Evaluation of matrix elements of the 8×8 k·p Hamiltonian with k-dependent spin-orbit contributions for the zinc-blende structure of GaAs

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The $\mathbf{k} \cdot \mathbf{p}$ method of band-structure calculation provides a detailed description of a crystal's energy dispersion near a high symmetry point in the first Brillouin zone. The resulting parameters of this calculation are a series of momentum matrix elements. Presented here is a set of band-structure parameters for the zinc-blende structure of GaAs at the Γ point that takes the lack of inversion symmetry into account as well as **k**-dependent spin-orbit contributions to the Hamiltonian. A comprehensive optimization was performed in order to satisfy effective mass data as well as conduction band spin-splitting data. It was found that the lack of inversion symmetry has a profound influence on the nonparabolicity of the conduction band and the contribution of the **k**-dependent spin-orbit effect cannot be ignored in the calculation of the effective mass of the conduction, light hole, and spin-orbit bands. [S0163-1829(96)03543-6]

Many semiconductor heterostructures and devices depend on GaAs or a compound with GaAs, such as $Al_xGa_{1-x}As$ or $In_xGa_{1-x}As$. Possibly important devices that depend on GaAs technology include quantum well modulators, gradedband-gap heterojunction transistors, high electron mobility transistors, vertical cavity lasers, quantum cascade lasers, and broad band light-emitting diodes. Growth techniques and more sophisticated experimental investigations¹⁻⁶ of these GaAs based heterostructures are increasing the demands on their theoretical treatments. We present a methodology for the accurate description of bulk GaAs in a model that can be applied to quantum heterostructures.

Many theoretical treatments of quantum heterostructures are based on bulk $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians in the envelope-function approximation. Reviews of these treatments include Bastard and co-workers,⁷⁻¹⁰ Smith,¹¹ and Marzin and co-workers.^{12,13} Typically, a transfer-matrix is applied to a bulk $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian in the envelope-function approximation. Effects such as strain, nonsquare wells, symmetry forbidden transitions, and electric and magnetic fields are addressed within the $\mathbf{k} \cdot \mathbf{p}$ model by a number of authors.^{14–22} All of these models depend on an estimation of the $\mathbf{k} \cdot \mathbf{p}$ matrix elements. Many authors^{18,23-29} have estimated some of these matrix elements to explain a given set of data, but the models used fall short of predicting other reliable data found elsewhere. The most influential differences that distinguish one model from another are the band levels considered, inversion asymmetry, and k-dependent spin-orbit coupling. The model that we consider here is an $8 \times 8 \mathbf{k} \cdot \mathbf{p}$ Kane Hamiltonian³⁰ that takes into account both the inversion asymmetry of GaAs and the k-dependent spin-orbit coupling of the Kane model.³¹ We present a set of matrix elements that reproduces physically measured effective mass and conduction band spin-splitting data. The data selected are based on the criteria discussed in Sec. II. The effective masses considered here are those of the conduction band, heavy and light hole bands in both the [001] and [111] directions, and the spin-orbit band. With the proper determination of its matrix elements, we expect this model to provide an improved basis for the theoretical treatment of quantum heterostructures.

In Sec. I, the $\mathbf{k} \cdot \mathbf{p}$ model considered will be developed, and the parameters that are to be optimized are identified and defined. In Sec. II, a review of effective mass and spinsplitting measurements over the past 35 years will be presented. Section III will illustrate the relationship between the Kane matrix elements and effective mass. The optimization of the Kane matrix elements to the relevant physical data discussed in Sec. II will be described. In Sec. IV, the findings of this model will be reviewed and compared to previous work.

I. BULK ZINC-BLENDE BAND STRUCTURE

Early band theory work concerning the importance of symmetry,^{32–34} boundary conditions,³⁴ and time-reversal symmetry³⁵ have led to some powerful methods currently in use today, such as the tight-binding method and the $\mathbf{k} \cdot \mathbf{p}$ method. The tight-binding (TB) method of crystal band-structure calculations has proven to be quite successful in the determination of semiconductor energy dispersion. In the TB approximation, the crystal wave functions are assumed to be composed of free atomic wave functions. The resulting dispersion is defined by a series of overlap-function matrix elements in the full zone \mathbf{k} representation.

The $\mathbf{k} \cdot \mathbf{p}$ method has been developed and utilized by a number of authors.^{23,30,31,36-43} Instead of free atomic wave functions, the $\mathbf{k} \cdot \mathbf{p}$ method assumes that a basis set of $u_{\mathbf{nk}_0}$ Bloch functions completely spans the space of functions periodic in the entire first zone. This set of states is referred to as the $\mathbf{k} \cdot \mathbf{p}$ representation. The result is a band structure that is defined by a series of momentum matrix elements. The relationship between TB and $\mathbf{k} \cdot \mathbf{p}$ has been illustrated by Priester and Lannoo,⁴¹ who have derived $\mathbf{k} \cdot \mathbf{p}$ parameters in terms of TB parameters. With a reduced basis set, the $\mathbf{k} \cdot \mathbf{p}$ method can provide detailed information about the band structure of a given crystal in the vicinity of an arbitrary point \mathbf{k}_0 . Since the free electrons and holes of a semiconductor are usually confined to a small region about a high symmetry point in the first zone, the $\mathbf{k} \cdot \mathbf{p}$ method can be an effi-

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cient and flexible model for the theoretical investigation of semiconductors and semiconductor quantum heterostructures. Full zone $\mathbf{k} \cdot \mathbf{p}$ schemes have been developed by Cardona and Pollak⁴⁰ and others, but its power lies in extracting detailed dispersion information in the vicinity of \mathbf{k}_0 .

Consider the general Hamiltonian eigenvalue equation

$$\left[\frac{p^2}{2m_0} + V(\mathbf{r})\right] \Psi_k(\mathbf{r}) = E(\mathbf{k}) \Psi_k(\mathbf{r})$$

Expressing the \mathbf{k} representation eigenvector in Bloch form

$$\Psi_k(\mathbf{r}) = e^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}}u_k(\mathbf{r})$$

leads to the equivalent form in the $\mathbf{k} \cdot \mathbf{p}$ representation

$$\left[\frac{p^2}{2m_0} + V(\mathbf{r})\right] e^{i\mathbf{k}\cdot\mathbf{r}} u_k(\mathbf{r}) = E(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}} u_k(\mathbf{r}),$$
$$\left[\frac{(\mathbf{p} + \hbar\mathbf{k})^2}{2m_0} + V(\mathbf{r})\right] u_k(\mathbf{r}) = E(\mathbf{k})u_k(\mathbf{r}),$$
$$\frac{p^2}{2m_0} + \frac{\hbar}{m_0}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar^2k^2}{2m_0} + V(\mathbf{r})\left] u_k(\mathbf{r}) = E(\mathbf{k})u_k(\mathbf{r}).$$

With the inclusion of the spin-orbit interaction, the Hamiltonian becomes

$$H_{\text{Tot}} = \frac{p^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} + V(\mathbf{r}) + H_{\text{pso}} + H_{\text{kso}},$$
(1.1)

$$H_{\rm pso} = \frac{\hbar}{4m_0^2 c^2} (\nabla V) \times \mathbf{p} \cdot \boldsymbol{\sigma},$$
$$H_{\rm kso} = \frac{\hbar^2}{4m_0^2 c^2} (\nabla V) \times \mathbf{k} \cdot \boldsymbol{\sigma},$$

where H_{pso} corresponds to Kane's³¹ H_1 and H_{kso} corresponds to Kane's H_2 . Solutions to Eq. (1.1) can be obtained

by approximating the unknown Bloch states as an expansion in the known Bloch states of a high symmetry point located at \mathbf{k}_0 ,

$$u_{n\mathbf{k}}(\mathbf{r}) = \sum_{n} c_{nn} u_{n\mathbf{k}_0}(\mathbf{r}).$$

This can now be solved by perturbation theory, as is usually the case, or by Schur-complement decomposition.³⁷ Löwdin perturbation theory⁴⁴ will be considered here and the following results are after Kane³¹ and Bahder.³⁰ Löwdin perturbation theory divides all possible eigenvectors into two classes, *A* and *B*. The class-*A* states represent the primary states of interest. The class-*B* states consist of all states outside of the class-*A* states and are to be treated by perturbation theory. Here, the class-*A* states are taken to be the band-edge eightdimensional manifold defined as

$$\nu_{1} = |s\rangle\chi_{\uparrow}, \quad \nu_{2} = |x\rangle\chi_{\uparrow}, \quad \nu_{3} = |y\rangle\chi_{\uparrow}, \quad \nu_{4} = |z\rangle\chi_{\uparrow}, \quad (1.2a)$$
$$\nu_{5} = |s\rangle\chi_{\downarrow}, \quad \nu_{6} = |x\rangle\chi_{\downarrow}, \quad \nu_{7} = |y\rangle\chi_{\downarrow}, \quad \nu_{8} = |z\rangle\chi_{\downarrow}, \quad (1.2b)$$

where

$$\chi_{\uparrow} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \chi_{\downarrow} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

The class-*B* states have a small effect on the class-*A* states, meaning

$$|H_{ik}| \ll |H_{ii} - H_{kk}|, \quad i \text{ in class-}A, \quad k \text{ in class-}B.$$

Renormalization of the class-*A* interactions of $\{\nu_i\}$ results in an 8×8 Kane-like interaction Hamiltonian matrix. Transforming $\{\nu_i\}$ by unitary transformation to a basis for the $\{\Gamma_6, \Gamma_7, \Gamma_8\}$ irreducible representations of the T_d double group gives $\{u_i\}$ as defined in Appendix A.³⁰ Now, renormalization of the class-*A* interactions of $\{u_i\}$ results in the Hamiltonian matrix given by Bahder,³⁰ which will be denoted as \mathbf{H}_0 ,

$u_{-1/2}^{\Gamma_6}$	$u_{1/2}^{\Gamma_{6}}$	$u_{-3/2}^{\Gamma_8}$	$u_{-1/2}^{\Gamma_8}$	$u_{1/2}^{\Gamma_8}$	$u_{3/2}^{\Gamma_{8}}$	$u_{-1/2}^{\Gamma_{7}}$	$u_{1/2}^{\Gamma_{7}}$
A	0	$T^* + V^*$	0	$-\sqrt{3}(T-V)$	$\sqrt{2}(W-U)$	W-U	$\sqrt{2}(T^*+V^*)$
0	Α	$\sqrt{2}(W-U)$	$-\sqrt{3}(T^*+V^*)$	0	T-V	$-\sqrt{2}(T-V)$	$W^* + U$
T+V	$\sqrt{2}(W^*-U)$	-P+Q	$-S^{*}$	R	0	$(\frac{3}{2})^{1/2}S$	$-\sqrt{2}Q$
0	$-\sqrt{3}(T+V)$	- <i>S</i>	-P-Q	0	R	$-\sqrt{2}R$	$(\frac{1}{2})^{1/2}S$
$-\sqrt{3}(T^*-V^*)$	0	R*	0	-P-Q	<i>S</i> *	$(\frac{1}{2})^{1/2}S^*$	$\sqrt{2}R^*$
$\sqrt{2}(W^*-U)$	$T^* - V^*$	0	<i>R</i> *	S	-P+Q	$\sqrt{2}Q$	$(\frac{3}{2})^{1/2}S^*$
$W^* - U$	$-\sqrt{2}(T^*-V^*)$	$(\frac{3}{2})^{1/2}S^*$	$-\sqrt{2}R^*$	$(\frac{1}{2})^{1/2}S$	$\sqrt{2}Q$	Ζ	0
$\sqrt{2}(T+V)$	W + U	$-\sqrt{2}Q$	$(\frac{1}{2})^{1/2}S^*$	$\sqrt{2}R$	$(\frac{3}{2})^{1/2}S$	0	Ζ

The constants in matrix (1.3) are defined as follows:

$$A = E_c + \left[A' + \frac{\hbar^2}{2m_0} \right] (k_x^2 + k_y^2 + k_z^2), \qquad (1.4a)$$

$$U = \frac{1}{\sqrt{3}} P_0 k_z, \qquad (1.4b)$$

$$V = \frac{1}{\sqrt{6}} P_0(k_x - ik_y), \qquad (1.4c)$$

$$W = i \frac{1}{\sqrt{3}} B k_x k_y, \qquad (1.4d)$$

$$T = \frac{1}{\sqrt{6}} Bk_z(k_x + ik_y), \qquad (1.4e)$$

$$P = -E_v + \gamma_1 \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2 + k_z^2), \qquad (1.4f)$$

$$Q = \gamma_2 \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2 - 2k_z^2), \qquad (1.4g)$$

$$R = -\sqrt{3} \frac{\hbar^2}{2m_0} [\gamma_2(k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y], \quad (1.4h)$$

$$S = \sqrt{3} \gamma_3 \frac{\hbar^2}{m_0} k_z (k_x - ik_y), \qquad (1.4i)$$

$$Z = E_v - \Delta - \gamma_1 \frac{\hbar^2}{2m_0} (k_x^2 + k_y^2 + k_z^2).$$
(1.4j)

The band structure given by matrix (1.3) is parametrized by the constants A', B, E_p , γ_1 , γ_2 , and γ_3 , which are defined in Appendixes B and C. A' is the momentum matrix element that couples class-*B* states to the class-*A* conduction band edge, Γ_6 , in the double group notation. *B* accounts for the inversion asymmetry of the zinc-blende structure (T_d point group, Schoenflies notation). If B=0, then the structure will be that of diamond (O_h point group, Schoenflies notation). E_p is the energy associated with the P_0 matrix element that couples Γ_6 to the class-*A* valence band edge Γ_8 and is defined as

$$E_p = \frac{2m_0}{\hbar^2} P_0^2.$$

 γ_i are the modified Luttinger parameters where the standard Luttinger parameters will be denoted as γ_i^l . Matrix (1.3) accounts for the interactions given in Eq. (1.1), except for the **k**-dependent spin-orbit interaction $H_{\rm kso}$. This is accounted for by the matrix $\mathbf{M}_{\rm kso}$ (after Bahder³⁰),

$$\mathbf{M}_{kso} = \langle u_i | H_{kso} | u_j \rangle = \begin{bmatrix} u^{\Gamma_6} & u^{\Gamma_8} & u^{\Gamma_7} \\ 0 & \mathbf{M}_1 & \mathbf{M}_2 \\ \mathbf{M}_1^{\dagger} & 0 & 0 \\ \mathbf{M}_2^{\dagger} & 0 & 0 \end{bmatrix}, \quad (1.5)$$

where

$$\begin{split} \mathbf{M}_{1} = & \frac{C_{0}}{\sqrt{2}} \\ \times \begin{bmatrix} u_{-3/2}^{\Gamma_{8}} & u_{-1/2}^{\Gamma_{8}} & u_{1/2}^{\Gamma_{8}} & u_{3/2}^{\Gamma_{8}} \\ -(k_{x} + ik_{y}) & 0 & -\sqrt{3}(k_{x} - ik_{y}) & 2k_{z} \\ 2k_{z} & \sqrt{3}(k_{x} + ik_{y}) & 0 & k_{x} - ik_{y} \end{bmatrix}, \\ & u_{-1/2}^{\Gamma_{7}} & u_{1/2}^{\Gamma_{7}} \\ \mathbf{M}_{2} = 2C_{0} \begin{bmatrix} -k_{z} & k_{x} + ik_{y} \\ k_{x} - ik_{y} & k_{z} \end{bmatrix}, \\ & C_{0} = \frac{1}{\sqrt{3}} \frac{\hbar^{2}}{4m_{0}^{2}c^{2}} \left\langle s \left| \frac{\partial V}{\partial x} \right| x \right\rangle. \end{split}$$

The complete Hamiltonian matrix is then given by

$$\mathbf{H}_T = \mathbf{H}_0 + \mathbf{M}_{\rm kso} \,. \tag{1.6}$$

 \mathbf{M}_{kso} couples class-*A* and class-*B* states in the second-order perturbation. This results in the coupling of Γ_6 to both Γ_8 and Γ_7 to first order in **k**. H_{kso} also generates matrix elements in $\langle x | \partial V / \partial x | z \rangle$, which have been shown to be zero by Bir and Pikus.⁴⁵

Now the dispersion near the Γ point is defined and parametrized by E_g , Δ , A', B, E_p , C_0 , γ_1 , γ_2 , and γ_3 . The energy gap is defined as $E_g = E(\Gamma_6) - E(\Gamma_8)$ and the spinorbit splitting as $\Delta = E(\Gamma_8) - E(\Gamma_7)$. E_g and Δ have been determined to a reasonable degree of accuracy and will be considered as known parameters, or constants, here. The set of unknown parameters, S, is then taken to be

$$S = \{\gamma_1^l, \gamma_2^l, \gamma_3^l, A', B, C_0, E_p\}.$$
 (1.7)

We wish to optimize *S* to effective mass and spin-splitting data within the described model. To do this, it will be necessary to pay considerable attention to the choice of data used in the optimization.

Over the past 35 years, substantial experimental effort has gone into the determination of the effective masses (electron and hole) of GaAs. Here, we review this body of work and determine a set of effective masses to be used in the determination of S [Eq. (1.7)].

II. DETERMINATION OF PARAMETER SET

A. Conduction electron mass

Early work on determining the Γ point conduction bandedge effective mass consisted of infrared reflectivity and Faraday rotation experiments as well as some cyclotron reso-

TABLE I. Experimentally determined conduction band mass and spin-orbit splitting for GaAs.

Source	m_c^*/m_0	$\gamma \ (eV \ Å^3)$	Temp. (K)	Method
Aspnes (Ref. 76)	0.067	*	0	Hall coefficient data
	0.063	*	295	
Stradling and Wood (Ref. 77)	0.0665	*	60	magnetophonon magnetoresistance
	0.0636	*	290	
Miller et al. (Ref. 63)	0.0665	*	77	quantum well transitions ^a
Fetterman et al. (Ref. 51)	0.06649	*	4.2	cyclotron resonance, 337 μ m
Stillman et al. (Ref. 50)	0.0665	*	1.5 - 4.2	Zeeman effect, shallow donors
Narita and Miyao (Ref. 78)	0.067	*	4.2	Zeeman effect, shallow donors
Marushchak et al. (Ref. 72)	*	22	4.2	electron spin relaxation
Aronov et al. (Ref. 71)	*	20.9	4.2	electron spin relaxation

^aSquare and parabolic wells, GaAs/Al_{0.3}Ga_{0.7}As, $L_w = 51 - 521$ Å.

nance experiments. Work by Spitzer and Whelan⁴⁶ with infrared reflectivity data and later refinements by Ehrenreich⁴⁷ lead to a conduction band-edge mass of $m_c = 0.072m_0$. Faraday rotation experiments by Moss and Walton⁴⁸ and Cardona⁴⁹ lead to measurements that were in close agreement with this infrared reflectivity work. Although there existed a great deal of agreement between most of these early results, they tended to overestimate the conduction band effective mass with respect to more recent results listed in Table I. The mass that was measured in most of these early experiments was the optical mass, m_{opt} , and is influenced by impurities and electron concentration, thus requiring a correction for polaron interactions. The nonparabolicity of the conduction band also had the effect of producing larger effective masses if $\mathbf{k} \neq \mathbf{0}$ contributions were not kept to a minimum.

The results of later work are given in Table I for a number of different temperatures and experimental techniques. Stillman and co-workers⁵⁰ utilized the Zeeman effect on shallow donors and obtained a value of $m_c = (0.0665 \pm 0.0005)m_0$ at liquid helium temperatures. Fetterman and co-workers⁵¹ employed cyclotron resonance with high purity GaAs. Narrow cyclotron resonance absorption was observed at 337 μ m and 311 μ m, where the magnetic field used was accurately characterized using NMR techniques and corrections that accounted for the nonparabolicity of the conduction band were made resulting in a value of $m_c = (0.06649 \pm 0.00003)m_0$ at 4.2 K. Other work utilizing magnetophonon magnetoresistance, Hall coefficient data, and quantum well transitions all yielded similar results. Using cyclotron resonance, Chamberlain and Stradling⁵² found no detectable change in m_c over the temperature range 4 K to 115 K. Considering the agreement between the bulk of these more refined measurements, a value of $m_c = 0.0665m_0$ will be used in the determination of S at OK.

B. Valence hole masses

The problems that researchers faced when measuring the effective masses of the Γ_8 valence band edge, $m_{\rm hh}$ and $m_{\rm lh}$, were very similar to the problems that were overcome in measuring m_c , yet there still remains a considerable spread in the experimentally obtained values for $m_{\rm hh}$ and $m_{\rm lh}$. This is due to the fact that the Γ_8 band edge is not spherical. There exists a considerable anisotropy such that,

for example, $m_{\rm hh}^{001} \neq m_{\rm hh}^{111}$. As a result, early measurements that were influenced by off Γ point contributions tended to overestimate the effective mass in the [001] direction and underestimated the effective mass in the [111] direction. Due to GaAs's inversion asymmetry and the electronic properties of its cation and anion, it is slightly ionic. Therefore, cyclotron resonance measurements,^{42,43,53,54} where $\omega < \omega_{\rm lo}$, actually measure the polaron mass and must be corrected.^{55,56} This correction depends on the Fröhlich polaron coupling constant, α_F , which describes the coupling of electrons and longitudinal optical phonons, and is fairly well known for the conduction band, but is not so well known for the light and heavy holes bands due to the anisotropy of these bands.

Table II lists various results for $m_{\rm hh}$ and $m_{\rm lh}$ obtained by a variety of experimental methods. Generally, it is difficult to correct bulk data from cyclotron resonance and magnetooptic measurements for effects due to the \mathbf{k}_{H} dependence of low-lying Landau levels, line shape broadening, hole concentration, and polaron mass. Looking at Table II, the data seems to form two, fairly distinct, groups. Studying bulk materials, Vrehen,⁵⁷ Seisyan and co-workers,⁵⁸ Balslev,⁵⁹ and Skolnick and co-workers⁶⁰ all obtained similar values for $m_{\rm hh}$ and $m_{\rm lh}$ in the [001] direction, but their results vary dramatically in the [111] direction. The second group of measurements incorporates both bulk and quantum well systems. Hess and co-workers,⁶¹ Yamanaka and co-workers,⁶² Miller and co-workers,⁶³ and Shanabrook and co-workers⁶⁴ all obtained similar results for $m_{\rm hh}$ and $m_{\rm lh}$ in the [001] direction. Measurements of $m_{\rm hh}$ and $m_{\rm lh}$ in the [111] direction were done on bulk GaAs by Hess and co-workers, and on GaAs/Al_{0.3}Ga_{0.7}As quantum wells of varying well thickness by Shanabrook and co-workers. The results of these two experiments are in fair agreement, but their differences should be discussed. The work done by Hess and co-workers utilized high field magnetoreflectance of free excitons to study bulk GaAs. Their data fit well within an adiabatic description of free excitons in a high magnetic field,⁶⁵ but the resulting band-structure parameters, from which effective masses are calculated, are very sensitive to the bandstructure model used. Experimental data derived from quantum well experiments are dominated by the new symmetry of the quantum well system. The effective masses are primarily defined by the bulk band structure (in the absence of strain,

TABLE II. Valence band effective masses and Luttinger parameters for GaAs.

Source	$m_{ m hh}^{001}$	$m_{ m hh}^{111}$	$m_{ m lh}^{001}$	$m_{ m lh}^{111}$	γ_1^l	γ_2^l	γ_3^l	Temp (K)	Method
Skolnick et al. (Ref. 60)	0.45	0.57	0.082	0.079	7.21	2.49	2.73	50-77	CR ^a
Vrehen (Ref. 57)	0.45	0.45	0.082	0.082	7.21	2.49	2.49	77	MOA ^b
Seisyan et al. (Ref. 58)	0.434	0.469	0.0829	0.0817	7.18	2.44	2.53	77	MOA ^b
Balslev (Ref. 59)	0.45	0.99	0.088	0.080	6.79	2.29	2.87	$T \leq 100$	PT^{c}
	0.46	1.03	0.083	0.075	7.11	2.47	3.09	$T \ge 200$	
Mears and Stradling (Ref. 73)	0.475	*	0.087	*	6.80	2.35	*	50	CR^d
Miller et al. (Ref. 63)	0.34	*	0.094	*	6.79	1.92	*	77	QWT ^e
Hess et al. (Ref. 61)	0.38	0.95	0.090	0.070	6.85	2.10	2.90	5	HFMR ^f
Yamanaka et al. (Ref. 62)	0.34	*	0.12	*	5.64	1.35	*	295	PCS ^g
Shanabrook et al. (Ref. 64)	0.34	0.75	0.094	0.082	6.80	1.90	2.73	10	ERS^h

^aCyclotron resonance, 337 μ m and 2.2 mm.

^bInterband magneto-optic absorption.

^cPiezotransmission.

^dCyclotron resonance, 155 GHz, high purity epitaxial films.

^eQuantum well transitions in square and parabolic GaAs/Al_{0.3}Ga_{0.7}As, $L_w = 21 - 521$ Å.

^fHigh field magnetoreflectance of excitons.

^gPhotocurrent spectroscopy, GaAs/Al_{0.34}Ga_{0.66}As quantum wells.

^hElectronic Raman scattering, GaAs/Al_{0.3}Ga_{0.7}As qauntum wells, $L_w = 100 - 400$ Å.

with strain, band mixing effects must be taken into account) of a specific constituent material, but the effect of mass on experimental data is dominated by the quantum well structure. Shanabrook and co-workers utilized electronic Raman scattering to measure intersubband quantum well transitions in GaAs/Al₀₃Ga₀₇As. The drawback to this kind of investigation is that knowledge of the precise dimensions of the quantum well system is required in order to extract information on energy levels and effective mass. Shanabrook and co-workers characterized the widths of their quantum wells by growth characteristics, intersubband transitions of photoexcited electrons, and photoreflectance spectroscopy. Since intersubband transitions of holes were examined, the data is more sensitive to changes in effective mass than the determination of the interband exciton energies themselves. Also, this type of measurement is fairly insensitive to changes in the band offset of the quantum well.⁶³ Thus, for the determination of S [see Eq. (1.7)], we will employ the effective mass measurements of Shanabrook and co-workers (see Table II).

Measurements on the spin-orbit band mass, m_{s0} , were done by Vrehen⁵⁷ using interband magnetoabsorption. He obtained a value of $0.159m_0$ at 77 K. Later work by Reine and co-workers⁶⁶ utilized stress-modulated interband magnetoreflectivity data. They obtained a value of $0.154m_0$ at about 30 K. Like m_c , no detectable change in this mass is anticipated to 0 K. Reine and co-workers results have since been widely accepted and cited by a number of authors;^{67–69} therefore, a value of $0.154m_0$ at 0 K will be used for the determination of S.

C. Conduction band spin spitting

Table III lists experimental and theoretical values of the conduction band spin-splitting parameter, γ , defined by the conduction band dispersion relation⁷⁰

$$E_{\Gamma_6}(k) = \frac{\hbar^2}{2m_c} k^2 + (\alpha + s\beta)k^4 \pm \gamma(s - 9t)^{1/2}k^3, \quad (2.1)$$

where

$$s = \frac{1}{k^4} (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2), \qquad (2.2)$$
$$t = \frac{1}{k^6} (k_x^2 k_y^2 k_z^2).$$

The experimental values were obtained by electron spin relaxation measurements. The analysis of this data depends, in part, on the Fröhlich polaron coupling constant, α_F , which itself depends on a number of previously measured quantities.⁵⁵ The experimental methods of Aronov⁷¹ and Marushchak⁷² are similar, but Aronov used a value for the Fröhlich polaron coupling constant of $\alpha_F = 0.06$. Estimates of α_F vary to some degree, but the most often cited value^{69,60,73,74} is $\alpha_F = 0.06$. Aronov's result is in fair agreement with most of the theoretical calculations, especially the results of Zawadzki²⁸ using a five level $\mathbf{k} \cdot \mathbf{p}$ analysis. As a result, we will use Aronov's value of $\gamma = 20.9$ eV Å³ in the determination of *S*.

III. DETERMINATION OF S

We now wish to determine the band-structure parameter set *S* that produces the measured observable set *T* by \mathbf{H}_T [see Eq. (1.6)].

$$S = \{\gamma_{1}^{l}, \gamma_{2}^{l}, \gamma_{3}^{l}, A', B, C_{0}, E_{p}\},$$

$$T = \{m_{c}, m_{hh}^{001}, m_{hh}^{111}, m_{lh}^{001}, m_{lh}^{111}, m_{so}, \gamma\},$$
(3.1)

where the elements of T were defined previously as

$$m_c = 0.0665, \quad m_{\rm hh}^{001} = 0.34,$$

 $m_{\rm hh}^{111} = 0.75, \quad \gamma = 20.9 \text{ eV } \text{\AA}^3,$ (3.2)

Source	$-\alpha \ (eV \ Å^4)$	$-\beta$ (eV Å ⁴)	$\gamma \;({\rm eV}\;{\rm \AA}^3)$	E_p (eV)	E'_p (eV)	Temp (K)	Method
Balslev (Ref. 59)	*	*	*	22.93	*	205-295	piezotransmission
Aspnes (Ref. 76)	*	*	*	22.53	*	0-295	Hall coefficient data
Lawaetz (Ref. 23)	*	*	*	25.7	*	0	k ⋅p ^a
Rössler (Ref. 24)	1984	1380	19	*	*	0	8×8 k ∙p
	2132	2493	30	*	*	0	14×14 k ⋅p
Christensen and Cardona (Ref. 25)	*	*	18	26.29	3.55	0	five level $\mathbf{k} \cdot \mathbf{p}$
	*	*	17	*	*	0	modified LMTO
Yoo (Ref. 26)	1937	*	*	*	*	0	$8 \times 8 \mathbf{k} \cdot \mathbf{p}^{b}$
Hermann and Weisbuch (Ref. 27)	*	*	*	28.9	6	0	five level k · p
Zawadzki et al. (Ref. 28)	*	*	20.7	28.9	5.72	0	five level k · p
Eppenga et al. (Ref. 18)	*	*	*	28.8	*	0	$8 \times 8 \mathbf{k} \cdot \mathbf{p}^{c}$
Marushchak et al. (Ref. 72)	*	*	22	*	*	4.2	electron spin relaxation
Aronov et al. (Ref. 71)	*	*	20.9	*	*	4.2	electron spin relaxation

TABLE III. Experimental and calculated nonparabolicity parameters (α , β , γ) and momentum matrix element energy E_p for GaAs.

^aSemiempirical five level.

^bTransfer matrix applied to GaAs/Al_xGa_{1-x}As quantum wells.

^cApplied to GaAs/Al_{0.25}Ga_{0.75}As quantum wells in the envelope-function approximation.

$$m_{\rm so} = 0.154, \quad m_{\rm lb}^{001} = 0.094, \quad m_{\rm lb}^{111} = 0.082.$$

It should be understood that the given electron and hole masses are in terms of the bare electron rest mass m_0 , and that the valence band masses are actually negative quantities. The parameters of \mathbf{H}_T that are taken to be constant are, for T=0 K,

$$E(\Gamma_6) = 1.519 \text{ eV}, \quad E(\Gamma_8) = 0 \text{ eV},$$
 (3.3)
 $\Delta = E(\Gamma_7) = 0.341 \text{ eV}, \quad a = 5.652.28 \text{ Å}.$

A first attempt at solving this problem might consist of solving for the eigenvalues of \mathbf{H}_T , $\{\lambda_i(S, \mathbf{k})\}$, analytically and then simply solving for the masses of the respective bands. This would involve selecting two specific directions for \mathbf{k} , \mathbf{k}_{001} , and \mathbf{k}_{111} and solving for the respective eigenvalues (one direction at a time) $\{\lambda_i(S, \mathbf{k}_{001})\}$ and $\{\lambda_i(S, \mathbf{k}_{111})\}$. The elements of *S* could then be solved for from the resulting expressions for the six possible effective masses and the conduction band spin splitting of the observable set *T*. This is not possible owing to the overwhelming complexity of the analytic representations of $\{\lambda_i(S, \mathbf{k}_{001})\}$ and $\{\lambda_i(S, \mathbf{k}_{111})\}$ as well as the time required to complete (if possible) such a task.

A second attempt might be to tackle the problem as a whole with a multiparameter search method such as utilizing a seven-dimensional closed simplex in an eight-dimensional Euclidean space. The problem with this and other similar methods is that a simple closed form function does not exist in this application. Here, \mathbf{H}_T must be diagonalized and evaluated numerically for a number of values of \mathbf{k} , and then curvefit to obtain any member of the observable set T.

Examine Figs. 1–6. These were generated by successive numerical solutions for the eigenvalues of \mathbf{H}_T . With this information, the problem could be simplified by obtaining a linear approximation of these curves about a trial sevendimensional solution point and solving for the elements of S by general matrix methods. Since these curves are sensitive to changes in parameters that are assumed to be held fixed, successive iterations from one solution to the next will have to be made until a final, stable, point is reached. The problem with this method is that the function space defined here is extremely sensitive to this kind of linear approximation. Attempts at linearizing all seven dimensions and solving by general matrix methods has proven to be divergent, meaning successive, finer, iterations diverge quadratically, regardless of the initial point chosen.

The problem has been solved by linearizing only one dimension at a time. In order to do this, prior knowledge of the one-dimensional partial derivatives is used to preprogram a given path through the seven-dimensional parameter space as discussed below. Figures 1–6 illustrate the dependence of effective mass on the different elements of S. Matrix element B (see Appendix B for definition) has no effect on any of the effective masses, but it does have a sizable influence on the third- and fourth-order nonparabolicity parameters as will be



FIG. 1. Effective mass in the [001] direction as a function of γ_1^l . The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.



FIG. 2. Effective mass in the [001] direction as a function of γ_2^l . The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.

discussed in the next section. Figures 1-8 were made with the final data given in Table IV for A'=0. The data for the original versions of Figs. 1-8 used in the determination of *S* were derived from an initial guess (a seven-dimensional initial point, S_i) and showed the same trends and dependencies as the final figures.

Both *S* and *T* have seven elements, but it turns out that this system is still underdefined. There are four valence band hole masses, two in the [001] direction, and two in the [111] direction. Within the 4×4 Luttinger Hamiltonian, these four valence band effective masses, $m_{hh(lh)}^{001}$ and $m_{hh(lh)}^{111}$, are completely defined by the three Luttinger parameters, γ_1^l , γ_2^l , and γ_3^l ,

$$m_{\rm hh(lh)}^{001} = (\gamma_1^l \mp 2 \gamma_2^l)^{-1},$$
 (3.4a)



FIG. 3. Effective mass in the [111] direction as a function of γ_3^l . The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.



FIG. 4. Effective mass in the [001] direction as a function of Ep. The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.

$$m_{\rm hh(lh)}^{111} = (\gamma_1^l \mp 2\gamma_3^l)^{-1}.$$
 (3.4b)

Within the 8×8 Hamiltonian discussed here, \mathbf{H}_T , the above relation for $m_{\rm hh}$ in both directions still holds. Under a unitary transformation, the heavy hole valence band will completely decouple from the 8×8 Hamiltonian matrix in both the [001] and the [111] directions. For $m_{\rm lh}$, which remains coupled to the Γ_6 and Γ_7 states, Eqs. (3.4) are not exact, but are still a good approximation. What this means is that a given set of parameters, *S*, will produce specific values for the four valence band effective masses, but no set *S* exists that can manipulate the value of one of these effective masses without affecting the other masses as defined by Eq. (3.4). Another way to look at this is to define the three Luttinger parameters by rewriting Eq. (3.4) as



FIG. 5. Effective mass in the [001] direction as a function of A'. The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.



FIG. 6. Effective mass in the [001] direction as a function of C_0 . The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.

$$\gamma_1^l = \frac{1}{2} \left(\frac{1}{m_{\rm hh}^{001}} + \frac{1}{m_{\rm lh}^{001}} \right),$$
 (3.5a)

$$\gamma_2^l = \frac{1}{4} \left(\frac{1}{m_{\rm lh}^{001}} - \frac{1}{m_{\rm hh}^{001}} \right),$$
 (3.5b)

$$\gamma_3^l = \frac{1}{4} \left(\frac{1}{m_{\rm hh}^{001}} + \frac{1}{m_{\rm lh}^{001}} \right) - \frac{1}{2m_{\rm hh}^{111}}.$$
 (3.5c)

Therefore, within the 4×4 Luttinger model, only three effective masses are required to completely define the three Luttinger parameters. Equations (3.5a)-(3.5c) are not exact when applied to the case defined by \mathbf{H}_T , but the approximation is strong enough to reduce by one the number of degrees of freedom of the observable set *T*. Thus, to a large extent, the seven members of *T* will actually behave as six with



FIG. 7. Nonparabolicity parameters as a function of B. The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.



FIG. 8. Nonparabolicity parameters as a function of C_0 . The values of the matrix elements used in the calculation of the curves are given in the first row of Table IV.

respect to the parameters in S. One parameter in S will have to be fixed at a constant value during the search process.

The search process involved in the determination of *S* depended on the linearization of $m_{\rm lh}^{001}$ vs γ_1^l . From an initial point S_0 , two $m_{\rm lh}^{001}$ vs γ_1^l points were determined from $\gamma_1^+ = \gamma_{1(0)}^l + h/2$ and $\gamma_1^- = \gamma_{1(0)}^l - h/2$, where *h* is some initial iteration step. Two sets, S^+ and S^- , were constructed from γ_1^+ and γ_1^- as follows.

from γ_1^+ and γ_1^- as follows. (1) Data for $\gamma_1^{+/-}$, m_{hh}^{001} , and m_{hh}^{111} were used to obtain γ_2^l and γ_3^l for each of S^+ and S^- . They will be denoted as $\gamma_2^{+/-}$ and $\gamma_3^{+/-}$.

(2) Dispersion data for m_c vs E_p and m_{so} vs C_0 were linearized about S_0 for $\gamma_1^{+/-}$, $\gamma_2^{+/-}$, and $\gamma_3^{+/-}$ in order to obtain $E_p^{+/-}$ and $C_0^{+/-}$. This procedure completed S^+ and S^- for the first iteration.

(3) To complete the first iteration, a pair of points for $m_{\rm lh}^{001}$ vs γ_1^l was obtained by \mathbf{H}_T and $S^{+/-}$. From these points, a different value for γ_1^l was calculated from the known value for $m_{\rm lh}^{001}$.

(4) A procedure analogous to lines 1-3 was used to calculate a new central point S_0 . Dispersion for this new central point was calculated and used to generate a first iteration approximation of the observable set *T*. This iteration process was then continued until the approximation of *T* fell within a predetermined tolerance.

The primary line of iteration, m_{lh}^{001} vs γ_1^l , was chosen based on two criteria, linear approximation and the magnitude of its slope about S_0 . Examination of Fig. 1 shows that m_{lh}^{001} vs γ_1^l is approximately linear about $\gamma_1^l = 7.0$ and has a slope large enough to have a fairly predictable influence over the search process. Also, all of the valence band masses are influence by γ_1^l with the same sign of their partial derivatives. This adds to the predictability of the search process.

We have chosen A' to be fixed at one of two values, 0 and $-14.70 \text{ eV } \text{Å}^2$. Table IV shows the final results of both values. An estimate of A' was determined from Bahder's³⁶ analytic dispersion relation for the conduction band which considers C_0 to be zero.

<i>A'</i> (eV Å ²)	γ_1^l	γ_2^l	γ_3^l	E_p (eV)	C ₀ (eV Å)	<i>B</i> (eV Å ²)
0.0	6.672	1.866	2.669	22.827	0.1257	41.90
-14.70	6.669	1.864	2.668	29.112	0.1564	39.11

TABLE IV. Final optimized values of the Kane 8×8 band-structure parameters, T=0 K. Both sets of parameters will produce T.

$$\frac{m_0}{m_c} = 1 + \frac{2m_0}{\hbar^2} A' + E_p \frac{E_g + \frac{2}{3}\Delta}{E_g(E_g + \Delta)}.$$
 (3.6)

Now, Hermann and Weisbuch²⁷ have defined the conduction electron's effective mass in terms of the band parameters of a five level $\mathbf{k} \cdot \mathbf{p}$ model. Their result is given by

$$\frac{m_0}{m_c} = 1 + \frac{E_p}{3} \left(\frac{2}{E_g} + \frac{1}{E_g + \Delta} \right) - \frac{E_{p'}}{3} \left(\frac{2}{E(\Gamma_8^c) - E_g} + \frac{1}{E(\Gamma_7^c) - E_g} \right) + C. \quad (3.7)$$

Solving for A' gives

$$\frac{2m_0}{\hbar^2}A' \cong -\frac{E_{p'}}{3} \left(\frac{2}{E(\Gamma_8^c) - E_g} + \frac{1}{E(\Gamma_7^c) - E_g} \right) + C.$$
(3.8)

Zawadzki²⁸ defined $E_{p'} = 5.72$ eV (see Table III), and Hermann and Weisbuch defined C = -2 (in terms of $2m_0/\hbar^2$). This gives an estimate of A' = -14.70 eV Å². This is only an estimate, meaning that the sign and order of magnitude are probably the most one could hope to glean from this value, but it does illustrate the dependence of the other band parameters to changes in A' (see Table IV.) This is not to say that the other elements of *S* depend explicitly, or analytically, on A', but changing A' to a different constant value will force the other elements of *S* to change in order to produce the same observable set *T* by \mathbf{H}_T .

The elements of *S* can now be calculated as a set of parametric relations in *A*'. This was done by simply determining a set *S* for each of ten different arbitrary values of *A*' and then curve fitting the results for each element of *S*. The result is given below and assumes *A*' in units of eV $Å^2$,

$$\gamma_1^l = 6.6723 + 1.9027 \times 10^{-4} A',$$
 (3.9a)

$$\gamma_2^l = 1.8655 + 9.4762 \times 10^{-5} A',$$
 (3.9b)

$$\gamma_3^l = 2.6695 + 9.4762 \times 10^{-5} A',$$
 (3.9c)

$$E_p = 22.827 - 0.42760A',$$
 (3.9d)

$$C_0 = 0.12568 - 2.0881 \times 10^{-3} A',$$
 (3.9e)

$$B = 41.90 + 0.18978A'. \tag{3.9f}$$

The three parameters E_p , B, and C_0 are the most sensitive to changes in A' (see Appendix B and Table IV). The effective hole mass in the [011] direction has also been calculated and appears to be independent of the choice made for A'. The masses are $m_{\rm hh}^{011} = 0.593m_0$ and $m_{\rm h}^{011} = 0.0841m_0$. The data

given in Table IV and in Eqs. (3.9a)-(3.9f) provide a detailed description of the band-structure parameters for the eight-band $\mathbf{k} \cdot \mathbf{p}$ model discussed here. The original model was defined by seven independent parameters. The parametrization has now been reduced to one, A'. With the parameter values given in Eq. (3.9) and Table IV, the model now reproduces some of the best physical measurements made on effective mass and conduction band spin splitting.

IV. DISCUSSION

A. Kane nonparabolicity parameters

One of the most interesting results of this study is the dependence of α and β on matrix element B. Recall Eqs. (2.1) and (2.2), in order to determine α and β , a fourth order, in k, curve fit of the energy dispersion in two different directions must be performed. Then, α and β can be solved for by way of Eqs. (2.1) and (2.2). Table V lists the results of this calculation for four different high symmetry directions of the zinc-blende structure. The data corresponding to B=0 gives consistent results for α and β for all possible combinations of the four directions examined. The data for $B \neq 0$ produces inconsistent results for α and β . Only the data from the two main cubic axes, [001] and [111] produces a result that is consistent with Fig. 7, which illustrates how α and β vary with matrix element B. A maximum magnitude value for β occurs at B=0 and the curve shows a parabolic symmetry for $B \neq 0$. Therefore, we conclude that the fourth-order term of Eq. (2.1) neglects the lack of inversion symmetry of the zinc-blende structure as well as the k-dependent spin-orbit interaction which, in reality, has a

TABLE V. Fourth-order nonparabolicity parameter, $(\alpha + s\beta)k^4$, dependence on matrix element *B* (*A*'=0).

Directions	$B (eV Å^2)$	$\alpha \ ({\rm eV} \ {\rm \AA}^4)$	β (eV Å ⁴)
[001][011]	0	-1919.74	-1211.56
[001][111]	0	-1919.74	-1211.55
$[001][1\frac{1}{2}0]$	0	-1919.74	-1211.56
[011][111]	0	-1919.73	-1211.52
$[011][1\frac{1}{2}0]$	0	-1919.74	-1211.56
$[111][1\frac{1}{2}0]$	0	-1919.74	-1211.54
[001][011]	36	-1919.74	+74889.20
[001][111]	36	-1919.74	-410.58
$[001][1\frac{1}{2}0]$	36	-1919.74	+93714.19
[011][111]	36	+73380.06	-226309.92
$[011][1\frac{1}{2}0]$	36	+6446.94	+41422.56
$[111][1\frac{1}{2}0]$	36	+27041.75	-87294.98

TABLE VI. Final optimized values of the Kane nonparabolicity parameters α , β , γ and their dependence on A' and B, T=0 K.

$ \begin{array}{c} A' \\ (eV Å^2) \end{array} $	<i>B</i> (eV Å ²)	α (eV Å ⁴)	β (eV Å ⁴)	γ (eV Å ³)
0.0	0.0	-1919.86	-1211.56	0.0
0.0	41.90	-1919.86	-126.38	20.90
-14.70	39.11	-1827.17	-599.01	20.90

strong influence on the nonparabolicity of the conduction band (see Fig. 8). The results shown in Table VI are from calculations using the optimized band-structure parameters of Eq. (3.9). The first row of Table VI used the same data as the second row, except *B* was set to equal zero. The results in Table VI should be compared to the previous work done on determining α and β given in Table III. The data corresponding to A', B=0 seems to agree with the work done by Rössler.²⁴ The magnitude of α and β given here are smaller than those proposed by Rössler since the **k**-dependent spinorbit interaction was not taken into account (see Fig. 8), nor was *B* explicitly taken into account. Table VI suggests a smaller value for β than shown previously, since *B* cannot be zero (in order to account for conduction band spinsplitting data.) The third-order parameter, γ , is best calculated by determining the spin splitting of the conduction band and fitting to Eq. (2.1). This calculation produces consistent values of γ $(B \neq 0)$ for all directions of high symmetry. If *B* is set to zero, then γ will be zero. By examination of Fig. 8, It should be apparent that the matrix element C_0 , which accounts for the **k**-dependent spin-orbit coupling interaction, has a measurable effect on γ . Analytic expressions offered by other workers^{25,31,28} neglect this effect and produce varying results.

B. Valence band parameters

The valence band parameters are defined by Dresselhaus as^{38}

$$E_{\Gamma_8}(k) = Ak^2 \pm [B^2k^4 + C^2(k_x^2k_y^2 + k_y^2k_z^2 + k_z^2k_x^2)]^{1/2}.$$
(4.1)

Table VII lists a number of values by different authors. As a result of the work done here, we propose the following valence band parameters for T=0 K:

$$A = -6.672, \quad B = -3.731, \quad C^2 = 43.75$$

TABLE VII. Valence Danu parameters for GaA	TABLE VII.	Valence	band	parameters	for	GaAs
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Source	-A	-B	C^2	Temp (K)	Method
This work	6.67	3.73	43.75	0	A'=0
	6.67	3.73	43.72	0	A' = -14.70
Skolnick et al. (Ref. 60)	6.98	4.4	38.4	50-77	CR^{a}
Vrehen (Ref. 57)	7.2	5	0	77	MOA ^b
Seisyan et al. (Ref. 58)	7.183	4.88	12.82	77	MOA ^b
Balslev (Ref. 59)	6.77	4.55	37.45	$T \leq 100$	PT^{c}
	7.13	4.98	39.56	$T \ge 200$	
Cardona (Ref. 79)	5.5	4.5	-1	0	five level k · p ^d
Pollak et al. (Ref. 80)	7.39	4.93	25.7	0	five level k ∙p
Bowers and Mahan (Ref. 29)	5.80	2.43	27.7	0	$15 \times 15 \mathbf{k} \cdot \mathbf{p}^{e}$
Lawaetz (Ref. 23)	7.65	4.82	59.40	0	five level $\mathbf{k} \cdot \mathbf{p}^{f}$
Miller et al. (Ref. 63)	6.79	3.84	*	77	QWT ^g
Hess et al. (Ref. 61)	6.85	4.20	48.0	5	HFMR ^h
Yamanaka et al. (Ref. 62)	5.64	2.70	*	295	PCS ⁱ
Shanabrook et al. (Ref. 64)	6.8	3.8	46.1	10	ERS ^j
Eppenga et al. (Ref. 18)	7.06	4.43	49.5	295	$8 \times 8 \mathbf{k} \cdot \mathbf{p}^{k}$
Mears and Stradling (Ref. 73)	6.80	4.69	*	50	CR ¹

^aCyclotron resonance, 337 μ m and 2.2 mm.

^bInterband magneto-optic absorption.

^cPiezotransmission.

 ${}^{d}T_{d}$ symmetry wave functions approximated by antisymmetric perturbing potential applied to diamond structure.

^eMatrix elements evaluated by zinc-blende pseudopotential.

^fSemiempirical model, considers the dependence of matrix elements on lattice constant, ionicity, and *d*-electron shells.

^gQuantum well transitions, square and parabolic GaAs/Al_{0.3}Ga_{0.7}As, $L_w = 51 - 521$ Å.

^hHigh field magnetoreflectance of excitons.

ⁱPhotocurrent spectroscopy of GaAs/Al_{0.34}Ga_{0.66}As quantum wells.

^jElectronic Raman scattering, GaAs/Al_{0.3}Ga_{0.7}As quantum wells, $L_w = 100 - 400$ Å.

^kApplied to GaAs/Al_{0.25}Ga_{0.75}As quantum wells.

¹Cyclotron resonance, 155 GHz, high purity epitaxial films.

This result is virtually independent of the choice made for A'. There should be no confusion between matrix element B and valence band parameter B. The above valence band parameters were calculated from the Luttinger parameters given in Table IV (also see Appendix C.) It should be no surprise that the parameters given above are very close to those of Shanabrook and co-workers⁶⁴ and Miller and co-workers,⁶³ since it was their values for effective hole masses that were used in the optimization, but take note that there is some difference.

C. Momentum matrix element energy E_p

Table III lists some of the previous work done in the determination of E_p . A comparison with the values obtained here in Table IV shows that E_p varies between 22.827 eV for A'=0 and 29.112 eV for A'=-14.70. This range encompasses all but one of the previously obtained values in Table III. Zawadzki²⁸ used a five-level $\mathbf{k} \cdot \mathbf{p}$ to obtain $\gamma = 20.7$ eV Å³ and $E_p = 28.9$ eV, both of which are close to the values obtained here for A' = -14.70. The work done which ignores A' or its equivalent produces values of E_p around 22 to 23 eV, while the work that took A' or its equivalent into account obtained values of E_p that are 25 eV or greater.

V. SUMMARY

We have fit the matrix elements of an eight-band $\mathbf{k} \cdot \mathbf{p}$ model for the zinc-blende structure of GaAs to experimental data on effective masses and conduction band spin splitting. This model is now parametrized by only one matrix element, A', and reproduces reliably measured values for effective masses and the conduction band spin splitting of GaAs. Future work will involve the definition of the final matrix element by further analysis of reliable experimental data. The data already available for the nonparabolicity parameters, α and β , are too model dependent and varied to determine A'. It was found that the fourth-order conduction band dispersion terms are greatly influenced by matrix elements Band C_0 . The effective masses also showed a strong sensitivity to C_0 . This model is well suited for the theoretical examination of semiconductor heterostructures.

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APPENDIX A: T_d SYMMETRY BASIS FUNCTIONS

The class-A states as basis functions for the $\{\Gamma_6, \Gamma_7, \Gamma_8\}$ irreducible representations of the T_d double group are given by³⁰

$$u_{-1/2}^{\Gamma_6} = |s\rangle \chi_{\downarrow}, \qquad (A1a)$$

$$u_{1/2}^{\Gamma_6} = |s\rangle \chi_{\uparrow},$$
 (A1b)

$$u_{-3/2}^{\Gamma_8} = \frac{-i}{\sqrt{6}} [|x\rangle + i|y\rangle] \chi_{\downarrow} + i \sqrt{\frac{2}{3}} |z\rangle \chi_{\uparrow}, \qquad (A1c)$$

$$u_{-1/2}^{\Gamma_8} = \frac{i}{\sqrt{2}} [|x\rangle + i|y\rangle] \chi_{\uparrow}, \qquad (A1d)$$

$$u_{1/2}^{\Gamma_8} = \frac{-i}{\sqrt{2}} [|x\rangle - i|y\rangle] \chi_{\downarrow}, \qquad (A1e)$$

$$u_{3\backslash 2}^{\Gamma_8} = \frac{i}{\sqrt{6}} [|x\rangle - i|y\rangle] \chi_{\uparrow} + i \sqrt{\frac{2}{3}} |z\rangle \chi_{\downarrow}, \qquad (A1f)$$

$$u_{-1/2}^{\Gamma_7} = \frac{-i}{\sqrt{3}} [|x\rangle - i|y\rangle] \chi_{\uparrow} + \frac{i}{\sqrt{3}} |z\rangle \chi_{\downarrow}, \qquad (A1g)$$

$$\mu_{1/2}^{\Gamma_7} = \frac{-i}{\sqrt{3}} [|x\rangle + i|y\rangle] \chi_{\downarrow} - \frac{i}{\sqrt{3}} |z\rangle \chi_{\uparrow} .$$
 (A1h)

APPENDIX B: DEFINITION OF THE KANE MATRIX ELEMENTS

1

The Kane matrix elements that make up Eq. (1.3) are defined as follows:

$$A' = \frac{\hbar^2}{m_0^2} \sum_{nj} \frac{\left| \langle s | p_x | n \Gamma_5 j \rangle \right|^2}{E_c - E_{n, \Gamma_5}}, \qquad (B1a)$$

$$B = 2\frac{\hbar^2}{m_0^2} \sum_{nj} \frac{\langle s|p_x|n\Gamma_5 j\rangle \langle n\Gamma_5 j|p_x|z\rangle}{(E_c + E_v)/2 - E_{n,\Gamma_5}}, \qquad (B1b)$$

$$M = H_1 + H_2, \tag{B1c}$$

$$L' = F' + 2G, \tag{B1d}$$

$$N' = F' - G + H_1 - H_2,$$
 (B1e)

$$P_0 = -i\frac{\hbar}{m_0} \langle s | p_x | x \rangle, \qquad (B1f)$$

$$G = \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_3 j\rangle|^2}{E_v - E_{n,\Gamma_3}},$$
 (B1g)

$$F' = \frac{\hbar^2}{m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_1 j\rangle|^2}{E_v - E_{n,\Gamma_1}},$$
 (B1h)

$$H_1 = \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_5 j\rangle|^2}{E_v - E_{n,\Gamma_5}},$$
 (B1i)

$$H_2 = \frac{\hbar^2}{2m_0^2} \sum_{nj} \frac{|\langle x|p_x|n\Gamma_4j\rangle|^2}{E_v - E_{n,\Gamma_4}}.$$
 (B1j)

The above sums involving $|n\Gamma j\rangle$ terms run over the single group class-*B* states of the indicated irreducible representation. The notation used for the irreducible representations is that of Koster-Dimmock-Wheeler-Statz,⁷⁵ see Bahder³⁰ and Bir and Pikus⁴⁵ for more information.

APPENDIX C: LUTTINGER PARAMETERS AND VALENCE BAND PARAMETERS

The standard Luttinger parameters are defined from the Dresselhaus³⁸ $\mathbf{k} \cdot \mathbf{p}$ matrix elements, (L, M, N) as follows:

$$\gamma_1^l = -\frac{2m_0}{3\hbar^2}(L+2M) - 1,$$
 (C1a)

$$\gamma_2^l = -\frac{m_0}{3\hbar^2}(L-M),$$
 (C1b)

$$\gamma_3^l = -\frac{m_0}{3\hbar^2}N.$$
 (C1c)

The modified Luttinger parameters are defined from the Kane^{31,70} $\mathbf{k} \cdot \mathbf{p}$ matrix elements, (L', M, N') as follows:

$$\gamma_1 = -\frac{2m_0}{3\hbar^2}(L'+2M) - 1,$$
 (C2a)

$$\gamma_2 = -\frac{m_0}{3\hbar^2}(L' - M),$$
 (C2b)

$$\gamma_3 = -\frac{m_0}{3\hbar^2}N'. \tag{C2c}$$

The difference between these two developments is that Kane used a $\{|s\rangle, |x\rangle, |y\rangle, |z\rangle\}$ manifold for his class-A states, while Dresselhaus used a $\{|x\rangle, |y\rangle, |z\rangle\}$ manifold. The two are related by

$$\gamma_1^l = \gamma_1 + \frac{E_p}{3E_g + \Delta},\tag{C3a}$$

$$\gamma_2^l = \gamma_2 + \frac{1}{2} \frac{E_p}{3E_g + \Delta},\tag{C3b}$$

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 $\gamma_3^l = \gamma_3 + \frac{1}{2} \frac{E_p}{3E_p + \Delta}, \qquad (C3c)$

where

$$F = F' + \frac{P_0^2}{E'_v - E_c}, \quad E'_v = E_v - \frac{\Delta}{3}, \quad (C4)$$
$$L = F + 2G,$$
$$N = F - G + H_1 - H_2.$$

The Dresselhaus^{38,53} valence band parameters are defined as follows.

$$A = \frac{1}{3}(L+2M) + \frac{\hbar^2}{2m_0},$$
 (C5a)

$$B = \frac{1}{3}(L - M), \tag{C5b}$$

$$C^{2} = \frac{1}{3} [N^{2} - (L - M)^{2}].$$
 (C5c)

The standard Luttinger parameters are related to the valence band parameters by

$$\gamma_1^l = -A \quad (A < 0), \tag{C6a}$$

$$\gamma_2^l = -\frac{1}{2}B$$
 (B<0), (C6b)

$$(\gamma_3^l)^2 = \frac{1}{12}(C^2 + 3B^2),$$
 (C6c)

$$C^{2} = 12[(\gamma_{3}^{l})^{2} - (\gamma_{2}^{l})^{2}].$$
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