

shallow_donors

April 22, 2014

```
In [21]: from wand.image import Image as WImage
         from wand.display import display
         img = WImage(filename='/home/dominique/BTSync/SolidState/Brno/SemiCon/Humlicek/TA_Notes/Donor_9
         print img.size
         print img.format
         img.resize(2*595L, 2*842L)
         print img.size
         img
         converted = img.convert('jpeg')
         converted
```

(3306L, 4678L)

PDF

(1190L, 1684L)

Out[21]:

Table 2
The calculated energy levels spacing in eV compared with experiment [19]

Band-gap energy (eV)	GaSb		InSb		InAs		GaAs	
	Cal	Exp	Cal	Exp	Cal	Exp	Cal	Exp
$\Gamma^c - \Gamma^v$	0.72	0.72	0.17	0.18	0.36	0.36	1.42	1.42
$X^c - \Gamma^v$	1.01	1.05	1.63	1.63	1.37	1.37	1.95	1.91
$L^c - \Gamma^v$	0.77	0.76	0.93	0.93	1.07	1.07	1.73	1.73

seen, for InAs, Nakwaski [18] has recommended for the electron effective mass a value of $0.023 m_0$, where m_0 stands for the electron mass in free space. Our calculated value is bigger than this one, but is in a good agreement with those measured by Ukhonov and Mal'tsev [21] and Kazakova et al. [22]. For InSb, our calculated value is much higher than that of Ref. [3]. Unfortunately, we have no other experimental data which are available for comparison. Similarly, as for InSb, we have only one available experimental value of the electron effective mass taken from Ref. [3], which is in a reasonable agreement with our calculated value. However, in the case of GaAs, many theoretical and experimental values of effective masses are available from the scientific literature. A nearly general agreement between many researchers using different theoretical approaches or experimental techniques shows that the value $m_e^* = 0.067 m_0$ of the band-edge electron effective mass in GaAs seems to be determined very correctly [18], which is in a very good agreement with our calculated one. We may then conclude that our calculated electron effective masses and experiment compare favorably, although the agreement is not quite as good as for GaAs and GaSb. This can be explained by the fact that the energy band gap of both materials InAs (0.36 eV) and InSb (0.17 eV) is less than those of GaSb (0.72 eV) and GaAs (1.42 eV), since the narrow gap between the conduction and valence bands in InAs and InSb leads to a strong interaction between them which makes the energy dispersion relation $E(k)$ vary non-parabolically with k (E not proportional to k^2). The conduction band non-parabolicity is a result of mixing between states in different bands, especially conduction and valence bands. Due to the non-parabolic nature of the energy band, the polar interactions of the electrons with the longitudinal phonons through the electric field of

polarization wave play an important role at room temperature for these materials, where in this interaction, the phonon energy is comparable to the electron energy. Another complication which is due also to the narrowness of the band gap implies a non-negligible number of thermally excited electrons, so screening has to be taken into consideration. The inclusion of screening and the subband wave-function effects decreases, however, the mass correction appreciably [27–29]. This may improve our calculated electron effective masses of InAs and InSb.

The calculated heavy-hole effective masses for our studied materials are tabulated and compared with other theoretical estimates and available experimental data in Table 4. We notice that the agreement between our theoretical results and the experiment is generally very good.

Since we have neglected spin–orbit coupling in our work, we cannot say anything about the so-called split-off mass band resulting from the spin–orbit coupling.

Let us now try to find relations for the band-edge density of states electron and heavy-hole effective masses in the ternary compounds $\text{InAs}_x\text{Sb}_{1-x}$ and $\text{Ga}_x\text{In}_{1-x}\text{Sb}$.

Table 3
Conduction band-edge electron effective mass (in units of free electron mass) in InAs, InSb, GaSb and GaAs determined by various experimental and theoretical methods

Material	m_e^*	Method
InAs	0.018 [20] ^b	Self-consistent ab-initio calculations
	0.029 [21] ^c	Faraday rotation
	0.030 [22] ^c	Reflection
	0.04 [23] ^b	Thermoelectric power
	0.026 [3]	
	0.023 [18]	Recommended value
InSb	0.034 ^{a,b}	Pseudo-potential method
	0.015 [3]	
GaSb	0.03 ^{a,b}	Pseudo-potential method
	0.047 [3]	
GaAs	0.05 ^{a,b}	Pseudo-potential method
	0.0636 [24] ^c	Photoluminescence
	0.069 [25] ^c	Faraday rotation
	0.07 [26] ^{b,c}	Thermoelectric power
	0.07 [3]	
	0.067 [18]	Recommended value
	0.07 ^{a,b}	Pseudo-potential method

^aPresent work. ^bAt room temperature. ^cAt 300 K.

In [5]: `import scipy.constants as cst`

```

import math

In [13]: r = 0.067 * (1.0/12.5)**2 * (cst.e**4*cst.m_e/(2.0*cst.hbar**2))*(1.0/(4.0*math.pi*cst.epsilon_0))

In [16]: r/cst.e*1000.0

Out[16]: 5.8341209654160515

In [8]: cst.epsilon_0

Out[8]: 8.854187817620389e-12

In [9]: cst.physical_constants["Rydberg constant"][0]

Out[9]: 10973731.568539

In [10]: cst.physical_constants["Rydberg constant"][1]

Out[10]: 'm^-1'

In [12]: cst.e**4*cst.m_e/(2.0*cst.hbar**2)

Out[12]: 2.698660275393679e-38

In []:

```