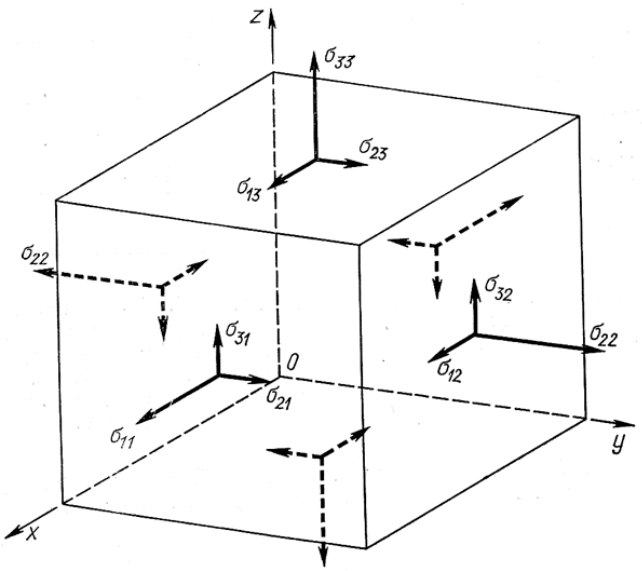
Lecture contents

- Stress and strain
- Deformation potential

Few concepts from linear elasticity theory : Stress and Strain

6 independent components

Stress = force/area (3x3 symmetric tensor !) $\sigma_{ij} = \sigma_{ji}$



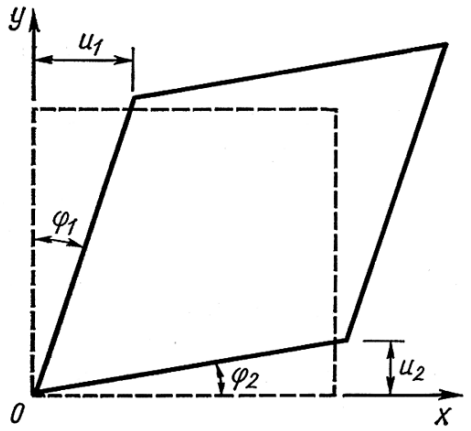
Stresses applied to a infinitely small volume:

Strain = Δdisplacement/ Δcoordinate
(3x3 symmetric tensor !)

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

6 independent components

Diagonal (axial) strain components: $\varepsilon_{ii} = \frac{\partial u_i}{\partial x_i}$



Explanation of shear strain components:

Few concepts from linear elasticity theory : Hooke's law

Stress-Strain relation: extension of Hooke's law (linear regime):

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\\ \sigma_{32}\\ \sigma_{13}\\ \sigma_{21}\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16}\\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{24} & c_{25} & c_{26}\\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} & c_{34} & c_{35} & c_{36}\\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}\\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56}\\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66}\\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}\\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56}\\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66}\end{bmatrix} \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \varepsilon_{23}\\ \varepsilon_{31}\\ \varepsilon_{12}\\ \varepsilon_{32}\\ \varepsilon_{13}\\ \varepsilon_{21}\end{bmatrix}$$

Due to symmetry of stress-strain tensors the matrix of elastic moduli (elastic stiffness constants) can be reduced to 6x6:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16}\\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26}\\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36}\\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46}\\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56}\\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66}\end{bmatrix} \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \gamma_{23}\\ \gamma_{31}\\ \gamma_{12}\end{bmatrix}$$

Note: $\gamma_{ij} = 2\varepsilon_{ij}$ for non-diagonal strain components

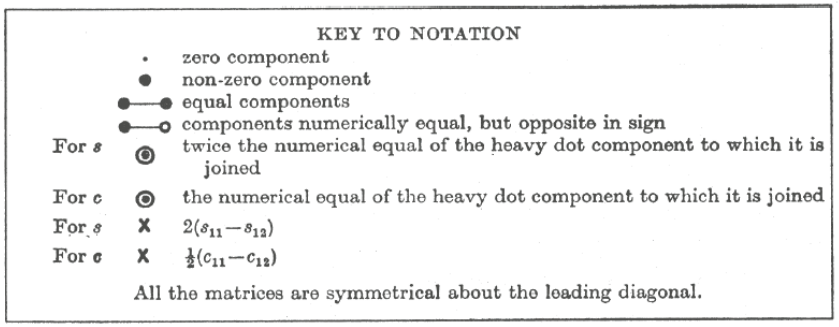
For cubic crystals,

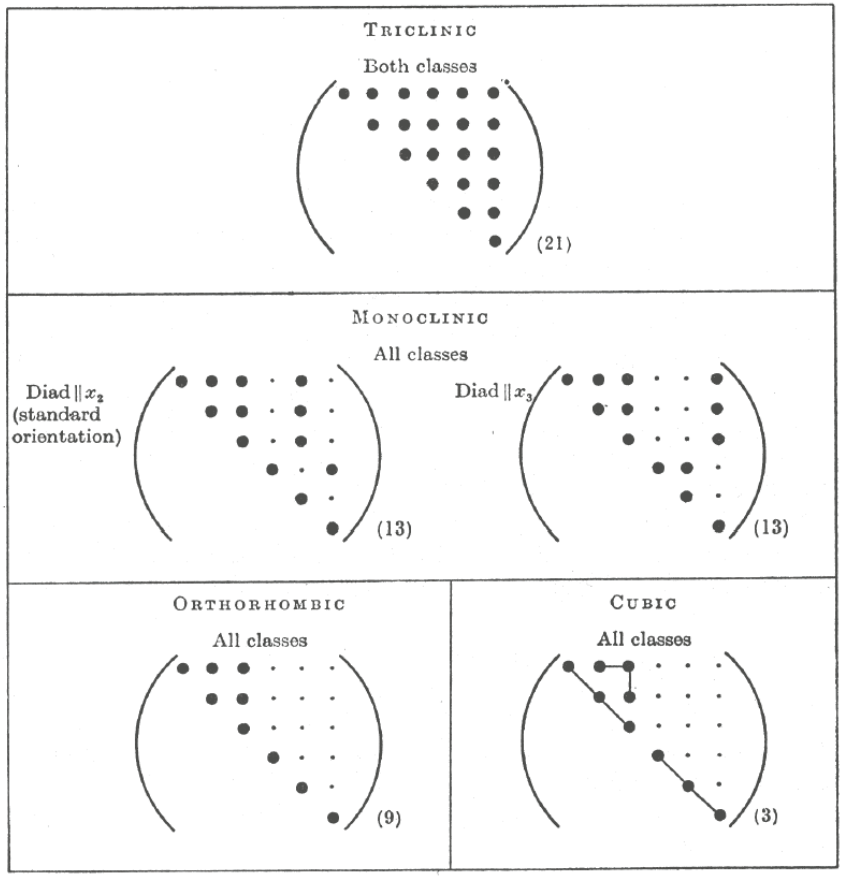
only 3 constants are independent:

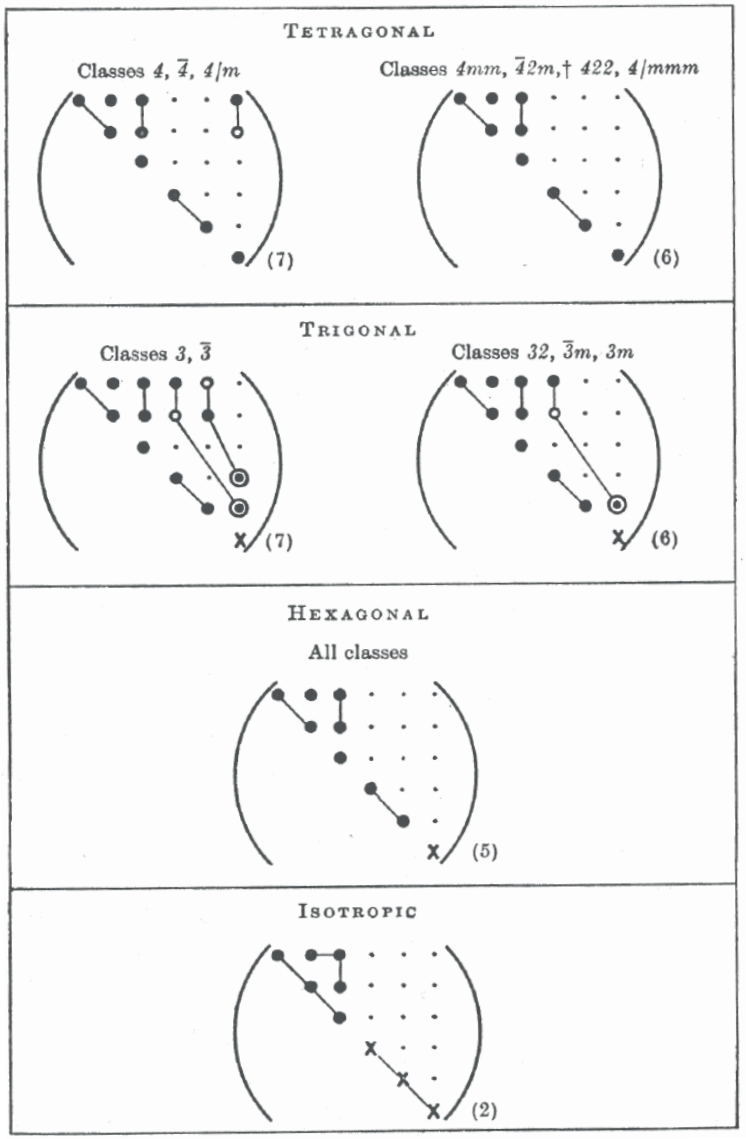
$$c_{mn} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44}\end{bmatrix}$$

$$\begin{aligned}
\sigma_{11} &= c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{12}\varepsilon_{33};\\
\sigma_{22} &= c_{12}\varepsilon_{11} + c_{11}\varepsilon_{22} + c_{12}\varepsilon_{33};\\
\sigma_{33} &= c_{12}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{11}\varepsilon_{33};\\
\sigma_{23} &= 2c_{44}\varepsilon_{23};\\
\sigma_{31} &= 2c_{44}\varepsilon_{31};\\
\sigma_{12} &= 2c_{44}\varepsilon_{12}.
\end{aligned}$$

Effects of crystal symmetry on elastic constants







Definitions for other elastic constants

For cubic crystal (3 constants are independent) :

$$\sigma_{11} = c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{12}\varepsilon_{33};$$
$$\sigma_{22} = c_{12}\varepsilon_{11} + c_{11}\varepsilon_{22} + c_{12}\varepsilon_{33};$$
$$\sigma_{33} = c_{12}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{11}\varepsilon_{33};$$
$$\sigma_{23} = 2c_{44}\varepsilon_{23};$$
$$\sigma_{31} = 2c_{44}\varepsilon_{31};$$
$$\sigma_{12} = 2c_{44}\varepsilon_{12}.$$

Anisotropy ratio $A = \dfrac{2c_{44}}{c_{11} - c_{12}}$

For <u>isotropic material,</u> A=1, only two elastic constants are independent

$$2c_{44} = c_{11} - c_{12}$$

Lamé coefficient λ and shear modulus μ :

$$\sigma_{11} = (\lambda + 2\mu)\,\varepsilon_{11} + \lambda\varepsilon_{22} + \lambda\varepsilon_{33};$$
$$\sigma_{22} = \lambda\varepsilon_{11} + (\lambda + 2\mu)\,\varepsilon_{22} + \lambda\varepsilon_{33};$$
$$\sigma_{33} = \lambda\varepsilon_{11} + \lambda\varepsilon_{22} + (\lambda + 2\mu)\,\varepsilon_{33};$$
$$\sigma_{23} = 2\mu\varepsilon_{23};$$
$$\sigma_{31} = 2\mu\varepsilon_{31};$$
$$\sigma_{12} = 2\mu\varepsilon_{12};$$

Material	C_{11}(N/m^2)	C_{12}(N/m^2)	C_{41}(N/m^2)
Si	1.66 x 10^{11}	0.64 x 10^{11}	0.8 x 10^{11}
Ge	1.29 x 10^{11}	0.48 x 10^{11}	0.67 x 10^{11}
GaAs	1.2 x 10^{11}	0.54 x 10^{11}	0.59 x 10^{11}
C	10.76 x 10^{11}	1.25 x 10^{11}	5.76 x 10^{11}

Material	C_{13}(N/m^2)	C_{33}(N/m^2)
GaN	10.9 x 10^{11}	35.5 x 10^{11}
AlN	12 x 10^{11}	39.5 x 10^{11}

From Singh, 2003

Fractional change of crystal volume under uniform deformation

$$\frac{\delta V}{V} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$$

Definitions of other elastic constants

Young's modulus

$$E = \frac{\mu(3\lambda + 2\mu)}{\mu + \lambda} = \frac{9\mu B}{3B + \mu} = 2\mu(1 + \nu);$$

Poisson ratio

$$\nu = \frac{3B - 2\mu}{2(3B + \mu)} = \frac{\lambda}{2(\mu + \lambda)} = \frac{E - 2\mu}{2\mu};$$

Shear modulus

$$\mu = \frac{E}{2(1 + \nu)};$$

Lamé coefficient

$$\lambda = \frac{\nu E}{(1 + \nu)(1 - 2\nu)} = \frac{2\nu\mu}{1 - 2\nu}.$$

Bulk modulus

$$B = \frac{3\lambda + 2\mu}{2}$$

Another useful set of equations for <u>isotropic</u> material (only 2 constants are independent) :

$$\varepsilon_{11} = \frac{1}{E}[\sigma_{11} - \nu(\sigma_{22} + \sigma_{33})];$$

$$\varepsilon_{22} = \frac{1}{E}[\sigma_{22} - \nu(\sigma_{11} + \sigma_{33})];$$

$$\varepsilon_{33} = \frac{1}{E}[\sigma_{33} - \nu(\sigma_{11} + \sigma_{22})];$$

$$\varepsilon_{23} = \frac{1}{2\mu}\sigma_{23};$$

$$\varepsilon_{31} = \frac{1}{2\mu}\sigma_{31};$$

$$\varepsilon_{12} = \frac{1}{2\mu}\sigma_{12}.$$

Strain in heterostructures

Lattice mismatch:

Strain relaxed:

Strain: $\varepsilon = \frac{a_S - a_I}{a_I}$

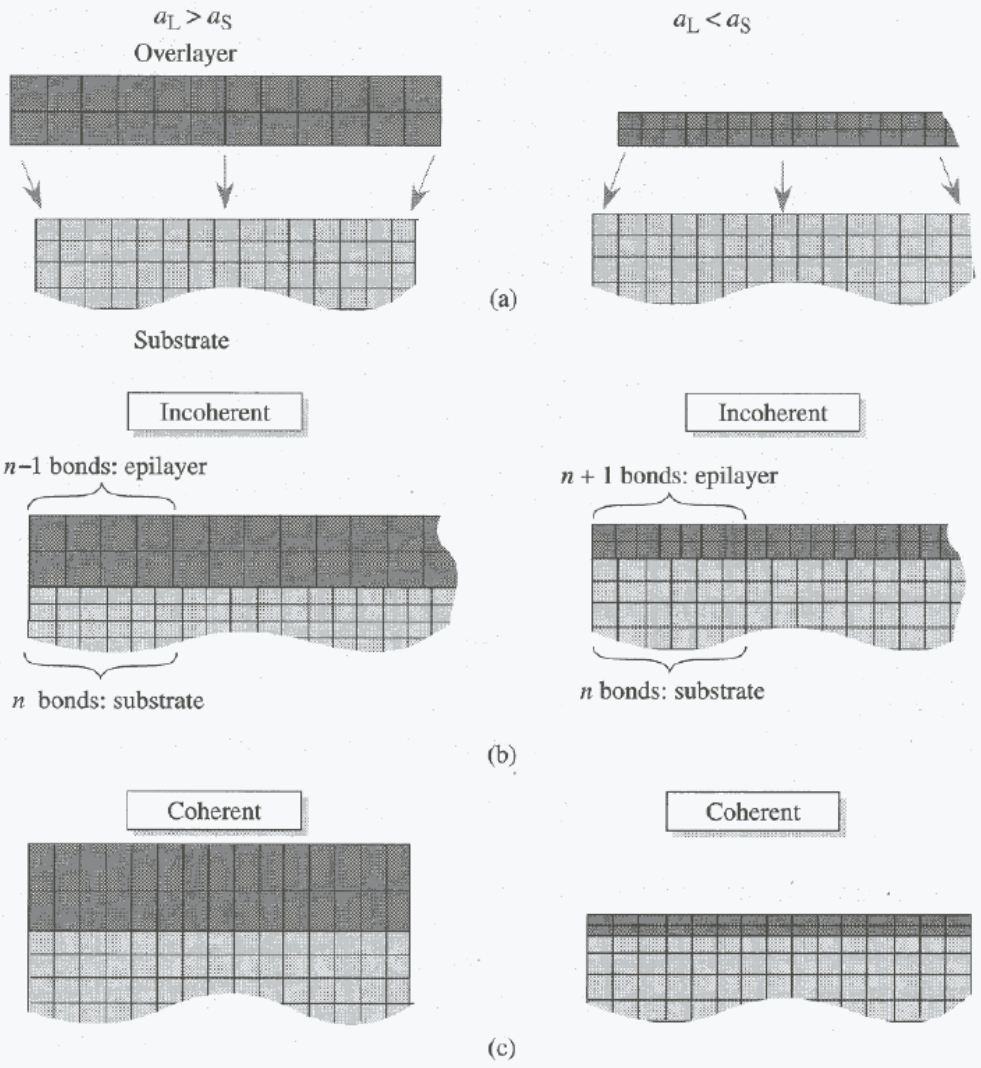


Figure 1.20: (a) The conceptual exercise in which an overlayer with one lattice constant is placed without distortion on a substrate with a different lattice constant. (b) Dislocations are generated at positions where the interface bonding is lost. (c) The case is shown where the overlayer is distorted so that no dislocation is generated.

Ref: Singh

Stress in pseudomorphic epitaxial films

$$e_{\parallel} = \frac{a_S}{a_L} - 1 = \epsilon$$

Biaxial strain.
No stress along the growth direction!

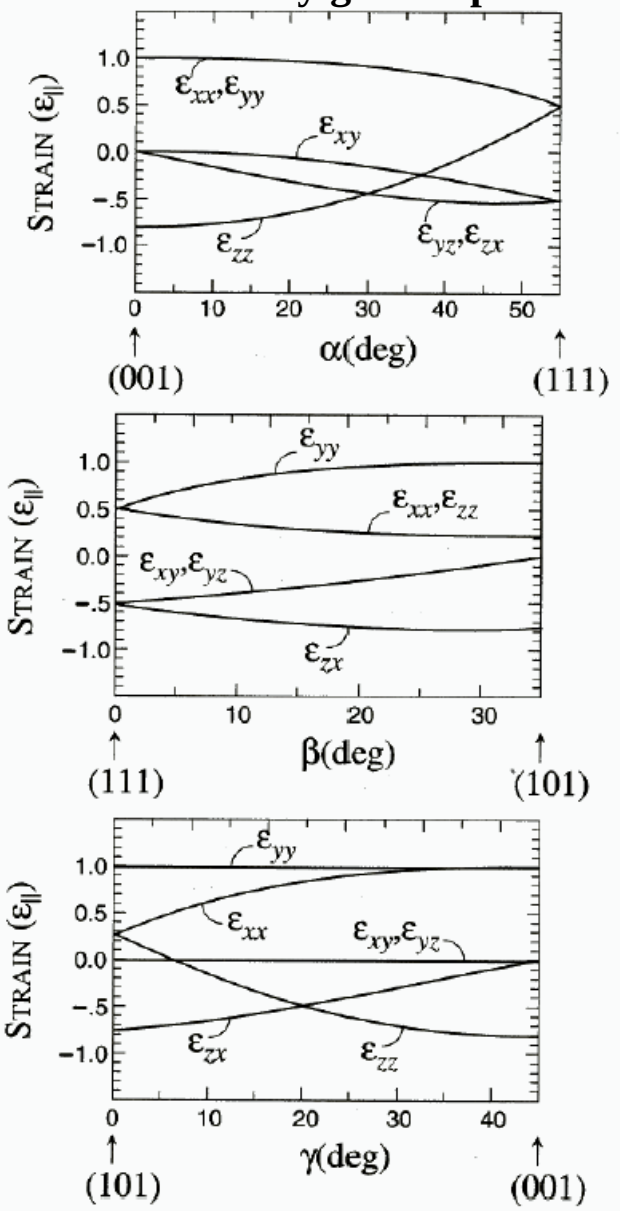
$$\begin{aligned}
\epsilon_{xx} &= \epsilon_{\parallel} \\
\epsilon_{yy} &= \epsilon_{xx} \\
\epsilon_{zz} &= \frac{-2c_{12}}{c_{11}}\epsilon_{\parallel} \\
\epsilon_{xy} &= 0 \\
\epsilon_{yz} &= 0 \\
\epsilon_{zx} &= 0
\end{aligned}$$

For strained growth on (001) substrate & fcc lattice

For strained growth on (111) substrate & fcc lattice (xyz's are along the cube axes)

$$\begin{aligned}
\epsilon_{xx} &= \left[\frac{2}{3} - \frac{1}{3}\left(\frac{2c_{11}+4c_{12}-4c_{44}}{c_{11}+2c_{12}+4c_{44}}\right)\right]\epsilon_{\parallel} \\
\epsilon_{yy} &= \epsilon_{xx} \\
\epsilon_{zz} &= \epsilon_{xx} \\
\epsilon_{xy} &= \left[\frac{-1}{3} - \frac{1}{3}\left(\frac{2c_{11}+4c_{12}-4c_{44}}{c_{11}+2c_{12}+4c_{44}}\right)\right]\epsilon_{\parallel} \\
\epsilon_{yz} &= \epsilon_{xy} \\
\epsilon_{zx} &= \epsilon_{yz}
\end{aligned}$$

On arbitrary growth planes



Ref: Singh

Strained tensor for self-organized quantum dots

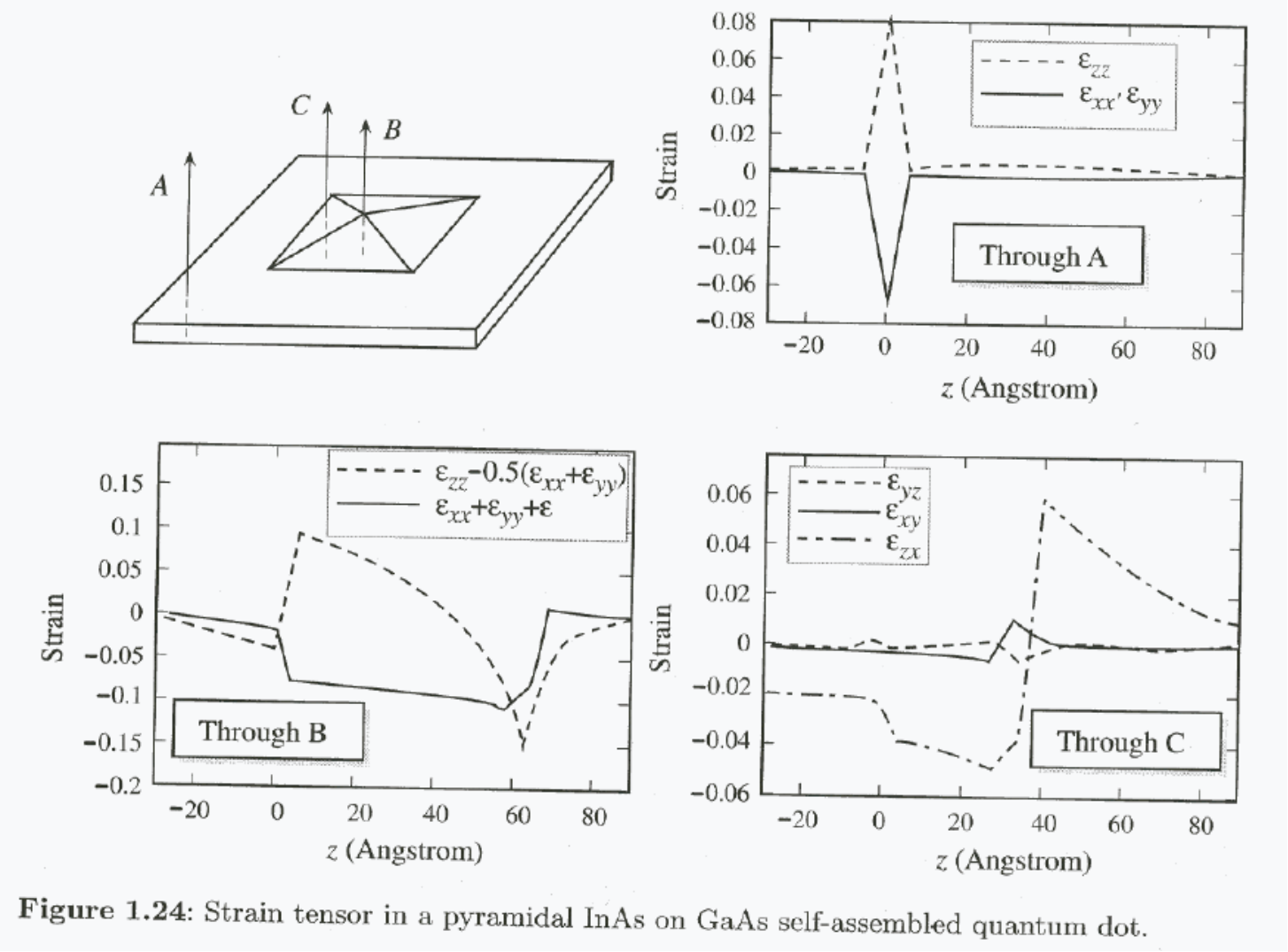
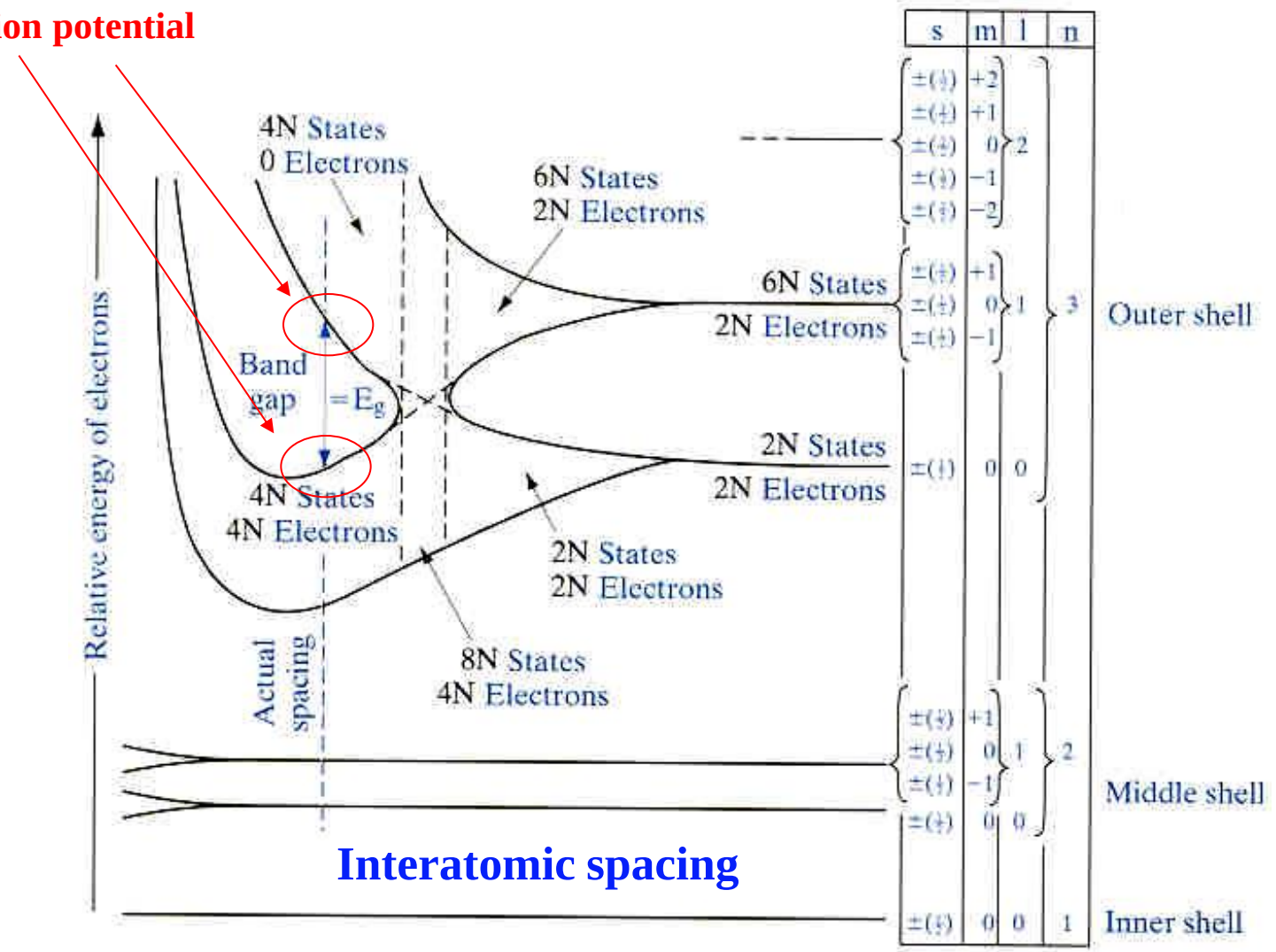


Figure 1.24: Strain tensor in a pyramidal InAs on GaAs self-assembled quantum dot.

Ref: Singh

Energy levels of Si as a function of interatomic spacing

Energy band shift vs. strain:
Deformation potential



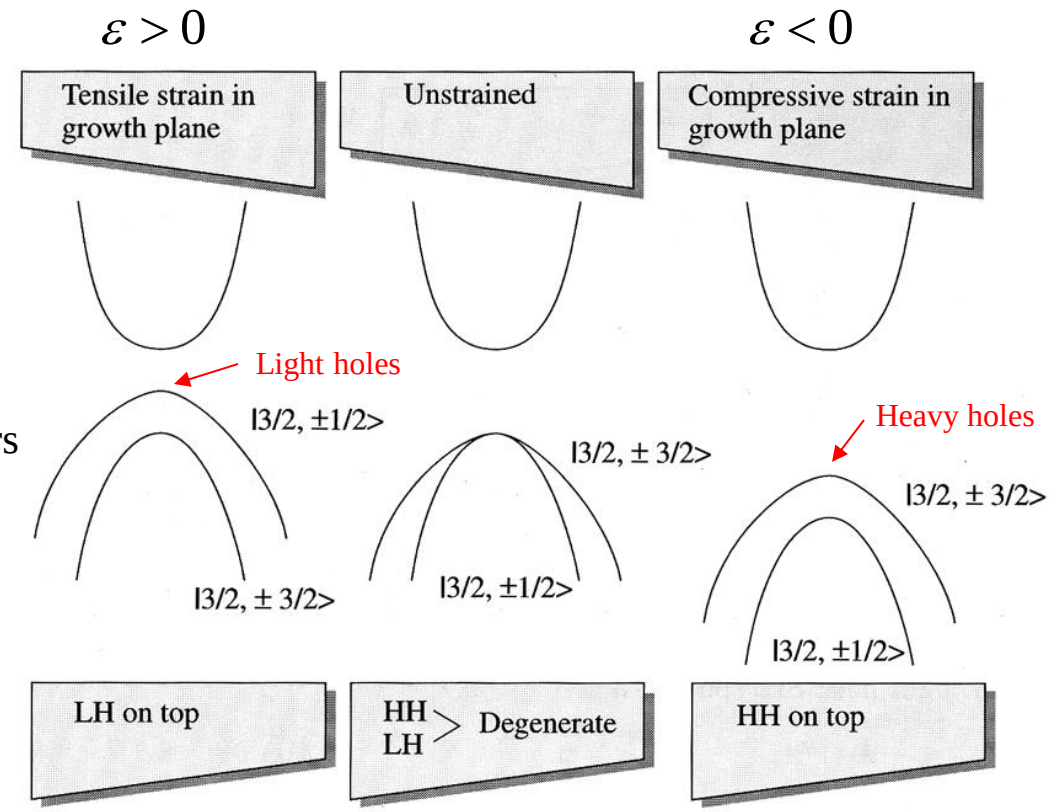
Deformation potential

Once the strain ε_{ij} is known, the effects of strain on various band states (α) can be calculated using Deformation potential theory:

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

- Number of independent non-zero D_{ij}^{α} depends on symmetry of the state α
- Tensile strain in sp^3 – bonded semiconductors reduces bandgap; compressive increases bandgap.
- Axial strain splits the valence band: strain effect on heavy holes is less
- Axial strain lifts degeneracy of indirect conduction band valleys and reduce the electron effective masses
- Strain induces piezoelectric field in polar semiconductor structures

Effect of strain on direct band-edges



From Singh, 2003

Values of D's are usually of the order of few eV

Deformation potential

Table 3.1. Deformation potentials for the conduction and valence band extrema in diamond and zinc-blende semiconductors (in eV). a denotes the volume deformation potential for the lowest energy Γ_{1c} conduction band minimum or the highest energy Γ_{15v} valence band maximum (zinc-blende notation). b and d are the shear deformation potentials for the Γ_{15v} valence band maximum. Ξ_d and Ξ_u denote deformation potentials at zone boundaries. Most of the data are taken from [3.30]

	Ξ_d	Ξ_u	$a(\Gamma_{1c})$	$a(\Gamma_{1c}) - a(\Gamma_{15v})$	b	d
Si	$\approx 5^a$	8.77^a		−10	−2.2	−5.1
Ge	-12.3^b	16.3^b		−12	−2.3	−5.0
GaP		13		−9.3	−1.8	−4.5
GaAs	6.5^a	14.5^b	−8.6	−9	−2.0	−5.4
GaSb				−8.3	−1.8	−4.6
InP			−7	−6.4	−2.0	−5.0
InAs				−6.0	−1.8	−3.6
InSb				−7.7	−2.0	−5.0
ZnS				−4.0	−0.62	−3.7
ZnSe				−5.4	−1.2	−4.3
ZnTe				−5.8	−1.8	−4.6
CdTe				−3.4	−1.2	−5.4

[a] [100] valleys;

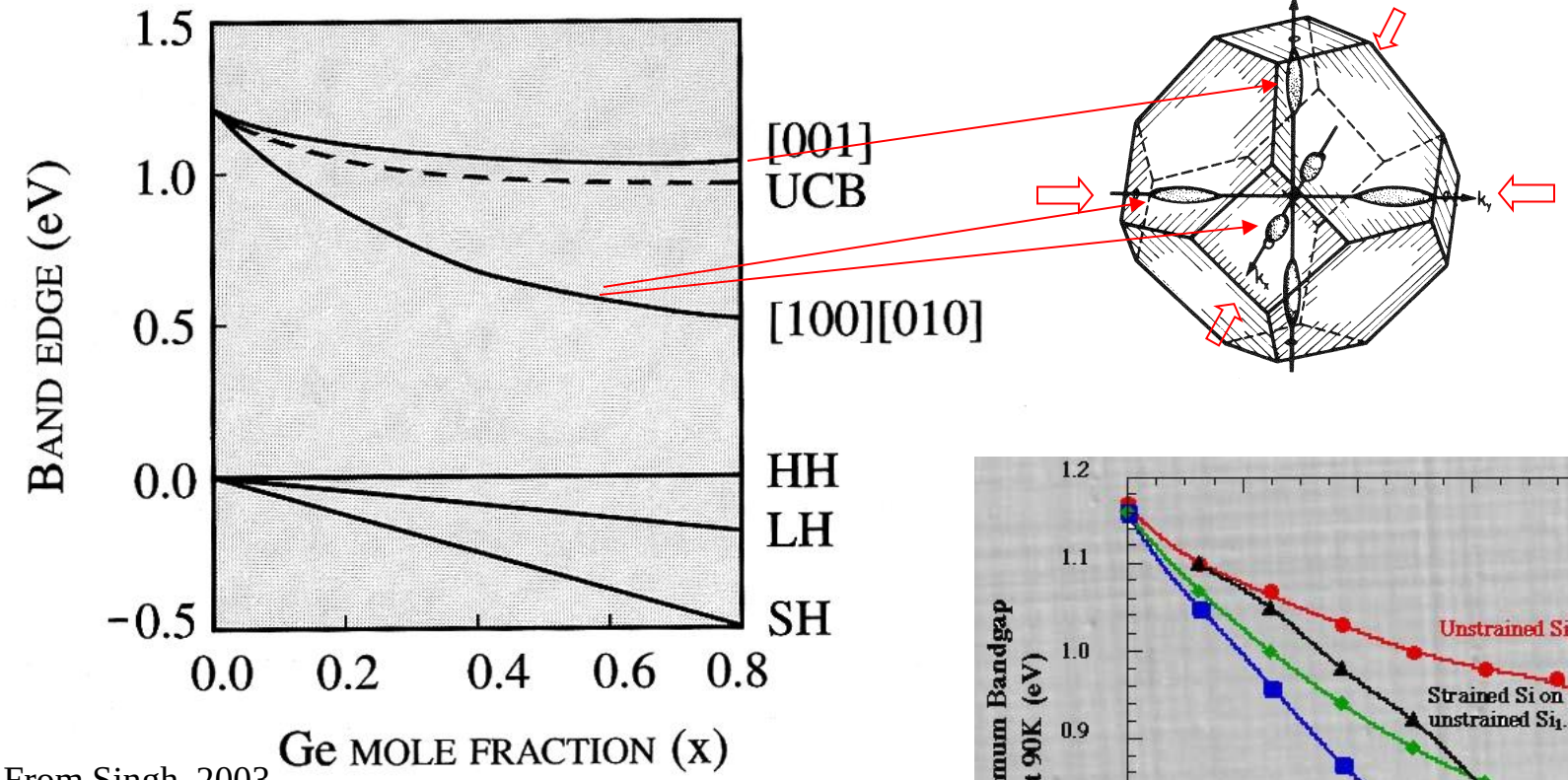
[b] [111] valleys, D.N. Mirlin, V.F. Sapega, I.Ya. Karlik, R. Katilius: Hot luminescence investigation of L-valley spliting in GaAs. Solid State Commun. **61**, 799–805 (1987)

Volume DP for the bandgap

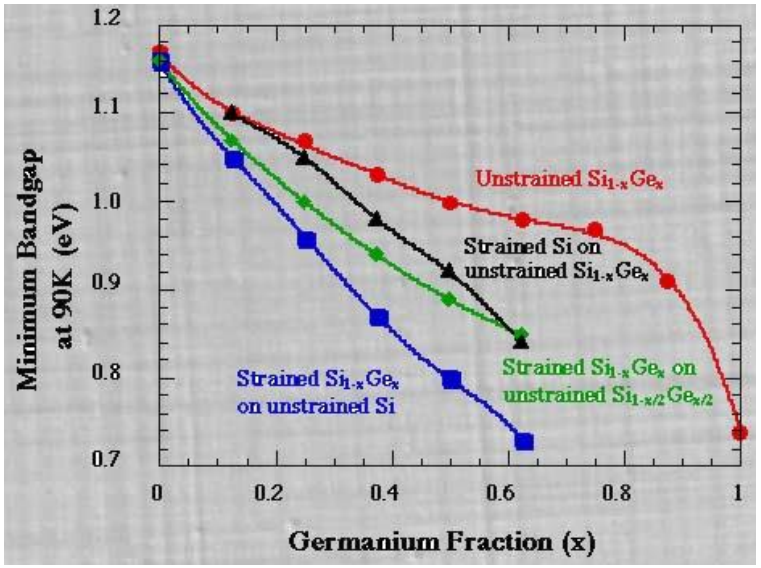
From Yu and Cordona, 2003

Strained $Si_{1-x}Ge_x$ / Si

Effect of strain on indirect band-edges



From Singh, 2003



Biaxial compressive strain causes:

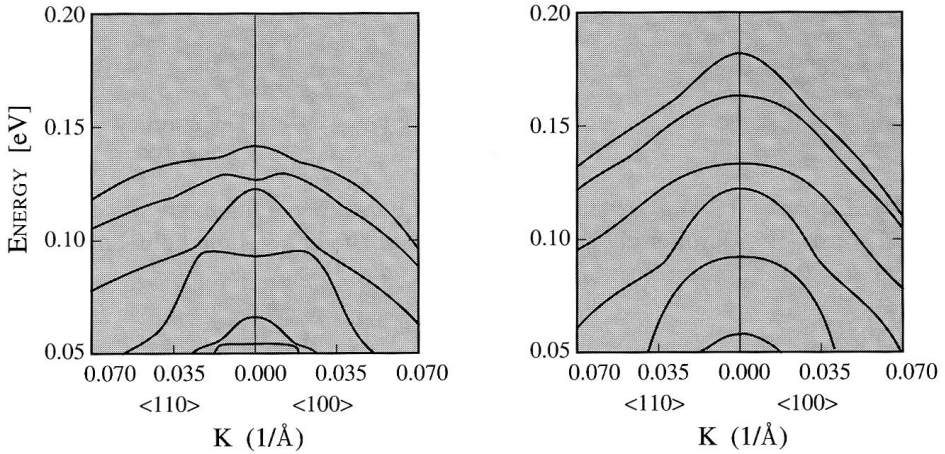
- Strong lowering of 4-fold in-plane valleys
- Weak lowering of 2-fold out-of plane valleys
- Reduction of masses and density of states

Strained quantum wells

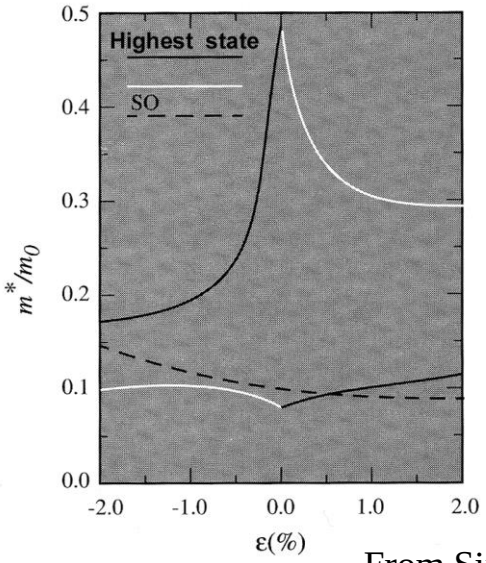
- Strained heterostructures are usually grown in a form of quantum-confined structures to prevent plastic relaxation
- Both quantum confinement and stress should be considered
- The strain bandgap energy shift for QWs can be over 100 meV – larger than quantum confinement energies
- Strain reduces hole effective masses due to the splitting of LH and HH
- Tensile strain can compensate quantum confinement energy and restore degeneracy of the valence band

100 Å QW valence band dispersion in

AlGaAs/GaAs **AlGaAs/$In_{0.1}Ga_{0.9}As$**

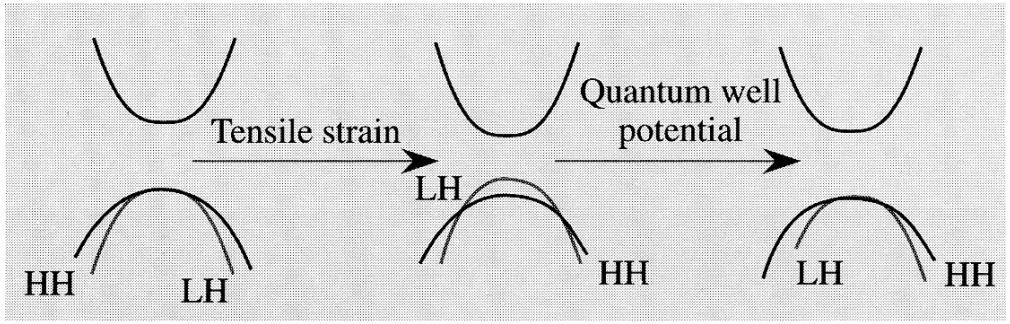


Effect of biaxial strain on hole masses



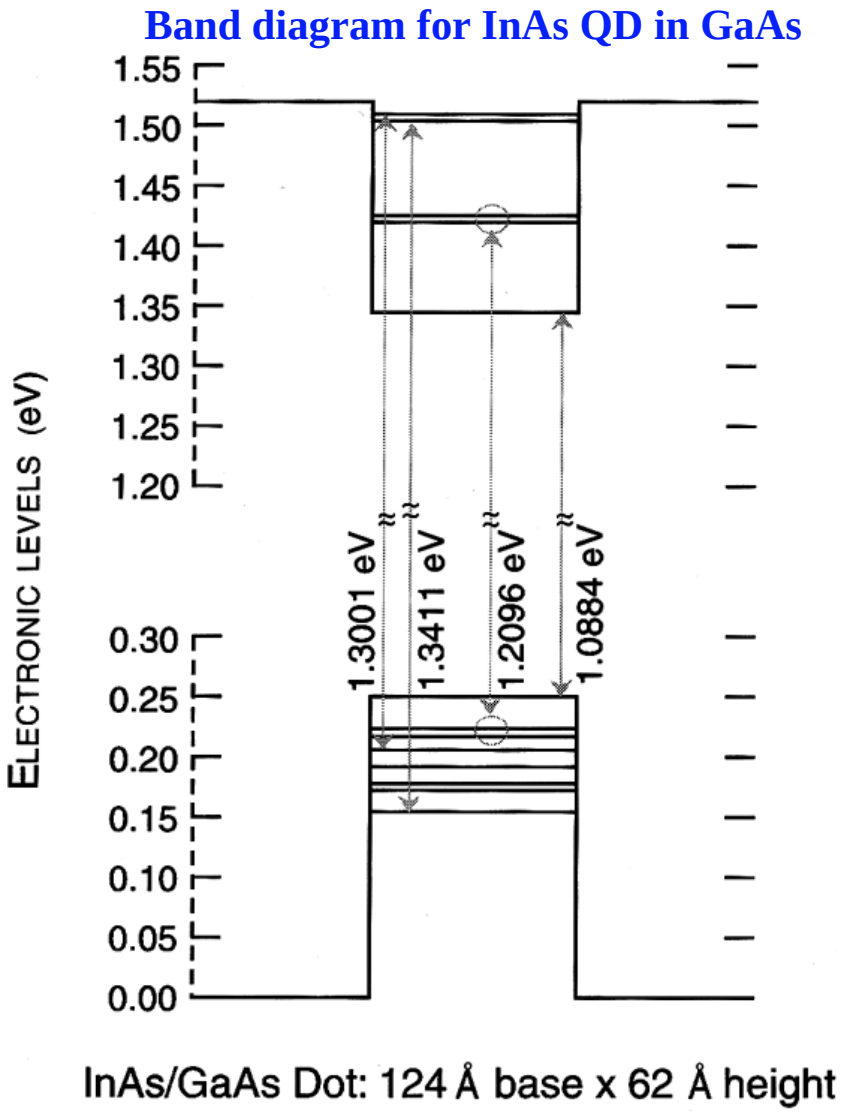
From Singh, 2003

Effect of biaxial tensile strain and quantum confinement on band edges



Self-assembled quantum dots

- The highest elastic stain can be obtained in all-epitaxial self-assembled QDs
- Example: InAs bandgap = 0.35 eV
- The bandgap of strained InAs with a GaAs lattice parameter =1.09 eV
- The strain bandgap energy shift for InAs QD can be over 740 meV ! much larger than quantum confinement energies



From Singh, 2003