shallow_donors

April 29, 2014

In [24]:
```
import scipy.constants as cst
import math
from wand.image import Image as WImage
from wand.display import display
from IPython.display import HTML
```

In [15]:
```
img = WImage(filename='/home/dominique/BTSync/SolidState/Brno/SemiCon/[Peter_Y._Yu,_Manuel_Car
             resolution=400)
#print img.size
#print img.format
img.resize(2*595L, 2*842L)
#print img.size
img
#converted = img.convert('jpeg')
#converted
```

Out[15]:

notations are used to denote the bound states of shallow impurities. The energies of these bound states are given by the **Rydberg series**:

$$E - E_c(\mathbf{0}) = -R/N^2 \quad (N = 1,2,3,\ldots). \tag{4.23}$$

R is the **Rydberg constant** for the donor electron and is related to the Rydberg constant for the hydrogen atom $[e^4 m_0/(2\hbar^2)]$ by

$$R = \left(\frac{m^*}{m_0}\right)\left(\frac{1}{\varepsilon_0^2}\right)\left(\frac{e^4 m_0}{2\hbar^2}\right)\frac{1}{(4\pi\varepsilon_0)^2}, \tag{4.24}$$

m_0 being the free electron mass. A schematic diagram of some of the bound states of a donor atom near a simple parabolic conduction band is shown in Fig. 4.1.

- The extent of the bound-state electron wave functions in real space is measured in terms of a *donor Bohr radius* a^*. It is related to the Bohr radius in the hydrogen atom $[\hbar^2/(m_0 e^2)]$ by

$$a^* = \left(\frac{\varepsilon_0 m_0}{m^*}\right)\left(\frac{\hbar^2}{m_0 e^2}\right)(4\pi\varepsilon_0). \tag{4.25}$$

In particular, the wave function of the 1s state is given by

$$C_{1s}(\boldsymbol{R}) = \left(\frac{1}{\pi}\right)^{1/2}\left(\frac{1}{a^*}\right)^{3/2}\exp\left(\frac{-R}{a^*}\right). \tag{4.26}$$

In order that $\boldsymbol{R}$ can be considered continuous rather than discrete, we require $a^* \gg a_0$. This condition also ensures that it is meaningful to approximate the entire conduction band structure by an effective mass m^*. The reason is that the extent in $\boldsymbol{R}$ of an envelope function $C(\boldsymbol{R})$ corresponding to the electron wave function $\Psi(\boldsymbol{r})$ scales as a^*. On the other hand, the extent in $\boldsymbol{k}$-space of Bloch functions (which are indexed by $\boldsymbol{k}$) to be summed over in the reciprocal space to construct $\Psi(\boldsymbol{r})$ can be small. This is because of an "uncertainty principle" for two variables that are related by Fourier

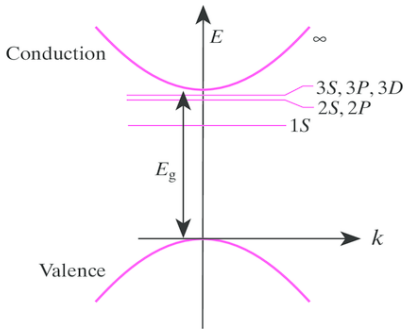

Fig. 4.1. Schematic diagram of the n=1, 2, and 3 bound states of a shallow donor electron near a nondegenerate and parabolic conduction band (corresponding to $n = \infty$). E_g is the bandgap

In [10]: img = WImage(filename='/home/dominique/BTSync/SolidState/Brno/SemiCon/Humlicek/TA_Notes/Donor_

```
                    resolution=400)
#print img.size
#print img.format
img.resize(2*595L, 2*842L)
#print img.size
img
#converted = img.convert('jpeg')
#converted
```

Out[10]:

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_o, where m_o 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 Ukhanov 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 $m_e^* = 0.067\ m_o$ 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 $InAs_xSb_{1-x}$ and $Ga_xIn_{1-x}Sb$.

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
	0.034[a,b]	Pseudo-potential method
InSb	0.015 [3]	
	0.03[a,b]	Pseudo-potential method
GaSb	0.047 [3]	
	0.05[a,b]	Pseudo-potential method
GaAs	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

[a]Present work. [b]At room temperature. [c]At 300 K.

```
Out[25]: <IPython.core.display.HTML at 0xab9f5ac>

In [26]: HTML('<iframe src=http://www.semiconductors.co.uk/propiiiv5653.htm width=750 height=500></ifra

Out[26]: <IPython.core.display.HTML at 0xab9f82c>

In [27]: HTML('<iframe src=http://www.ioffe.ru/SVA/NSM/Semicond/InSb/basic.html width=700 height=500></

Out[27]: <IPython.core.display.HTML at 0xab9f8ac>

In [32]: def get_binding_energy(eff_mass, epsilon):
             return eff_mass/ epsilon**2 * (cst.e**4*cst.m_e/(2.0*cst.hbar**2))/(4.0*math.pi*cst.epsilo

In [37]: print "GaAs binding energy", get_binding_energy(0.07, 12.5), "meV"

GaAs binding energy 6.09535026237 meV

In [38]: print "InSb binding energy", get_binding_energy(0.014, 16.8), "meV"

InSb binding energy 0.674885543152 meV

In [8]: from wand.image import Image as WImage
        img = WImage(filename='shallow.pdf', resolution=400)
        #print img.size
        img.resize(2*img.size[0], 2*img.size[1])
        img

Out[8]:
```

Table 4.1. Experimental binding energies of the 1*s* state of shallow donors in some zinc-blende-type semiconductors (from [Ref. 4.4, p. 224]) compared with the predictions of (4.24)

Semiconductor	Binding energy from (4.24) [meV]	Experimental binding energy of common donors [meV]
GaAs	5.72	Si_{Ga}(5.84); Ge_{Ga}(5.88) S_{As}(5.87); Se_{As}(5.79)
InP	7.14	7.14
InSb	0.6	Te_{Sb}(0.6)
CdTe	11.6	In_{Cd}(14); Al_{Cd}(14)
ZnSe	25.7	Al_{Zn}(26.3); Ga_{Zn}(27.9) F_{Se}(29.3); Cl_{Se}(26.9)

```
In []:
```