Chapter

3

# BANDSTRUCTURE MODIFICATION

### **BANDSTRUCTURE MODIFICATION**

In bulk crystals the electronic properties (bandstructure) are determined by the nature of the atoms forming the crystal. We would like to modify the bandstructure for a variety of reasons, depending upon technology needs. There are three important ways of modifying bandstructure.



### ALLOYS: LATTICE CONSTANT

Lattice constant of an alloy  $A_x B_{1-x}$  is given by Vegard's Law

 $a_{\text{alloy}} = x a_A + (1 - x)a_B$ 



Composition of an alloy is usually chosen to produce lattice matching with a substrate.

### Alloys: Bandgap

In bulk crystals the electronic properties (bandstructure) are determined by the nature of the atoms forming the crystal. We would like to modify the bandstructure for a variety of reasons, depending upon technology needs. There are three important ways of modifying bandstructure.

Compound	Direct Energy Gap <i>E<sub>g</sub></i> (eV)		
$Al_x In_{1-x} P$	1.351 + 2.23x		
$Al_xGa_{1-x}$ As	1.424 + 1.247x		
$Al_x In_{1-x} As$	$0.360 + 2.012x + 0.698x^2$		
$Al_xGa_{1-x}$ Sb	$0.726 + 1.129x + 0.368x^2$		
$Al_x In_{1-x} Sb$	$0.172 + 1.621x + 0.43x^2$		
$\operatorname{Ga}_{x}\operatorname{In}_{1-x}\operatorname{P}$	$1.351 + 0.643x + 0.786x^2$		
$\operatorname{Ga}_{x}\operatorname{In}_{1-x}\operatorname{As}$	0.36 + 1.064x		
$Ga_x In_{1-x}$ Sb	$0.172 + 0.139x + 0.415x^2$		
$GaP_xAs_{1-x}$	$1.424 + 1.150x + 0.176x^2$		
$GaAs_xSb_{1-x}$	$0.726 + 0.502x + 1.2x^2$		
$InP_xAs_{1-x}$	$0.360 + 0.891x + 0.101x^2$		
$InAs_xSb_{1-x}$	$0.18 + 0.41x + 0.58x^2$		

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### Semiconductor heterostructures: How do bands line up?

An extremely important issue in the properties of a quantum well is the bandedge discontinuity,  $\Delta E_c$  (and  $\Delta E_v$ ) which defines the confining potential. The electron affinity rule suggests that the conduction band discontinuity is determined by the electron affinity difference. Unfortunately, the rule does not work.



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#### **BANDSTRUCTURE IN QUANTUM WELLS: SUBBANDS**

What is the electronic spectra in a 2-dimensional quantum well? Electrons are confined in the *z*-direction and are free to move in the *x*-plane.

The Schrödinger equation for the quantum well in which the confinement is along the *z*-axis can be separated into equations in the *x* and *y* direction and in the *z*-direction as follows:



Valence band quantum well
 ∞

POSITION z —

 $\infty$ 

Schematic of a quantum well and the sub-band levels. Note that in a semiconductor quantum well, one has a quantum well for the conduction band and one for the valence band. In the infinite barrier model, the barriers are chosen to have an infinite potential, as shown.

### SUBBAND STRUCTURE IN QUANTUM WELLS

In an infinite square well, the electron energies are

$$E(n,k_x,k_y) = \frac{\pi^2 \hbar^2 n^2}{2m^* W^2} + \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} ; n = 1,2,3...$$
(subband number)

In an finite barrier, an iterative method is to be used to solve the following transcendental equations. The solutions give the subband levels.

$$\alpha \tan\left(\frac{\alpha W}{2}\right) = \beta \qquad \qquad \alpha = \sqrt{\frac{2m^*E}{\hbar^2}}$$
  

$$\alpha \cot\left(\frac{\alpha W}{2}\right) = -\beta \qquad \qquad \beta = \sqrt{\frac{2m^*(V_o - E)}{\hbar^2}}$$



Schematic of a quantum well and the subband levels. In the *x*-*y* plane, the subbands can be represented by parabolas. Subbands are produced in the conduction band and the valence band.

#### LOW-DIMENSIONAL STRUCTURES: DENSITY OF STATES

One of the most important motivations for low-dimensional systems is the ability they offer to modiy the density of statees.



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#### BANDSTRUCTURE IN A MOSFET CHANNEL

MOSFET is the most important electronic device. In the device electrons are confined (in inversion) in a triangular quantum well. A subband structure is formed for each of the six conduction band valleys.





## QUANTUM WELLS: VALENCE BANDSTRUCTURE

Due to the strong coupling between the heavy hole (HH) and light hole (LH) bands, the bandstructure in the valence band is quite non-parabolic.



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#### BANDSTRUCTURE MODIFICATION BY STRAIN

Strain changes the relative positions of atoms in a material.

- $\rightarrow$  causes changes in bandstructure.
- $\rightarrow$  degeneracies can be lifted.
- $\rightarrow$  selection rules for optical transitions can be altered.



#### Symmetries and deformation potentials

It is possible to predict which elements of the tensor  $D_{ij}^{\alpha\beta}$  are non-zero by examining the symmetry of the problem.



In fcc based structures it is useful to examine the following points:

- $\Gamma_2^1$ : bottom of the conduction band in direct gap material.
- $\Delta_l$ : direction along (100) and equivalent directions.
- $L_1$ : direction along (111) and equivalent directions.
- $\Gamma_{15}$ : top of the valence band.

#### DEFORMATION POTENTIAL THEORY

#### WHAT DOES STRAIN DO? DEFORMATION POTENTIAL THEORY

Deformation potential theory relates strain to changes in bandstructure (usually within first order perturbation theory).

$$H_{\varepsilon}^{\alpha\beta} = \sum_{ij} D_{ij}^{\alpha\beta} \varepsilon_{ij}$$

*ij*: *x*,*y*,*z* indices defining the strain tensor  $\varepsilon_{ij}$ .

 $\alpha,\beta$ : basis functions describing the electronic states

(eg.,  $s, p_{xy}, p_{xy}, p_z$ ).

- $H_{\epsilon}$ : perturbation due to strain.
- *D*: deformation potentials (usually determined from pressuredependent optical measurements.

#### STRAIN EFFECTS ON CONDUCTION BAND EDGES

Direct gap conduction band:  $\Gamma_2^l$  point: k = (0,0,0)

 $\delta E^{(000)} = \Xi_d^{(000)} \left( \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \right)$ 

This point is only influenced by the dilation due to the strain. Distortion of angles (off diagonal terms) have no influence on  $\Gamma_2$ .

Points along (100) and equivalent directions: There are six equivalent bands along these directions for fcc lattice based materials.  $\delta E^{(100)} = \delta E^{(\bar{1}00)} = \Xi_d^{(100)} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^{(100)} \varepsilon_{xx}$   $\delta E^{(010)} = \delta E^{(\bar{0}10)} = \Xi_d^{(100)} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^{(100)} \varepsilon_{yy}$   $\delta E^{(001)} = \delta E^{(00\bar{1})} = \Xi_d^{(100)} (\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + \Xi_u^{(100)} \varepsilon_{zz}$ If  $\varepsilon_{xx}$ ,  $\varepsilon_{yy}$ ,  $\varepsilon_{zz}$  are unequal, the six valleys can be split.

Points along (111) and equivalent directions:

$$\begin{split} \delta E^{(111)} &= D_{xx}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + 2D_{xy}(\varepsilon_{xy} + \varepsilon_{yz} + \varepsilon_{zx}) \\ \delta E^{(11\bar{1})} &= D_{xx}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + 2D_{xy}(\varepsilon_{xy} - \varepsilon_{yz} - \varepsilon_{zx}) \\ \delta E^{(1\bar{1}1)} &= D_{xx}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + 2D_{xy}(-\varepsilon_{xy} - \varepsilon_{yz} + \varepsilon_{zx}) \\ \delta E^{(\bar{1}11)} &= D_{xx}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + 2D_{xy}(-\varepsilon_{xy} + \varepsilon_{yz} - \varepsilon_{zx}) \end{split}$$

### STRAIN EFFECTS ON VALENCE BAND STATES

The top of the valence band is described by  $p_x, p_y, p_z$  states. The non-zero elements of the deformation potential tensor are:

$$D_{xx}^{xx} = l; D_{yy}^{xx} = m; D_{xy}^{xy} = n$$

where l,m,n are three independent valence band deformation potentials. Usually results are given in terms of another set of deformation potentials, a,b, and d where:

$$a = \frac{l+2m}{3}$$
;  $b = \frac{l-m}{3}$ ;  $d = \frac{n}{\sqrt{3}}$ 

The strain Hamiltonian for a 4x4 set of basis (i.e.,  $|3/2, \pm 3/2\rangle$  and  $|3/2, \pm 1/2\rangle$  is:

[	$H_{hh}^{\varepsilon}$	$H_{12}^{\varepsilon}$	$H_{13}^{\epsilon}$	0	3/2,3/2>
$H_{c}\Psi =$	$H_{12}^{\varepsilon*}$	$H_{lh}^{\epsilon}$	0	$H_{13}^{\varepsilon}$	3/2,1/2>
ε	$H_{13}^{\epsilon*}$	0	$H_{lh}^{\epsilon}$	$-H_{12}^{\varepsilon}$	3/2,-1/2>
	0	$H_{13}^{\epsilon*}$	$-H_{12}^{\epsilon*}$	$H_{hh}$	3/2,-3/2>

.....

where the matrix elements are given by

$$H_{hh}^{\varepsilon} = a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) - b\left[\varepsilon_{zz} - \frac{1}{2}(\varepsilon_{xx} + \varepsilon_{yy})\right]$$

$$H_{lh}^{\varepsilon} = a(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) + b\left[\varepsilon_{zz} - \frac{1}{2}(\varepsilon_{xx} + \varepsilon_{yy})\right]$$

$$H_{12}^{\varepsilon} = -d(\varepsilon_{xz} - i\varepsilon_{yz})$$

$$= \left\langle\frac{3}{2}, \frac{3}{2}\right|H_{\varepsilon}|\frac{3}{2}, \frac{1}{2}\right\rangle$$

$$H_{13}^{\varepsilon} = \frac{\sqrt{3}}{2}b(\varepsilon_{yy} - \varepsilon_{xx}) + id\varepsilon_{xy}$$

$$= \left\langle\frac{3}{2}, \frac{3}{2}\right|H_{\varepsilon}|\frac{3}{2}, \frac{-1}{2}\right\rangle$$

### VALENCE BAND EDGES FOR COHERENTLY STRAINED GROWTH ALONG (001)





The consequence of pseudomorphic strain on the bandedges of a direct bandgap semiconductor. The valence band degeneracy at k = 0 is lifted as the HH and LH states are split, as shown.

### STRAIN EFFECTS: CONDUCTION AND VALENCE BANDS OF SiGe ON Si

• Bulk Si and Si<sub>x</sub>Ge<sub>1-x</sub> (x > 0.15) have conduction bands which are 6-fold degenerate and *X*-like.

• If SiGe is grown on Si (100) the six bands are split into a 2-fold band and a 4-fold band.

• The valence band HH, LH degeneracy is also lifted.



Splittings of the conduction band and valence band are shown as a function of alloy composition.

UCB: unstrained conduction band, HH: heavy hole, LH: light hole, SH: split-off hole.