using the valence-force field method,[24] under the assumption of no distortion in the (001) atomic planes. This is consistent with the experimental situation, where the partially ordered $\text{Ga}_{0.5}\text{In}_{0.5}\text{P}$ alloy is grown pseudomorphically on a (001)-oriented GaAs substrate. By minimizing the elastic energy of the CuPt superlattice, we find the lattice constant to be $a_s=5.66$ Å, very close to the equilibrium lattice constant of GaAs. The band structure of the CuPt superlattice is then calculated using the density-functional theory in the local-density approximation (LDA), as implemented in the full-potential linearized augmented plane wave (LAPW) method.[25] We use the Ceperley-Alder exchange-correlation potential as parametrized by Perdew and Zunger.[26] Scalar relativistic effects are fully included, while spin-orbit splittings are obtained through a second variational procedure.[27] The LAPW method is known to give accurate ground-state properties, such as lattice constants and bulk moduli.[28] The derivatives occurring in Eqs. (1) and (2) are calculated numerically

TABLE I. Parameters used in the **k·p** calculations. E_g is the band gap of the disordered alloy, Δ_{SO} is the spin-orbit splitting, m_{el} is the electron effective mass, E_p is the Kane parameter, γ_1, γ_2, and γ_3 are the Luttinger parameters, a_c is the band-gap hydrostatic deformation potential, b and d are the strain-splitting parameters of the valence band, and c_{11}, c_{12} are the elastic constants. Also, Δ_{CF} is the crystal-field splitting of the fully ordered CuPt structure, and r is the ratio $\Delta E_g/\Delta_{\text{CF}}$ between the band-gap reduction and the crystal-field splitting (see text). When two references are given, they correspond to the experimental values for bulk GaP and InP, respectively. In this case, the parameter for the alloy is obtained as the average of the two bulk parameters.

Quantity	Value	Quantity	Value
E_g (eV)	1.991[a]	a_c (eV)	−8.25[c,c]
Δ_{SO} (eV)	0.103[a]	b (eV)	−1.52[c,c]
m_{el} (m_0)	0.092[b]	d (eV)	−4.40[c,c]
E_p (eV)	26[b]	c_{11} (kbar)	123.0[c,c]
γ_1	4.32[c,d]	c_{12} (kbar)	61.4[c,c]
γ_2	1.03[c,d]	Δ_{CF} (eV)	0.200[e]
γ_3	1.49[c,d]	r	−1.60[e]

[a] Reference 8.
[b] Reference 23.
[c] Reference 21.
[d] Reference 22.
[e] Reference 10.

from the LAPW band-structure using a simple finite-difference scheme. We estimate the numerical error involved in the effective mass and deformation potential calculations to be smaller than 1%.

The effective masses calculated within the LDA are affected by systematic errors,[29] reflecting the well-known band-gap underestimation of LDA. For example, our LAPW calculated electron effective mass of InP is $m_{\mathrm{el}}=0.034m_0$, compared to the experimental value[21] $m_{\mathrm{el}}=0.076m_0$. In the case of GaAs, the LDA effective mass calculated by Christensen[29] is $m_{\mathrm{el}}=0.012m_0$, while the observed value[21] is $m_{\mathrm{el}}=0.067m_0$. Note, however, that the LDA errors are expected to cancel to leading order when we consider the effective-mass *difference* between the disordered $\mathrm{Ga}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ alloy and the ordered CuPt structure. The LDA effective mass of the disordered alloy ($\eta=0$) is approximated by the average of the effective masses of pure GaP and InP, *calculated at the substrate lattice constant* a_s: $m_{\mathrm{LDA}}(0)=1/2[m_{\mathrm{GaP}}(a_s)+m_{\mathrm{InP}}(a_s)]$. This is expected to be a good approximation, because the bowing of the effective mass is primarily due to volume effects. Note that our value for $m_{\mathrm{LDA}}(0)$ is different from the usual average $1/2[m_{\mathrm{GaP}}(a_{\mathrm{GaP}})+m_{\mathrm{InP}}(a_{\mathrm{InP}})]$. The LDA effective mass of the ordered CuPt structure ($\eta=1$) is obtained from a direct band-structure calculation for a (111) monolayer superlattice with the same substrate lattice constant a_s. Then, to correct for the LDA error, we add the difference between the LDA effective masses of the ordered and disordered alloy to the experimental effective mass $m(0)$ of the disordered alloy,[23] obtaining the LDA-corrected effective mass of the fully ordered CuPt structure:

$$m(1)=m(0)+m_{\mathrm{LDA}}(1)-m_{\mathrm{LDA}}(0)\ . \tag{4}$$

Laks, Wei, and Zunger[30] have proved that the alloy properties that are invariant under atomic interchange depend quadratically on the degree of long-range order, provided that many-body effects can be neglected. Thus, for $0<\eta<1$ we use a quadratic interpolation formula for the inverse effective mass:

$$m^{-1}(\eta)=m^{-1}(0)+\eta^2[m^{-1}(1)-m^{-1}(0)]\ . \tag{5}$$

For our LDA calculations of the band-gap deformation potential as a function of the ordering parameter η we use a quadratic interpolation formula[30]

$$a(\eta)=a(0)+\eta^2[a_{\mathrm{LDA}}(1)-a_{\mathrm{LDA}}(0)]\ , \tag{6}$$

where $a(0)$ is the experimental band-gap deformation potential of the disordered alloy,[21] and $a_{\mathrm{LDA}}(1)-a_{\mathrm{LDA}}(0)$ is the difference between the LDA-calculated band-gap deformation potentials of the ordered CuPt structure and of the disordered alloy. The former is obtained directly from a band-structure calculation for a GaP/InP(111) monolayer superlattice, while the latter is approximated by the average of the LDA deformation potentials[11] of bulk GaP and InP, as shown in Table II.

TABLE II. LDA band-gap deformation potentials for (001) epitaxial strain (in eV).

	GaP	InP	Alloy
Γ_{1c}	−8.89	−4.60	−6.75
L_{1c}	−3.33	−2.05	−2.69

III. EFFECTIVE MASS

We start by discussing the qualitative physics of ordering-induced effects on the electron effective mass of the $\mathrm{Ga}_{0.5}\mathrm{In}_{0.5}\mathrm{P}$ alloy. Using nondegenerate second-order perturbation theory, the electron effective mass of the *disordered* alloy, $m^c_{\alpha\beta}$, can be written exactly[31] in terms of the eigenstates $|u_n\rangle$ and eigenvalues E_n at the zone center:

$$\frac{m_0}{m^c_{\alpha\beta}}=\delta_{\alpha,\beta}+\frac{2}{m_0}\mathrm{Re}\sum_{n\neq c}\frac{\langle u_c|p^\dagger_\alpha|u_n\rangle\langle u_n|p_\beta|u_c\rangle}{E_c-E_n}\ , \tag{7}$$

where m_0 is the bare electron mass and $\mathbf{p}$ is the momentum operator. From a qualitative point of view, two effects must be taken into account when considering the consequences of CuPt ordering on the electron effective mass. The first effect is the well-known reduction of the direct band gap upon ordering.[6–11] According to Eq. (7), the ordering-induced band-gap reduction tends to *decrease* the CBM effective mass. The second effect is the ordering-induced coupling between the Γ_{1c} and L_{1c} states, which causes a mixing of the corresponding wave functions in the ordered CuPt structure. Since the longitudinal effective mass of the bulk L_{1c} state is much larger than the Γ_{1c} effective mass, the Γ-L mixing tends to *increase* the CBM effective mass. The resulting electron effective mass depends on a delicate balance between these two competing effects.

Another consequence of CuPt ordering is the *anisotropy* of the conduction-band effective mass. While the effective mass of the perfectly random alloy is isotropic, the ordering-induced coupling between conduction and valence bands breaks the symmetry of the conduction-band minimum, inducing an anisotropy between the effective mass in the ordering direction and the effective mass in the plane orthogonal to the ordering direction. This anisotropy is *enhanced* by the Γ-L mixing, because the L_{1c} effective mass is larger in the ordering direction than in the perpendicular directions. The anisotropy of the conduction-band effective mass has been pointed out by Raikh and Tsiper.[32] Using a simple two-band model, these authors demonstrated that, because of the Γ-L mixing, the conduction-band effective mass is anisotropic, and estimated the anisotropy to be $(m_\parallel-m_\perp)/m_{\mathrm{alloy}}\sim 0.14$ in a partially ordered alloy with band-gap reduction $\Delta E_g=140$ meV (corresponding to $\eta\sim 0.66$ according to Table I). However, this method provides only a crude estimate, because the effects of the band-gap reduction on the effective mass are neglected, and because evaluating this model required several parameters that are difficult to obtain either from experiment or from first-principles calculations. O'Reilly and Meney[20] have recently dis-

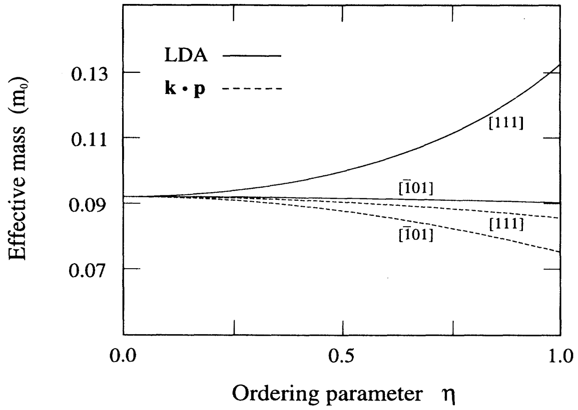

FIG. 1. Electron effective mass in the ordering direction [111] and in the perpendicular direction [$\bar{1}$01], as a function of the ordering parameter η. The **k**·**p** effective masses are obtained from numerical diagonalization of the 8×8 **k**·**p** Hamiltonian, while the LDA effective masses are calculated using Eqs. (4) and (5).

cussed the ordering-induced anisotropy of the hole effective mass between the [$\bar{1}$10] and [110] directions. Using the eight-band **k**·**p** model, these authors found that the heavy-hole effective mass of a disordered $Ga_{0.5}In_{0.5}P/Al_{0.2}Ga_{0.3}In_{0.5}P$ quantum well is isotropic in the $\langle 110 \rangle$ directions, with $m_{110} = m_{\bar{1}10} = 0.254 m_0$. Ordering effects break the symmetry of the heavy hole, leading to $m_{110} = 0.188 m_0$ and $m_{\bar{1}10} = 1.029 m_0$ in a partially ordered ($\eta \sim 0.57$) quantum well.

The electron effective mass of ordered and disordered $Ga_{0.5}In_{0.5}P$ alloys has been recently measured by a few groups. Using optically detected cyclotron resonance (ODCR) Emanuelsson *et al.*[23] found that the effective mass decreases upon ordering from $m_{el} = (0.092 \pm 0.003) m_0$ for the disordered alloy to $m_{el} = (0.088 \pm 0.003) m_0$ for the partially ordered alloy (band-gap reduction $\Delta E_g \simeq 50$ meV, corresponding to $\eta \sim 0.40$). The effective-mass reduction was ascribed primarily to the ordering-induced band-gap reduction. No effort was done to orient the magnetic field with respect to the ordering axis. Wong *et al.*[33] have measured the ODCR effective mass of two $Ga_{0.52}In_{0.48}P$ samples grown by molecular beam epitaxy (MBE) and by metalorganic vapor-phase epitaxy (MOVPE), obtaining $m_{el} = (0.088 \pm 0.005) m_0$ for the MBE sample and $m_{el} = (0.091 \pm 0.005) m_0$ for the MOVPE sample. Since the two samples have the same band gap (to within 3 meV), these authors conclude that the difference in the effective mass is unlikely to be caused by ordering effects.

The LDA and **k**·**p** electron effective mass calculated along the ordering direction [111] and along the perpendicular direction [$\bar{1}$01] are compared in Fig. 1 as a function of the ordering parameter η. The effective mass is isotropic in the plane orthogonal to the ordering direction. As can be seen from Fig. 1 the effective masses calculated with the **k**·**p** method always *decrease* when the ordering parameter η increases; this is a consequence of the ordering-induced band-gap reduction. On the other hand, the LDA effective mass slightly *decreases* in the [$\bar{1}$01] direction but *increases* significantly in the [111] direction when the degree of order increases. In fact the Γ-*L* mixing, which is neglected in the **k**·**p** model, is fully taken into account in the LDA band-structure calculation, and tends to increase the electron effective mass along the [111] direction. The **k**·**p** model predicts an anisotropy of the electron effective mass, which increases with the ordering parameter η; for the perfectly ordered CuPt structure we have: $(m_{111} - m_{\bar{1}01})/m_{\text{alloy}} \simeq 0.11$. This anisotropy is strongly enhanced by the Γ-*L* mixing: the LDA calculation yields $(m_{111} - m_{\bar{1}01})/m_{\text{alloy}} \simeq 0.46$ for the fully ordered CuPt structure.

From the point of view of theoretical rigor, the LDA calculation is more accurate than **k**·**p** since it includes the effects of folded bands, which are neglected by **k**·**p**. On the other hand, the experimental value of Ref. 23 for the partially ordered alloy ($m_{el} = 0.088 \pm 0.003 m_0$) agrees with **k**·**p** better than with LDA. This particular sample, however, has a low degree of ordering, so the *change* in the effective mass relative to the disordered sample is very small ($\Delta m_{el} \simeq -0.004 m_0$), and difficult to accurately compare with theory. Furthermore, in the experiment of Ref. 23 the magnetic field was not oriented with respect to the ordering direction, so the anisotropy predicted in Fig. 1 cannot be assessed. Finally, Ref. 33 suggests that effects other than ordering can produce effective-mass reductions comparable to that observed in Ref. 23. Thus, we call for additional, orientation-dependent measurements of anisotropic effective masses of significantly ordered samples to test our theory.

IV. STRAIN DEFORMATION POTENTIAL

Although the band-gap deformation potentials for epitaxial (001) strain have not been measured so far in the $Ga_xIn_{1-x}P$ alloy, it is likely that a certain amount of strain is present in many of the samples studied. In fact, $Ga_xIn_{1-x}P$ alloys can be grown coherently on a GaAs(001) substrate even when the alloy composition differs from the lattice-matched composition; in this case, the alloy film is subject to epitaxial (001) strain.[11,13,34] Also, the response of the substrate and the film to external fields can be different, so that a certain amount of strain can occur in a lattice-matched film when external fields (such as pressure or temperature) are applied. The deformation potentials of the partially ordered $Ga_{0.5}In_{0.5}P$ alloy are also interesting from a fundamental point of view. The band-gap deformation potential is expected to be relatively insensitive to the band-gap reduction induced by ordering in the $Ga_{0.5}In_{0.5}P$ alloy. Thus, the variations in the deformation potentials with the degree of order can reveal the extent of the Γ-*L* mixing of the conduction-band minimum.

Strictly speaking, the band-gap deformation potential of the perfectly random alloy for (001) strain is not a well-defined quantity. In fact, while the light-hole and heavy-hole states are degenerate in the cubic zinc-blende structure, they are split by (001) strain: the heavy-hole state becomes the valence-band maximum for in-plane compressive strain ($\epsilon < 0$), while the light-hole state be-

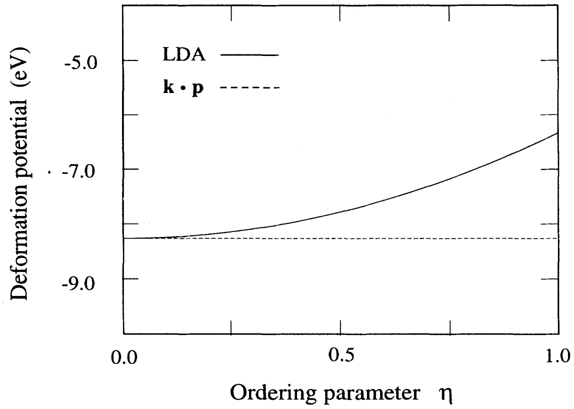

FIG. 2. Band-gap deformation potential for (001) epitaxial strain, as a function of the ordering parameter η.

comes the valence-band maximum for in-plane tensile strain ($\epsilon > 0$). Since the deformation potentials of the light hole and of the heavy hole are different, the band-gap deformation potential has a discontinuity at $\epsilon = 0$. However, there is no such discontinuity when an "effective band gap" is evaluated with respect to the average of the *three states* at the top of the valence band. Therefore, we define the band-gap deformation potential for (001) epitaxial strain as $a_{001} = \partial(E_c - \bar{E}_v)/\partial\epsilon$, where E_c is the CBM energy and $\bar{E}_v$ is the average energy of the three states at the valence-band maximum.

In the simple eight-band $\mathbf{k}\cdot\mathbf{p}$ model the conduction band is decoupled from the valence-band manifold at $\mathbf{k} = 0$, even in the presence of CuPt ordering and (001) strain. Since the ordering Hamiltonian does not depend on strain, the conduction-band deformation potential $\partial E_c/\partial\epsilon$ is independent of the ordering parameter η. Also, even though the valence eigenvalues depend on η, their sum does not. Therefore, the band-gap deformation potential in the eight-band model is independent of η, and its value is given by $a_{001} = 2a(1 - c_{12}/c_{11})$, where a is the *hydrostatic* band-gap deformation potential of the disordered alloy, and c_{11}, c_{12} are the alloy elastic constants.

The LDA and $\mathbf{k}\cdot\mathbf{p}$ band-gap deformation potentials for (001) epitaxial strain are compared in Fig. 2 as a function of the ordering parameter η. Since the L_{1c} deformation potential of the disordered alloy is *smaller* (in absolute value) than the Γ_{1c} deformation potential (Table II), the ordering-induced Γ-L mixing of the CBM is expected to *reduce* the magnitude of the band-gap deformation potential. This is what we observe in our LDA calculations, where we obtain $a_{001}(1) - a_{001}(0) = 1.92$ eV. Thus, from Eq. (6), we find that the band-gap deformation potential $|a_{001}|$ decreases from 8.26 eV in the disordered alloy to 6.34 eV in the fully ordered CuPt structure, primarily because of the ordering-induced Γ-L mixing of the conduction-band minimum.

V. SUMMARY

In conclusion, we have shown how long-range CuPt-type ordering affects the conduction-band effective mass and the band-gap strain deformation potential of $GaInP_2$ alloys. In the case of the effective mass, the final result depends on the balance between (i) the band-gap reduction induced by ordering and (ii) the Γ-L mixing of the conduction-band minimum wave function. The Γ-L mixing determines the strong anisotropy of the electron effective mass in ordered alloys. We find that the effective mass in the plane perpendicular to the ordering direction slightly decreases upon ordering, while the effective mass in the ordering direction increases significantly. In the case of the band-gap deformation potential for (001) epitaxial strain, we have shown that the main effect comes from the Γ-L mixing of the conduction-band minimum, which tends to decrease the absolute value of the deformation potential.

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