

Spring 5-31-2011

g-factors for ternary crystals of groups iii and v

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ABSTRACT

g-FACTORS FOR TERNARY CRYSTALS OF GROUPS III AND V

**by
Liviu Mateescu**

The objective of this thesis is to present a method of calculating the g-factors of ternary crystals of III-V group elements.

There is an increasing interest in knowing the magnetic behavior of different semiconductor materials, due to advances in the domain of spintronics. The g-factors were calculated for the conduction electrons, since they have the greatest contribution to the magnetic properties of the crystal. The thesis presented here proposes a method to calculate the magnetic g-factor of whole families of crystals made of three elements, of the form $A_{1-x}B_xC$, for eleven values, $x \in \{0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1\}$, that were considered sufficient for giving an accurate behavior of the magnetic properties of the conduction electrons.

The notion of g-factor is presented and then methods are shown that permit the calculation of the g-factor in cubic crystals. The algorithm is then applied to binary crystals and the results of calculations are compared to the scarce measurement data found in literature.

Finally, relying on a series of papers that approximate the lattice parameters for ternary III-V crystals (cubic determination), the g-factor is calculated for the families of $A_{1-x}B_xC$ for the x values mentioned above, and recommendations are given for an eventual enhancement of the precision.

The method presented here is but a first approximation, that is considered good enough for applications in the spintronics of the cubic crystals.

**g-FACTORS FOR TERNARY CRYSTALS
OF GROUPS III AND V**

**by
Liviu Mateescu**

**A Thesis
Submitted to the Faculty of
New Jersey Institute of Technology
in Partial Fulfillment of the Requirements for the Degree of
Master of Science in Physics**

Department of Applied Physics

May 2011

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APPROVAL PAGE

g-FACTORS FOR TERNARY CRYSTALS OF GROUPS III AND V

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2. Mateescu, L., Buna, D., *Radiation Protection in Radiology, a teaching guide for health science professionals*. Approved by the American Medical Association, May, 2001 and by the American Society of Radiologic Technologists, August 1999. Reference No. NJZ0189003.
3. Racolta, P.M., PopaSimil, L., Alexandreanu, B., Mateescu, L., *Thin layer activation-based evaluation of tribological behavior of light ion-implanted metallic samples*, Nuclear Instruments and Methods in Physics Research Section B, MAY 1997; v.127, p.949-953 Conference: 10th International Conference on Ion Beam Modification of Materials (IBMM-96); September 1-6, 1996; ALBUQUERQUE, NM
4. Mateescu, L., *Algorithm for interpolating data in m-dimensional spaces with polynomials of variable degree*. Bulletin of Geodynamics Institute, Bucharest, December 1999.

ACKNOWLEDGMENT

I wish to express my gratitude to my Thesis Advisor, Dr. Nuggehali Ravindra, for his continuous advice and support. I also thank the members of the Committee, for their time. I am indebted in particular to Dr. Vitaly Shneidman, whose lectures were always a challenge and a pleasure to attend to. I am thankful at the same time to the entire faculty in the Physics Department of NJIT and of Rutgers-Newark, whose dedication for Physics is exemplary.

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Chapter 1

INTRODUCTION

1.1 Objective

The objective of this study is to present a method of calculating the g-factors of ternary crystals of III-V group elements. A method is found that calculates the lattice parameters of $A_{1-x}B_xC$ cubic crystals and then the g-factor of these crystals is calculated for x sweeping the interval [0,1] with a step of 0.1, which is considered sufficient.

1.2 Defining the g-factor

Any quantum particle, be it considered simple, like an electron, or complex, such as a nucleus, has an associated magnetic moment $\boldsymbol{\mu}$, which characterizes the interaction of the said particle with an external magnetic field \mathbf{B} . The corresponding interaction energy between the magnetic moment and the external applied magnetic field is well known: $W = -\boldsymbol{\mu} \cdot \mathbf{B}$. Therefore, the magnetic moment is essential in defining the intensity of magnetic interactions.

Magnetic moments are quantized and there is always a common factor that appears in all their expressions for given families of particles. For example, in all magnetic moments associated with electrons, no matter the physical system they are a part of, the common factor (in International System), is

$$\mu_B = \frac{e\hbar}{2m_e} \quad (1.1)$$

where e is the elementary charge of the electron, \hbar is the reduced Planck constant, and m_e is the rest mass of the electron. The quantity defined above is called Bohr's magneton.

Similarly, where particles of a nucleus are involved, a common factor appears that is called *nuclear magneton*.

Therefore, the need has arisen to characterize the magnetic moment of a particle by a dimensionless number. If one takes a free electron, which is characterized by the spin quantum number, then its total magnetic moment will be

$$\bar{\mu}_s = g_e \mu_B \frac{\bar{S}}{\hbar} \quad (1.2)$$

where the vector \mathbf{S} is the spin angular momentum of the electron. The above relation is the definition of the (spin) g-factor of the electron, also called the gyromagnetic ratio of a particle. If the expression of Bohr's magneton is plugged in (1.2), then one sees that, after a projection on the Oz axis is made, g_e takes the value -2, since the spin number of the electron is $\pm \frac{1}{2}$.

All electron systems can have their own characteristic g-factor. For example, there is an orbital g-factor μ_L which characterizes the magnetic momentum of an electron strictly with respect of its orbital movement:

$$\bar{\mu}_L = g_L \mu_B \frac{\bar{L}}{\hbar} \quad (1.3)$$

and since the spin momentum and the orbital momentum can be added, respecting the composition rules for spins, there is also a gyromagnetic factor characterizing the electron in an atom:

$$\bar{\mu} = g_J \mu_B \frac{\bar{J}}{\hbar} \quad (1.4)$$

where \mathbf{J} is the total angular momentum of the electron ($\mathbf{J}=\mathbf{L}+\mathbf{S}$). g_J is also called the Landé g-factor, in honor of the first physicist who studied it. An intuitive presentation of the g-factor as studied by Landé can be found in [1].

1.3 The importance of g-factors

First and foremost, the importance of the g-factor resides in the fact that knowing it means knowing the effects within a system that is submitted to an external magnetic field. One of the main applications is in spintronics devices design.[8]

Spintronics is a multidisciplinary field, the main denominator of which is “the active manipulation of spin degrees of freedom in solid-state systems” (quoted from the above-mentioned reference).

Among the many uses, actual and potential, of spintronics, one can enumerate “giant magnetoresistive materials”, magnetic tunnel junction materials, magnetic sensors, spintronic couplers, and magnetic RAM (Random Access Memory). All these promise to be more efficient than the existing devices performing similar tasks (faster, more sensitive, tougher, more reliable).[9].

By control of the spin it is understood controlling either the population and the phase of the spin of an ensemble of particles, or a coherent spin manipulation of a single-spin or a few-spin system. The field has only very recently taken momentum, because only in 2001 a method was devised for spin-injecting of electrons at room temperature, according to [10].

Chapter 2

THE G-FACTOR CALCULATION,

WITH APPLICATION TO III-V BINARY CRYSTALS.

2.1 Band structure calculations with the k.p method

The k.p method is the instrument of choice for calculating band structure parameters, because it is the most convenient in finding band dispersion, effective masses and g-factors around the high-symmetry points, especially Γ point.

If a Bloch function $\Phi_{nk} = e^{i\vec{k} \cdot \vec{r}} u_{nk}(\vec{r})$ is introduced in the Schrödinger one-electron equation, the new equation in u_{nk} will become:

$$\left(\frac{p^2}{2m} + \frac{\hbar \vec{k} \cdot \vec{p}}{m} + \frac{\hbar^2 k^2}{2m} + V \right) u_{nk} = E_{nk} u_{nk} \quad (2.1)$$

For $k=0$, equation (2.1) simplifies significantly:

$$\left(\frac{p^2}{2m} + V \right) u_{n0} = E_{n0} u_{n0} \quad (2.2)$$

This equation is relatively easy to solve, since u_{n0} are periodic. Equation (2.2) will provide a set of eigenvalues E_{n0} and a complete orthogonal set of eigenfunctions u_{n0} , which will be the basis for perturbation calculations, where the perturbations will be $\frac{\hbar \vec{k} \cdot \vec{p}}{m}$ and $\frac{\hbar^2 k^2}{2m}$. This is the essence of the k.p method.

An application of the method is calculating the effective mass of a non-degenerate band, which is the case for most direct-gap semiconductors at the minimum of the conduction band:

Let E_{n0} be a stationary value of the energy, that is $\left. \frac{\partial E}{\partial k} \right|_{E=E_{n0}} = 0$, and let non degeneracy

occur at this value. Then, the unperturbed functions and energies are known, the perturbation theory gives:

$$u_{nk} = u_{n0} + \frac{\hbar}{m} \sum_{n \neq n'} \frac{\langle u_{n0} | \vec{k} \cdot \vec{p} | u_{n'0} \rangle}{E_{n0} - E_{n'0}} u_{n'0} \quad (2.3)$$

and also

$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2} \sum_{n \neq n'} \frac{|\langle u_{n0} | \vec{k} \cdot \vec{p} | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}} \quad (2.4)$$

But since $\left. \frac{\partial E}{\partial k} \right|_{E=E_{n0}} = 0$, the term linear in k will disappear, and therefore, at least around $k=0$, one

can write:

$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*} \quad (2.5)$$

m^* is by definition the effective mass of the electron in the given band.

By comparing (2.4) and (2.5), a general expression for m^* can be deduced:

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2} \sum_{n \neq n'} \frac{|\langle u_{n0} | \vec{k} \cdot \vec{p} | u_{n'0} \rangle|^2}{E_{n0} - E_{n'0}} \quad (2.6),$$

which is further processed. But conclusions can be drawn already, the most important being that the contribution of another band is determined by $E_{n0} - E_{n'0}$ (the closer the band, the bigger its influence).

Lower bands will contribute with a positive term, making $1/m^*$ bigger, and therefore m^* smaller than m_0 (the mass of the free electron). The contribution of upper bands is negative, and m^* can even become negative.

Symmetry reasons limit the number of mixed elements for the lowest conduction band in direct gap semiconductors. Here the only significant interaction is with the nearest valence band Γ_{4v} , and the approximate value of the effective mass is given by

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2} \frac{|\langle \Gamma_{1c} | \vec{k} \cdot \vec{p} | \Gamma_{4v} \rangle|^2}{E_0} \quad (2.7)$$

Here E_0 is the direct band gap. Moreover, the Γ_{4v} functions are denoted $|X\rangle$, $|Y\rangle$ and $|Z\rangle$, in an analogy with the p-type orbitals, and the only non-zero elements in (2.7) are

$$\langle X | p_x | \Gamma_1 \rangle = \langle Y | p_y | \Gamma_1 \rangle = \langle Z | p_z | \Gamma_1 \rangle = iP \quad (2.8)$$

P is specific for each crystal of such qualities. However, for most semiconductors of group IV or binary III-V and II-VI crystals, P is remarkably constant.

The value $E_p = 2P^2/m$ has a value that is around 20 eV, and the expression of the effective mass takes the simple form of:

$$\frac{m}{m_c^*} = 1 + 2 \frac{P^2}{E_0} \quad (2.9)$$

Here the subscript “c” shows that the expression is solely valid for the (lower) conduction band.

2.2 Examples of calculations of g-factors in bulk semiconductors using 3- and 5- band models

The theory in the precedent paragraph holds for most of the direct bandgap semiconductors. As stated, the formulae (2.8) and (2.9) are valid in the hypothesis that the only influence on the conduction band comes from the upmost valence band. That is, a three-band model of a band structure was used.

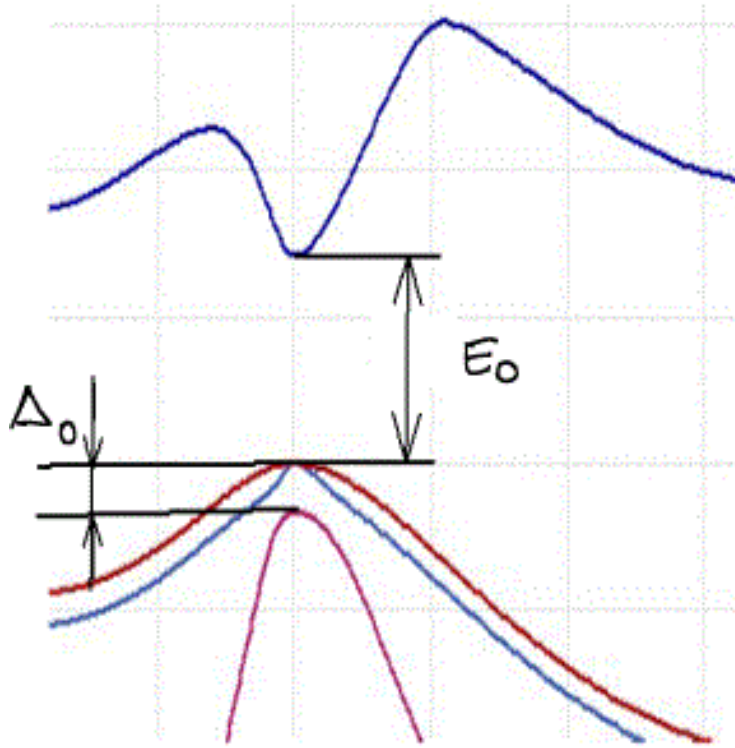


Figure 2.1. Typical 3-band model for a direct gap semiconductor.

Δ_0 is the relativistic spin-orbit split, and E_0 is the bandgap.

A direct consequence of this model is the expression of g^* for the first conduction band [14]. Applying a constant magnetic field to the crystal, in the approximation of the effective mass, the Schrödinger equation will have the following form:

$$\frac{\hbar^2}{2m_1}(\vec{p} + \frac{e\vec{A}}{c})\psi_1(\vec{r}) = (E_1 - E_{10})\psi_1(\vec{r}) \quad (2.10)$$

where \mathbf{A} is the magnetic vector potential, which will be chosen as

$$A_x = A_z = 0, A_y = -Hx.$$

Then, the energies and the wave functions will be the solutions of a set of coupled Schrödinger-like equations:

$$\sum_j [E_{j0} - E] \delta_{ij} \psi_j(\vec{r}) + \vec{P} \cdot (1/m^*)_{ij} \cdot \vec{P} \psi_j(\vec{r}) = 0 \quad (2.11)$$

where

$$(1/m^*)_{ij} = \frac{1}{m} \delta_{ij} \mathbb{I} + \frac{\hbar^2}{m^2} \sum_{\mu \neq i,j} \frac{\pi_{i\mu} \pi_{\mu j}}{E_{j0} - E_{\mu 0}} \quad (2.12)$$

Here

$$\pi_{i\mu} = \int u_{i0}(\vec{r}) [\vec{P} - \frac{\hbar^2}{4m} (\nabla V \times \sigma)] u_{\mu 0}(\vec{r}) d\vec{r} \quad (2.13),$$

due to the choice (which doesn't cancel its generality) of the magnetic field, and the fact that the general form of the Hamiltonian matrix element (in effective mass model) is

$$H_{ij} = \frac{1}{2} \vec{P} \cdot (1/m^*)_{ij} \cdot \vec{P} \delta_{ij} + \frac{1}{2} \mu_B \sigma_{ij} \cdot g \cdot \vec{H} \quad (2.14)$$

In this 2x2 effective mass Hamiltonian, μ_B is Bohr's magneton, the quantity $\frac{1}{2} \mu_B \sigma_{ij} \cdot g$ represents the magnetic moment of the electron, and g is a tensor supposed not to be influenced by the intensity \mathbf{H} of the applied magnetic field.

All one needs to do is identify the terms linear in \mathbf{H} . For the general case, this will have the form

$$\sigma_{ij} \cdot g = 4(s)_{ij} + \frac{2\hbar^2}{m^2} \sum_n \frac{\pi_{in} \times \pi_{ni}}{E_{0n}} \quad (2.15)$$

In the case of the spherical orbitals, the g tensor becomes a diagonal one, and the second term, after approximating \mathbf{P} with \mathbf{p} , the known expression is drawn:

$$\text{besides} \quad \frac{1}{2m^*} = \frac{1}{2m} + \frac{\hbar^2}{m^2} \sum_{n \neq 0} \frac{|p_{0n}^x|^2}{E_0 - E_{0n}} \quad (2.16),$$

one will have the expression of the magnetic moment of the electron:

$$\mu = \frac{e\hbar}{2m} + \frac{e\hbar}{2m^2} \frac{1}{i} \sum_{n \neq 0} \frac{p_{0n}^x p_{n0}^y - p_{0n}^y p_{n0}^x}{E_0 - E_{n0}} \quad (2.17)$$

After the Bohr magneton is factorized and expressing the matrix elements in the usual atomic orbitals X, Y, Z, the classical expressions appear:

$$\frac{1}{2m^*} = \frac{1}{2m} + \frac{1}{m^2} \frac{3E_g + 2\Delta_0}{3E_g(E_g + \Delta_0)} \left| \langle S | p_x | X \rangle \right|^2 \quad (2.18)$$

and

$$g = 2 \left(1 - \frac{\Delta_0}{3E_g(E_g + \Delta_0)} \left| \langle S | p_x | X \rangle \right|^2 \right) \quad (2.19)$$

or

$$g^* = 2 - \frac{2}{3} P^2 \frac{\Delta_0}{E_0(E_0 + \Delta_0)} \quad (2.20)$$

In the above-quoted paper, the relationship between the g-factor and the effective mass was first rigorously mentioned:

$$\frac{g^*}{g_0} = 1 - \frac{\Delta_0}{3E_0 + 2\Delta_0} \left(\frac{m_0}{m^*} - 1 \right) \quad (2.21)$$

This formula offers a good approximation of the g-factor for certain semiconductors, generally within 10% to the measured values, but for others the difference is very substantial; even the sign might be different between 3-band model and the measured value. In [15] the conclusion was taken that in formulae (2.3) and (2.6) supplementary terms must be taken into consideration, because the upper conduction bands Γ_8 and Γ_7 influence the lower conduction band at Γ_1 point. Thus a 5-band model was used.

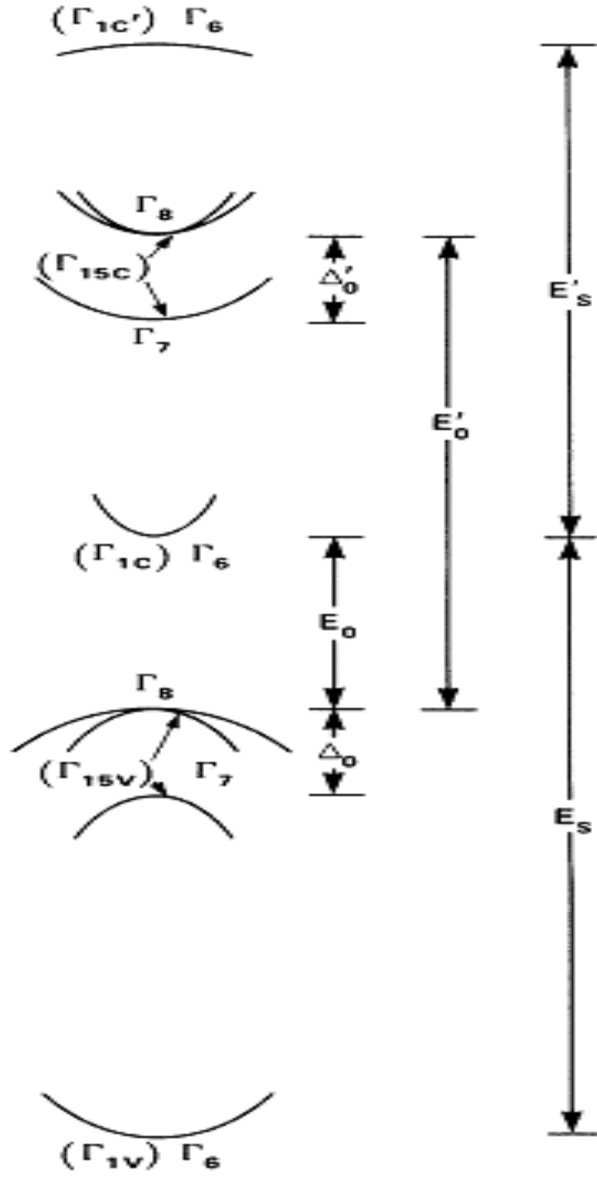


Figure 2.2 The 5-band model, used in [16]

A correction term was introduced, implying the existence of a parameter λ^2 , besides the band parameters visible in the figure above, and the P^2 interband term.

$$g^* = 2 - \frac{2}{3} P^2 \left(\frac{\Delta_0}{E_0(E_0 + \Delta_0)} + \lambda^2 \frac{\Delta'_0}{(E'_0 - E_0)(E'_0 - E_0 - \Delta'_0)} \right) \quad (2.22)$$

The term λ^2 can be found indirectly, since it is also present in the effective mass calculated by the 5-band model:

$$m / m^* = 1 + \frac{P^2}{3} \left(\frac{3E_0 + 2\Delta_0}{E_0(E_0 + \Delta_0)} - \lambda^2 \frac{3(E'_0 - E_0) - 2\Delta'_0}{(E'_0 - E_0)(E'_0 - E_0 - \Delta'_0)} \right) \quad (2.23)$$

The equation (2.23), which is an enhanced form of (2.21), is solved for λ^2 and the result is plugged in (2.22). Since the energies and the spin-orbit splits are generally known, and m^* is also known, the only imponderable is P^2 , the value of which is universally considered between 20 and 30, and very seldom bigger than 23.

The next table contains calculations of g^* using the 3-band and the 5-band model, compared with the measured values of g -factor for the first conduction band.

Table 2.1 Values of g -factor, calculated and measured, for binary crystals

	m^*/m_0	E_g	Δ_0	E'_0	Δ'_0	P^2	Calculated g^*		Measured g -factor
							3-band	5-band	
GaAs	0.066	1.519	0.341	4.659	0.171	29	-0.333	-0.48	-0.44
GaSb	0.045	0.81	0.8	3.69	0.25	23.93	-7.79	-8.4	-9.3
InP	0.08	1.42	0.11	5.66	0.41	19.50	+1.34	+1.21	+1.26
InAs	0.024	0.42	0.38	4.58	0.42	21.36	-14.104	-14.26	-14.7
InSb	0.0137	0.237	0.81	3.78	0.41	23.89	-49.99	-50.22	-51.4
AlP	0.272	5.12	0.05	5.18	0.03	22	1.972	-79 ^b	^f
AlAs	0.22	3.06	0.28	4.66	0.18	22	1.598	1.133	^f
AlSb	0.18	2.3	0.75	4.73	0.48	22	0.43	-0.16 ^c	^f
GaP	0.17	2.87	0.08	5.33	0.5	22	+1.86	+1.25 ^d	^f
GaN	0.625	3.62	-0.01	9.12	?	22	2.004	2.011	1.95 ^g
BN	0.752	5.9	0.021	13 ⁱ	0.008	23	1.991	1.990	^f
BP	^f	2.1	0.041	12 ⁱ	0.08	23	1.860	1.734	^f
BAs ^h	^f	1.25	0.216	1.75 ⁱ	0.086	23	+0.19	-2.37	^f
BSb	^f	0.527	0.366	^f	0.146	23	-9.92	-12.46 ^j	
ZnSe*	0.16	2.79	0.45	8.62	0.45	23	1.236	1.195	1.06-1.22
ZnTe*	0.12	2.39	0.93	5.85	0.45	23	+0.2	-0.06	-0.4
CdTe*	0.09	1.6	0.927	6.01	0.4	18.5	-0.827	-0.939	-1.65 ^k

*II-VI crystals in the zinc-blende system.

^f The value is not listed in Landold-Bornstein database or other sources.

^g Value listed in Landold-Bornstein database.

^h Very indirect bandgap. The approximations in the algorithm probably don't hold.

ⁱ Extrapolated from the band structure in LB database.

^j Incomplete, since E_0' is missing. Very scarce data for this substance.

^k The values of g_c in LB database are between -2.2 and -0.75. In paper [17] the -1.12 value is given.

^b The case of AIP is known in literature, and the algorithm is considered imprecise in this particular case, because E_0 and E_0' have very close values, as it is visible in the band structure of AIP (Source, LB database):

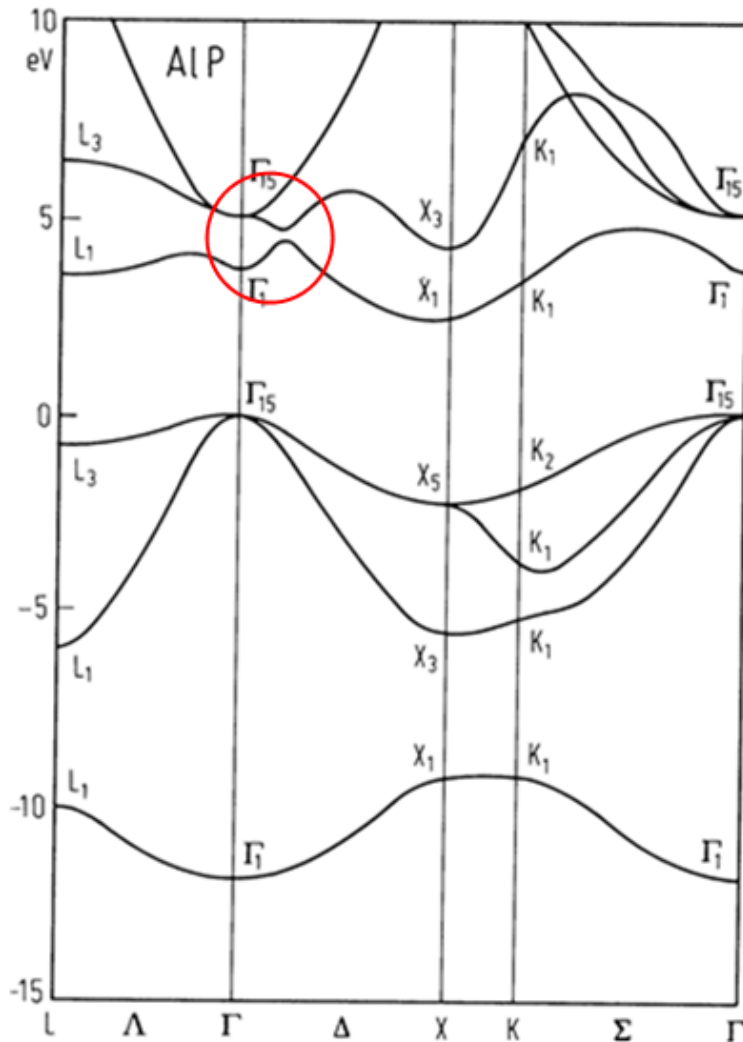


Figure 2.3 Band structure of AIP (calculated with an orthogonalized LCAO method).

As an observation, for positive g -factors, the 3-band and the 5-band methods give very similar results, and where there are data available, both values are in good agreement with the measured values. However, for negative g^* , a great discrepancy may appear between the two methods (but not necessarily). The 5-band model prevails in this case, with the notable exception of AlP.

Chapter 3

THE g-FACTORS of TERNARY III-V CRYSTALS

3.1 Results

The previous chapters' aim was to find and justify the validity of formulae (2.22) and (2.23).

The compounds of the type $A_{1-x}B_xC$ are in theory of an infinite variety, and all their band parameters cannot be found in databases. However, correlations exist between the x parameter and the band parameters of the compound, which can be calculated. Subsequently, the g -factor can be calculated as for the bulk materials. A similar method can be used for quaternary compounds of the type $A_{1-x}B_xC_{1-y}D_y$, though in this case there is no universal valid method to calculate the band parameters from x and the band parameters of the components.

In treating the g -factor for ternary and compounds, we will rely heavily on [25] and on the Landolt-Börnstein database, and also on the interpolation methods found in [17].

The real difficulty consists of interpolating the values of the parameters used in the formulae giving g^* . Where no method of finding the parameters as a function of x exists, a linear increase was postulated. A justification, at least for the dimensional parameters, can be seen in the observation that follows:

Families of binary crystals were analyzed from the point of view of the dependency of the lattice constant.

Crystal	Z1	Z2	Z1 + Z2	a_0 (Angstrom)
GaAs	31	33	64	5.65
GaSb	31	51	82	6.095
InP	49	15	64	5.86
InAs	49	33	82	6.05
InSb	49	51	100	6.479
AlP	13	15	28	5.467
AlAs	13	33	46	5.66
AlSb	13	51	64	5.35
GaP	31	15	46	5.45
GaN	31	7	38	4.52
BAs	5	33	38	4.77
BN	5	7	12	3.61
BP	5	15	20	4.538
BSb	5	51	56	5.12
InN	49	7	56	4.98

III	B	5
	Al	13
	Ga	31
	In	49
V	N	7
	P	15
	As	33
	Sb	51

Table 3.1 The lattice parameter dependence of the atomic number in binary crystals.

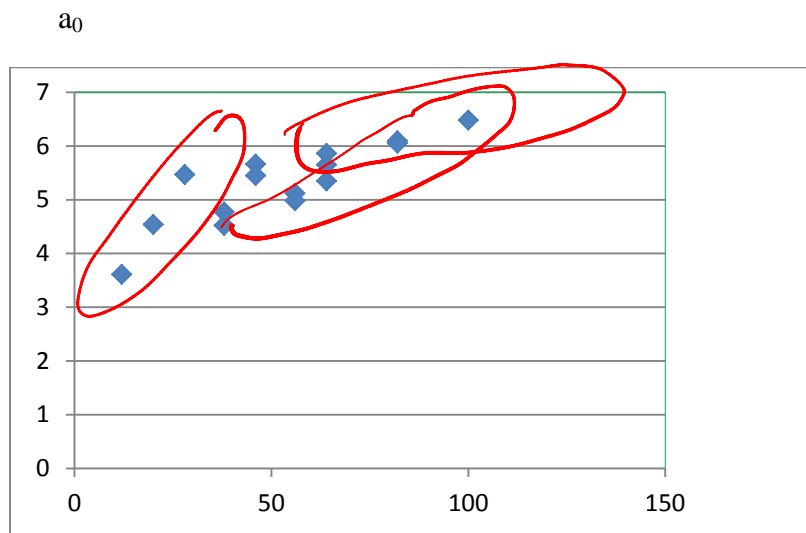


Figure 3.1
Dependency between
the atomic number and
the lattice parameter

A linear dependency is evident between the total atomic number and the lattice constant.

Where it was possible, interpolation parameters found in [25] were used. Where such interpolations do not exist in literature, a linear interpolation was performed.

Parameters were interpolated and the formulae for the g-factor of a cubic crystal were applied. The results are synthesized for families of $A_{1-x}B_xC$ ternary crystals.

Table 3.2 Band parameters of AlGaAs

x	Crystal	E_0	Δ_0	P^2	E_{0p}	Δ_{0p}	λ^2	g (3band)	g(5 band)
0	GaAs	1.519	0.341	29	4.569	0.171	0.4	-0.3334	-0.484
0.1		1.67274	0.3349	28.3	4.5781	0.1719	0.4	0.118535	-0.04481
0.2		1.8056	0.3288	27.6	4.5872	0.1728	0.4	0.430171	0.25491
0.3		1.92544	0.3227	26.9	4.5963	0.1737	0.4	0.663076	0.476256
0.4		2.04012	0.3166	26.2	4.6054	0.1746	0.4	0.849843	0.650932
0.5		2.1575	0.3105	25.5	4.6145	0.1755	0.4	1.008678	0.795786
0.6		2.28544	0.3044	24.8	4.6236	0.1764	0.4	1.149719	0.918919
0.7		2.4318	0.2983	24.1	4.6327	0.1773	0.4	1.278107	1.022267
0.8		2.60444	0.2922	23.4	4.6418	0.1782	0.4	1.395779	1.102211
0.9		2.81122	0.2861	22.7	4.6509	0.1791	0.4	1.502754	1.147868
1	AlAs	3.06	0.28	22	4.66	0.18	0.4	1.59819	1.1334

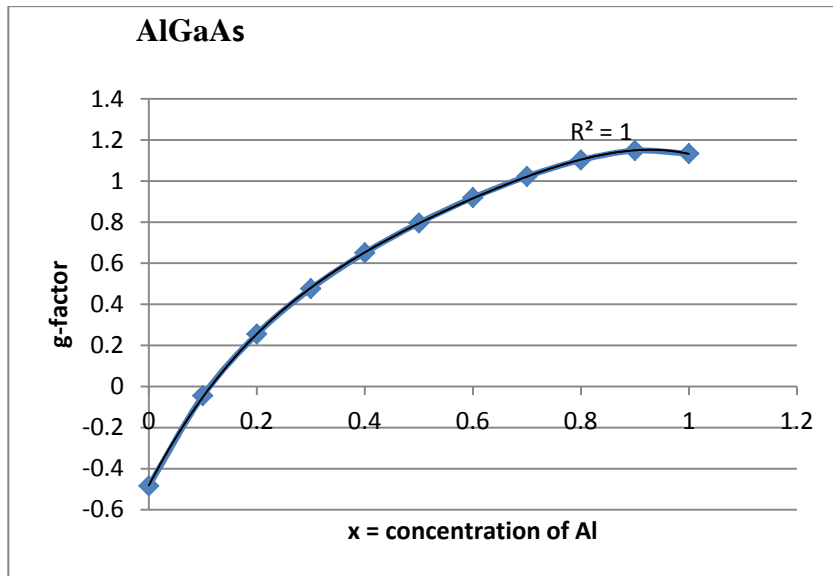


Figure 3.2 AlGaAs g-factor dependency on x

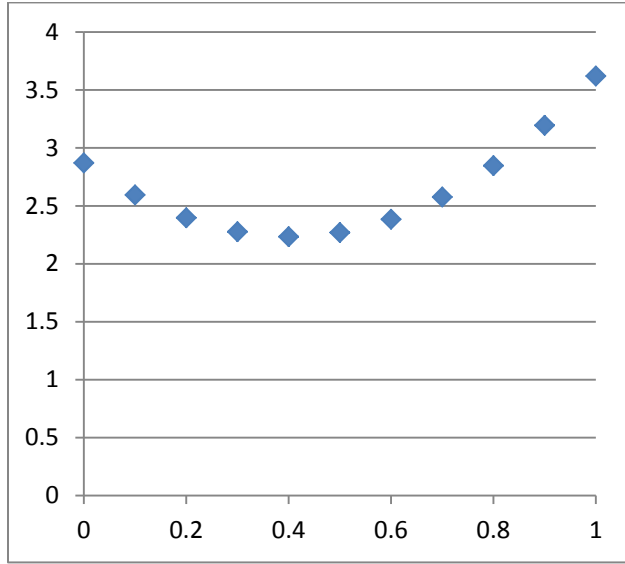


Figure 3.3 Variation of bandgap with x in GaPN alloys, apud [25]

Table 3.3 Band parameters of GaPN

x	Crystal	E ₀	Δ ₀	P ²	E _{0p}	Δ _{0p}	λ ²	g (3band)	g (5 band)
0	GaP	2.87	0.08	22	5.33	0.5	0.4	1.861415	1.253041
0.1		3.296	0.071	22	5.709	0.45	0.4	1.906166	1.348818
0.2		3.644	0.062	22	6.088	0.4	0.4	1.932665	1.462913
0.3		3.914	0.053	22	6.467	0.35	0.4	1.949936	1.584851
0.4		4.106	0.044	22	6.846	0.3	0.4	1.962128	1.698876
0.5		4.22	0.035	22	7.225	0.25	0.4	1.971412	1.794252
0.6		4.256	0.026	22	7.604	0.2	0.4	1.979075	1.867748
0.7		4.214	0.017	22	7.983	0.15	0.4	1.986016	1.9215
0.8		4.094	0.008	22	8.362	0.1	0.4	1.993013	1.960034
0.9		3.896	-0.001	22	8.741	0.05	0.4	2.000967	1.98834
1	GaN	3.62	-0.01	22	9.12	0	0.4	2.011223	2.011223

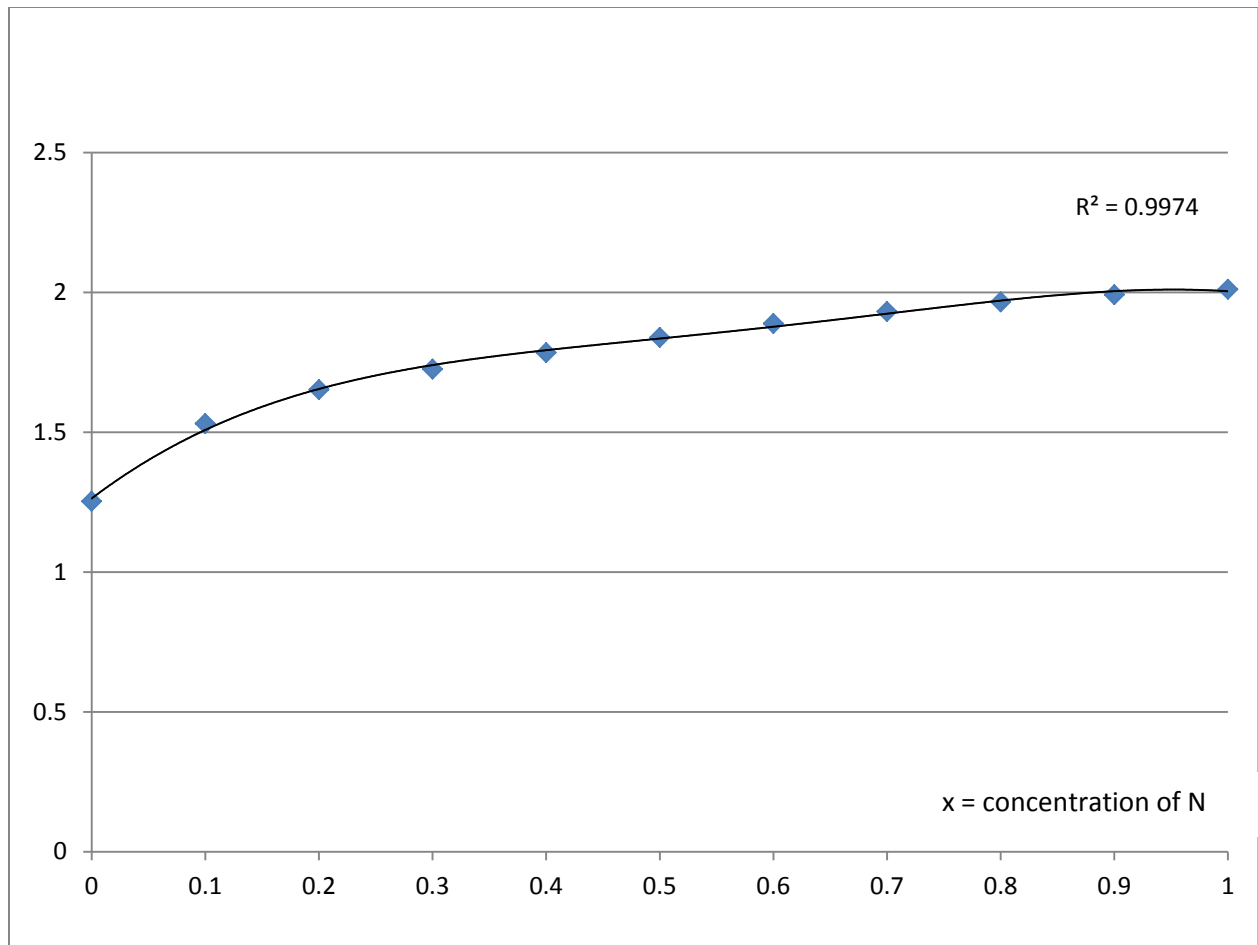


Figure 3.4 GaPN g-factor dependency on x

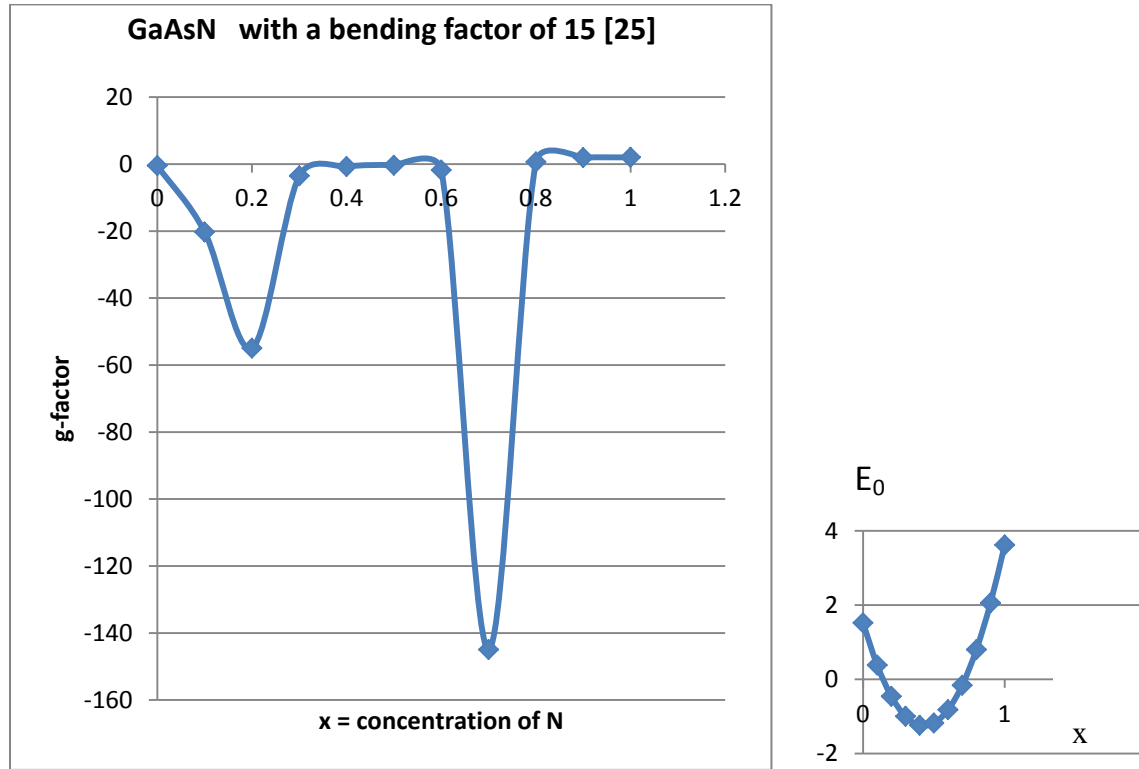


Figure 3.5 GaAsN g-factor and bandgap dependency on x (to the right)

Table 3.4 Band parameters of GaAsN

x	Crystal	E_0	Δ_0	P^2	E_{0p}	Δ_{0p}	λ^2	g (3band)	g(5 band)
0	GaAs	1.519	0.341	29	4.659	0.171	0.4	-0.33341	-0.47525
0.1		0.3791	0.3059	28.3	5.1051	0.1539	0.4	-20.2244	-20.2782
0.2		-0.4608	0.2708	27.6	5.5512	0.1368	0.4	-54.9115	-54.9401
0.3		-1.0007	0.2357	26.9	5.9973	0.1197	0.4	-3.52148	-3.53932
0.4		-1.2406	0.2006	26.2	6.4434	0.1026	0.4	-0.71566	-0.72797
0.5		-1.1805	0.1655	25.5	6.8895	0.0855	0.4	-0.34809	-0.35711
0.6		-0.8204	0.1304	24.8	7.3356	0.0684	0.4	-1.80858	-1.81544
0.7		-0.1603	0.0953	24.1	7.7817	0.0513	0.4	-144.951	-144.956
0.8		0.7998	0.0602	23.4	8.2278	0.0342	0.4	0.634659	0.630773
0.9		2.0599	0.0251	22.7	8.6739	0.0171	0.4	1.911558	1.909186
1	GaN	3.62	-0.01	22	9.12	0	0.4	2.011223	2.011223

Table 3.5 Band parameters of InPSb

x	Crystal	E_0	Δ_0	P^2	E_{0p}	Δ_{0p}	λ^2	g (3band)	g(5 band)
0	InSb	0.237	0.81	23.89	3.78	0.41	0.4	-49.9894	-50.2247
0.1		0.5263	0.8075	23.451	3.968	0.1959	0.4	-15.9841	-16.0938
0.2		0.7776	0.79	23.012	4.156	0.2208	0.4	-7.94257	-8.06959
0.3		0.9909	0.7575	22.573	4.344	0.2457	0.4	-4.57976	-4.7217
0.4		1.1662	0.71	22.134	4.532	0.2706	0.4	-2.78823	-2.94154
0.5		1.3035	0.6475	21.695	4.72	0.2955	0.4	-1.68248	-1.8428
0.6		1.4028	0.57	21.256	4.908	0.3204	0.4	-0.91868	-1.08136
0.7		1.4641	0.4775	20.817	5.096	0.3453	0.4	-0.33115	-0.49173
0.8		1.4874	0.37	20.378	5.284	0.3702	0.4	0.180556	0.025911
0.9		1.4727	0.2475	19.939	5.472	0.3951	0.4	0.701344	0.555602
1	InP	1.42	0.11	19.5	5.66	0.41	0.4	1.341802	1.210515

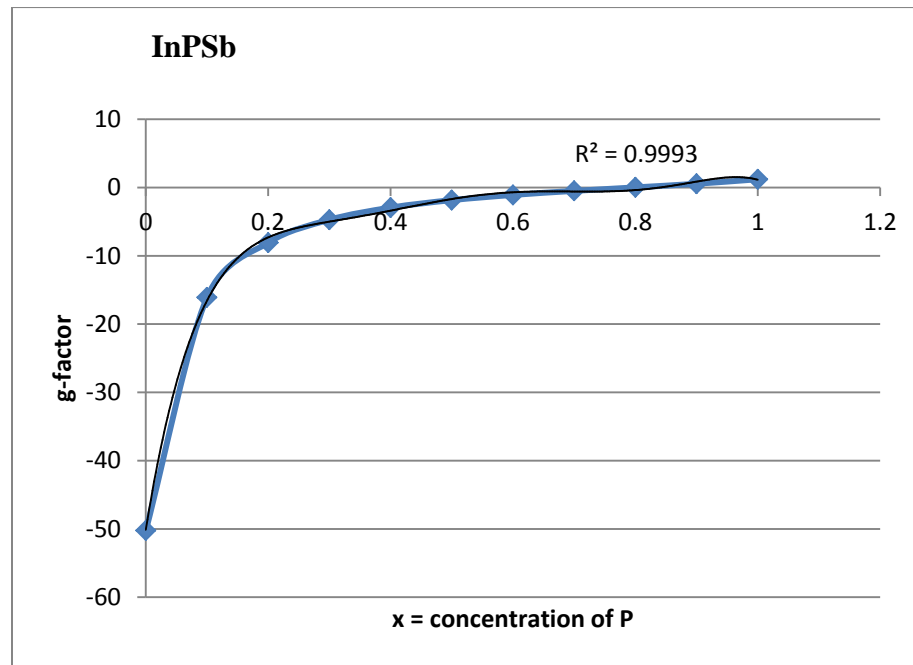


Figure 3.6 InPSb g-factor dependency on x

Table 3.6 Band parameters of GaPSb

x	Crystal	E_0	Δ_0	p^2	E_{0p}	Δ_{0p}	λ^2	g (3band)	g(5 band)
0	GaSb	0.81	0.8	23.93	3.69	0.25	0.4	-7.78657	-7.99719
0.1		0.773	0.728	23.737	3.854	0.1959	0.4	-7.92901	-8.06851
0.2		0.79	0.656	23.544	4.6432	0.2208	0.4	-7.01358	-7.11263
0.3		0.861	0.584	23.351	4.6353	0.2457	0.4	-5.30729	-5.42216
0.4		0.986	0.512	23.158	4.6274	0.2706	0.4	-3.35169	-3.48783
0.5		1.165	0.44	22.965	4.6195	0.2955	0.4	-1.60269	-1.76852
0.6		1.398	0.368	22.772	4.6116	0.3204	0.4	-0.26287	-0.47213
0.7		1.685	0.296	22.579	4.6037	0.3453	0.4	0.665186	0.388381
0.8		2.026	0.224	22.386	4.5958	0.3702	0.4	1.26665	0.875684
0.9		2.421	0.152	22.193	4.5879	0.3951	0.4	1.638978	1.029949
1	GaP	2.87	0.08	22	5.33	0.5	0.4	1.861415	1.253041

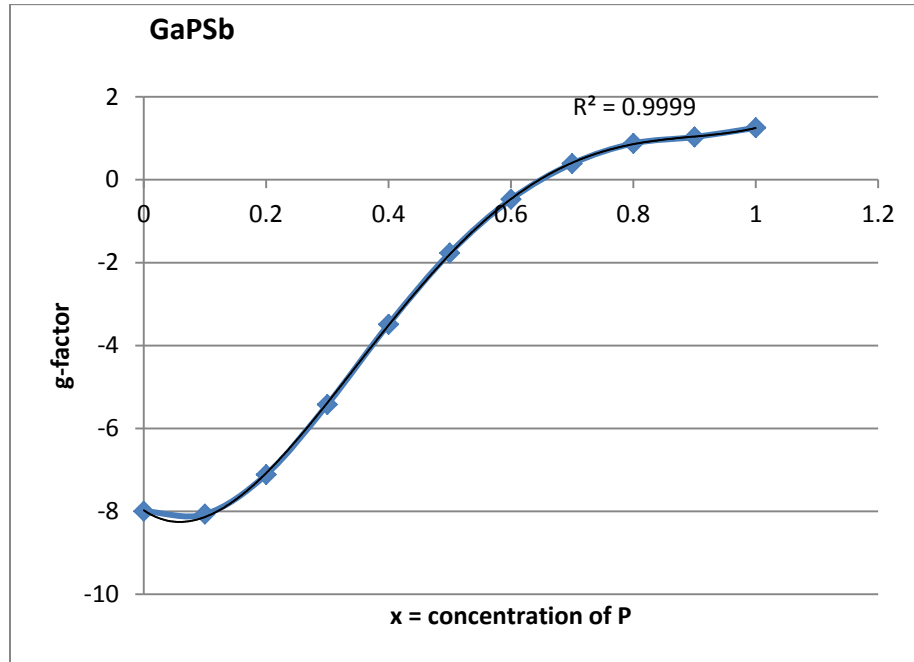


Figure 3.7 GaPSb g-factor dependency on x

Table 3.7 Band parameters of GaInAs

x	Crystal	E_0	Δ_0	P^2	E_{0p}	Δ_{0p}	λ^2	g (3band)	g(5 band)
0	GaAs	1.519	0.341	29	4.659	0.171	0.4	-0.33341	-0.47525
0.1		1.36617	0.3314	28.3692	4.6511	0.1959	0.4	-0.70256	-0.84861
0.2		1.22288	0.3248	27.7088	4.6432	0.2208	0.4	-1.17013	-1.31922
0.3		1.08913	0.3212	27.0188	4.6353	0.2457	0.4	-1.7666	-1.91786
0.4		0.96492	0.3206	26.2992	4.6274	0.2706	0.4	-2.53153	-2.68429
0.5		0.85025	0.323	25.55	4.6195	0.2955	0.4	-3.51525	-3.66901
0.6		0.74512	0.3284	24.7712	4.6116	0.3204	0.4	-4.77989	-4.93425
0.7		0.64953	0.3368	23.9628	4.6037	0.3453	0.4	-6.39841	-6.55303
0.8		0.56348	0.3482	23.1248	4.5958	0.3702	0.4	-8.44948	-8.60407
0.9		0.48697	0.3626	22.2572	4.5879	0.3951	0.4	-11.0049	-11.1592
1	InAs	0.42	0.38	21.36	4.58	0.42	0.4	-14.1048	-14.2585

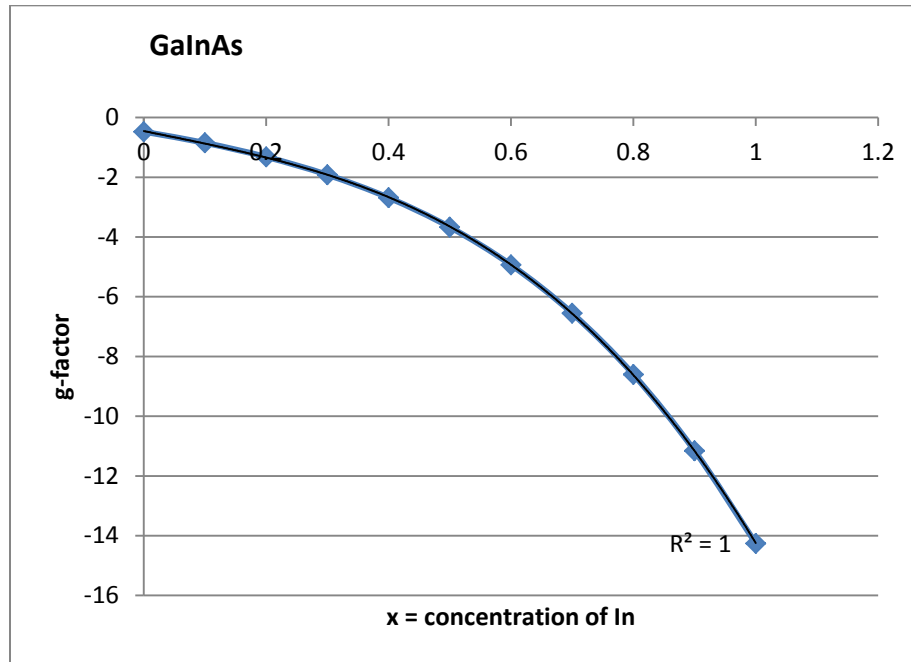


Figure 3.8 GaInAs g-factor dependency on x

3.2 Discussion

Of the compounds analyzed here, most have the expected monotonous behavior.

The “n” appearing in brackets in the graphs denotes the least degree of the interpolating polynomial that gives the acceptable value of R^2 .

AlGaAs is perhaps the most studied III-V alloy, due to its wide use in devices. The bowing parameter dependency on the Al concentration has been taken into consideration.

For GaPN, in spite of a very large bending coefficient for the bandgap, and in spite of difficulties posed by the presence of Nitrogen in other compounds, the g^* values have a well behaved, monotonous increasing.

A remarkable exception is the behavior of the g^* values for GaAsN compounds. The literature proposes many a value for the bending factor of the bandgap (between 10 and 20, and some opinions even stretch this interval, see [25]). All bending factors bigger than 4 yield to the highly uncharacteristic behavior seen in the figure 3.5. No matter what the actual value of the bending factor is, it determines a parabola-like $E_0(x)$, which has the above-said consequences. Since the discussion about the causes of such behavior of the bandgap are open, and the interpolation of bandgap values has not yet reached a consensus, the values of g^* for the intervals $[0, 0.3]$ and $[0.6, 0.8]$ of x are highly unreliable.

There is little data in literature for us to be able to compare the results. An exception is presented here, for AlGaAs, the compound of choice in many devices:

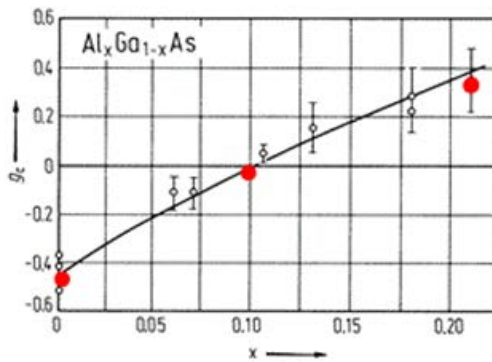


Figure 3.9 Comparison between measured values and the values calculated in this study (the full dots). [76C] represents the reference in the Landolt-Börnstein database.

Chapter 4

CONCLUSIONS

The present study offers, besides a series of values for six of the most used III-V ternary semiconductor alloys, also a method to follow for other families of such compounds.

This is perhaps the first systematic attempt to calculate the gyromagnetic factor for whole families of crystals, and it fits the scarce experimental data that exists.

Since the value of g-factor in ternary and further, quaternary crystals may become important with the development of the spintronics, the precision of calculation of g^* for families $A_{1-x}B_xC$ also becomes important. Better precision can deal with enhancing the interpolating methods for the parameters appearing in the equations of the 5-band model.

The results constitute themselves in a first (acceptable) approximation of the g-factors of the ternary crystals and may be a valid introduction in calculating the values of magnetic parameters of quaternary ones.

The advantage of the method consists of the ready-made values of the g-factors: instead of calculating everything from the beginning, one can simply interpolate the given values in the table for any value of x .

Further work should consist of a better approximation of the band parameters of complex crystals and the evaluation of the possibility to extend the method to quaternary crystals, which are more numerous and whose qualities might offer surprises with respect to their magnetic response and utility.

BIBLIOGRAPHY

1. *Magnetic Interactions and the Landé g-Factor*. Available from: <http://hyperphysics.phy-astr.gsu.edu/HBASE/quantum/Lande.html>.
2. Mohn, P., ed. *Magnetism in the Solid State: An Introduction*. Springer Series in Solid-State Sciences. 2005, Springer, p. 229.
3. Odom, B., et al., *New Measurement of the Electron Magnetic Moment Using a One-Electron Quantum Cyclotron*. Physical Review Letters, 2006. **97**(3): p. 801.
4. Schwinger, J., *On Quantum-Electrodynamics and the Magnetic Moment of the Electron*. Physical Review, 1948. **73**(4): p. 416.
5. Zee, A., *Quantum Field Theory in a Nutshell*. 2003: Princeton University Press.
6. Luttinger, J.M. and W. Kohn, *Motion of Electrons and Holes in Perturbed Periodic Fields*. Physical Review, 1955. **97**(4): p. 869.
7. Roth, L.M., *g Factor and Donor Spin-Lattice Relaxation for Electrons in Germanium and Silicon*. Physical Review, 1960. **118**: p. 1534.
8. Žutić, I., J. Fabian, and S. Das Sarma, *Spintronics: Fundamentals and applications*. Reviews of Modern Physics, 2004. **76**(2): p. 323.
9. Smith, C.H., *COMMERCIAL APPLICATIONS OF SPINTRONICS TECHNOLOGY*, in *Nanomaterials 2004*. 2004: Stamford, CT.
10. Oestreich, M. (2001) *Injection of Spin for Electronics*. PhysicsWorld.com.
11. Dietl, T., *Handbook of Semiconductors*, ed. S.M. Keller and T.S. Moss. Vol. 3. 1994, New York: North Holland.
12. Berciu, M., Janko B., *Nanoscale Zeeman localization of charge carriers in diluted magnetic semiconductor-permalloy hybrids*. Phys. Rev. Lett., 2003. **90** p. 43.
13. Snoke, D.W., *Solid State Physics: Essential Concepts*. Solid State Physics - Textbooks, ed. C. Benson. 2009, Addison-Wesley.
14. Roth, L.M., B. Lax, and S. Zwerdling, *Theory of Optical Magneto-Absorption Effects in Semiconductors*. Physical Review, 1959. **114**: p. 90.
15. Cardona, M., J. Phys. Chem. Solids 1963. **24**, p. 101.
16. Chadi, D.J., A.H. Clark, and R.D. Burnham, *Gamma 1 conduction electron g factor and matrix elements in GaAs and AlxGa1-xAs alloys*. Physical Review B, 1976. **13**: p. 4466.
17. Lawaetz, P., *Valence-Band Parameters in Cubic Semiconductors*. Physical Review B, 1971. **4**: p. 3460.

18. Hopfield, J.J., *Fine structure in the optical absorption edge of anisotropic crystals*. Phys. and Chem. of Solids, 1960. **15**(97).
19. Haberke, M.C.G., *GaN and InN conduction-band states studied by ellipsometry*, Phys Rev, 1965. **137**(1467).
20. E. Gutsche and E. Jahne, *Spin-Orbit Splitting of the Valence Band of Wurtzite Type Crystals*. Physica Status Solidi, 1967(19): p. 823-832.
21. Weisbuch, C. and C. Hermann, *Optical detection of conduction-electron spin resonance in GaAs, Ga_{1-x}In_xAs, and Ga_{1-x}Al_xAs*. Physical Review B, 1977. **15**: p. 816.
22. Yafet, Y. Solid State Physics, ed. R.A.W. F. Seitz. Vol. 14. 1963, New York: Academic Press.
23. Hermann, C. and C. Weisbuch, *k,p perturbation theory in III-V compounds and alloys: a reexamination*. Physical Review B, 1977. **15**(2): p. 823.
24. Ivchenko, E.L. and A.A. Kiselev, *Electron g factor in quantum wires and quantum dots*. Pis'ma Zh. Eksp. Teor. Fiz., 1998. **67**(1): p. 41-45.
25. Vurgaftman, I.M., J.R. Ram-Mohan L.R., *Band parameters for III–V compound semiconductors and their alloys*. Journal of Applied Physics, 2001. **89**(11)p. 5815.