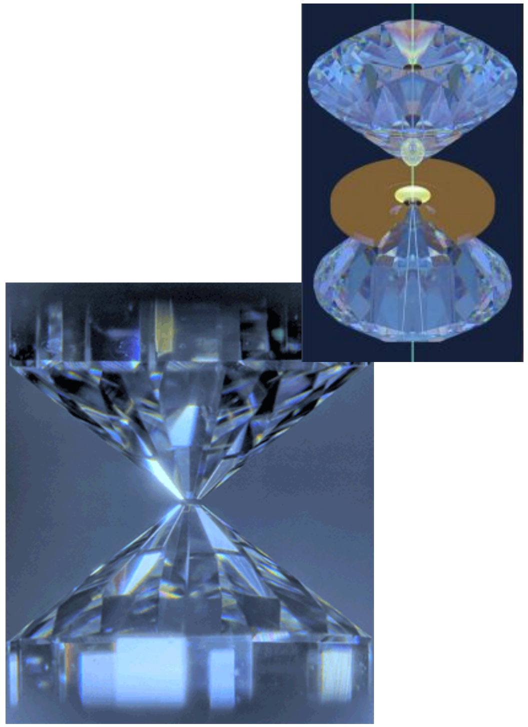
Lecture 4 – 02/10/2024

Strain effect on the band structure

- Introduction: strain, lattice-mismatch
- Elasticity theory



Summary Lecture 3

k.p method

$$u_{n,\mathbf{k}}(\mathbf{r})e^{i\mathbf{kr}}$$

$$\left[\frac{\mathbf{p}^2}{2m_0}+\frac{\hbar\mathbf{k}\cdot\mathbf{p}}{m_0}+\frac{\hbar^2\mathbf{k}^2}{2m_0}+V(\mathbf{r})\right]u_{n,\mathbf{k}}(\mathbf{r})=E_{n,\mathbf{k}}u_{n,\mathbf{k}}(\mathbf{r})$$

$$E_{n,\mathbf{k}}=E_{n,0}+\frac{\hbar^2k^2}{2m_0}+\frac{\hbar^2}{m_0^2}\sum_{n'\neq n}\frac{\left|\langle u_{n',0}|\mathbf{k.p}|u_{n,0}\rangle\right|^2}{E_{n,0}-E_{n',0}}$$

$$\boxed{E_{c,\mathbf{k}}=E_{c,0}+\frac{\hbar^2k^2}{2m_0}\left(1+\frac{P^2}{E_g}\right)=E_{c,0}+\frac{\hbar^2k^2}{2m^*}}$$

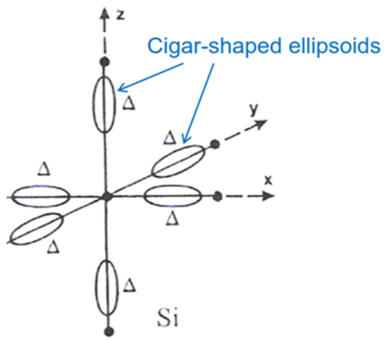
Effective mass

$$\boxed{m^*=m_0\left(1+\frac{P^2}{E_g}\right)^{-1}}$$

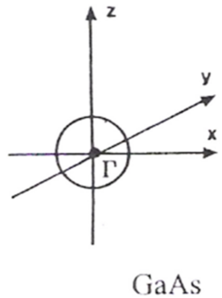
Effective mass

$$\boxed{m^*=\hbar^2\Big/\frac{d^2E}{d\mathbf{k}^2}}$$

$$\boxed{E_c(\mathbf{k})=E_c(0)+\hbar^2\left(\frac{k_1^2}{2m_1}+\frac{k_2^2}{2m_2}+\frac{k_3^2}{2m_3}\right)}$$



Anisotropic case



Isotropic case

Direct bandgap SC:

$$E_c(\mathbf{k})=E_c+\frac{1}{2}\frac{d^2E}{dk^2}k^2=E_c+\frac{\hbar^2k^2}{2m^*}$$

Indirect bandgap SC: $\left(k_\parallel=k_z,\ k_\perp=\sqrt{k_x^2+k_y^2}\right)$

$$E_c(\mathbf{k})=E_c+\frac{1}{2}\frac{d^2E}{dk_\parallel^2}\left(k_\parallel-k_0\right)^2+\frac{1}{2}\frac{d^2E}{dk_\perp^2}k_\perp^2=E_c+\boxed{\frac{\hbar^2}{2m_l^*}\left(k_\parallel-k_0\right)^2}+\boxed{\frac{\hbar^2}{2m_t^*}k_\perp^2}$$

m_l and m_t are the longitudinal and transverse effective masses, respectively

Summary Lecture 3

Valence band structure

- *s*-type (l = 0)
- *p*-type (l = 1), triply degenerate m_l = -1,0,1

Luttinger Hamiltonian because of symmetry:

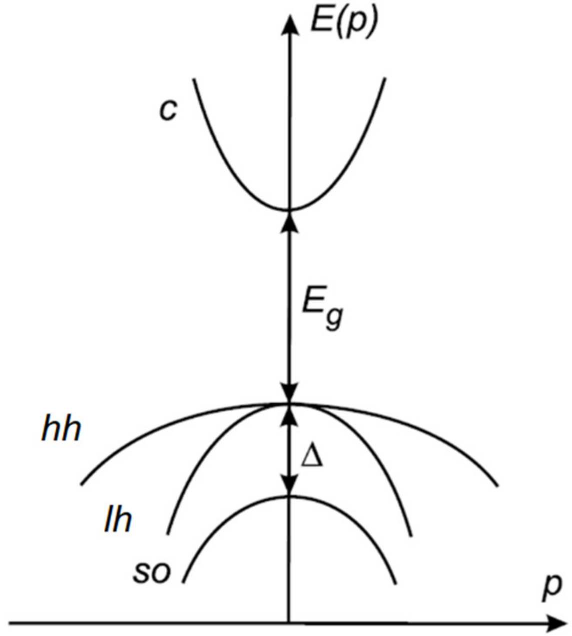
$$\boxed{H = Ap^2 I + B(\mathbf{pL})^2}$$ dim($\mathbf{L}$) = 3 × 3

$$\boxed{E_{hh}(p) = (A+B)p^2 \text{ for } L_z = \pm 1 \quad \text{and} \quad E_{lh}(p) = Ap^2 \text{ for } L_z = 0}$$

Impact of spin-orbit coupling on the VB

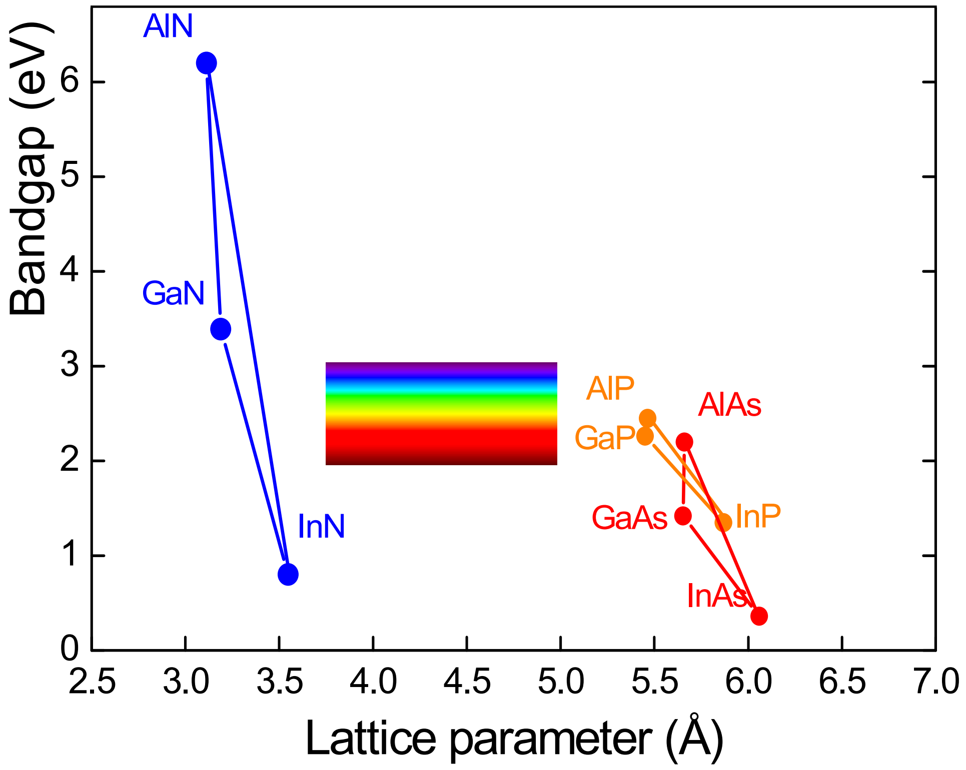
$$\boxed{H = Ap^2 I + B(\mathbf{pJ})^2}$$ dim($\mathbf{J}$) = 4 × 4

$$\boxed{\begin{aligned} E_{hh}(p) &= \left(A + \frac{9B}{4}\right)p^2 = \frac{p^2}{2m_{hh}} \quad (J_z = \pm 3/2) \\ E_{lh}(p) &= \left(A + \frac{B}{4}\right)p^2 = \frac{p^2}{2m_{lh}} \quad (J_z = \pm 1/2) \end{aligned}}$$



Band structure of a zinc-blende SC near the Γ-point

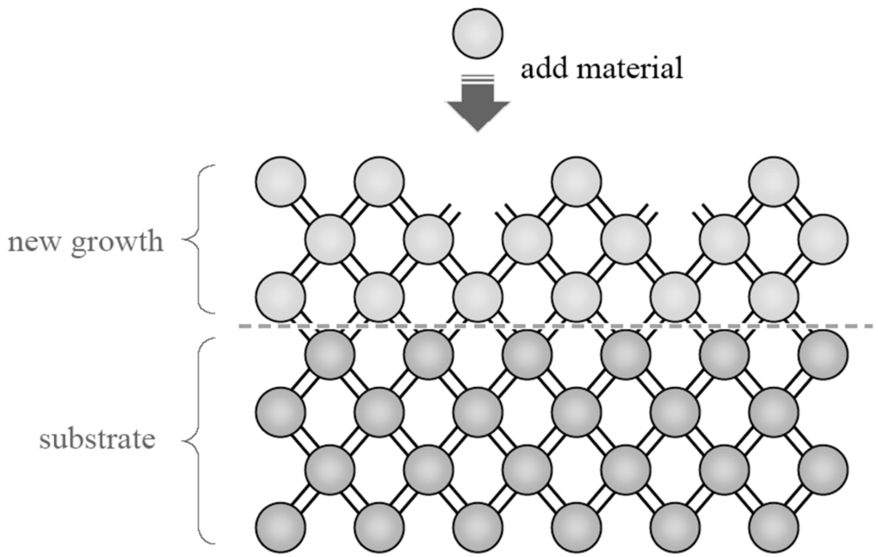
Lattice-mismatch in III-V semiconductors

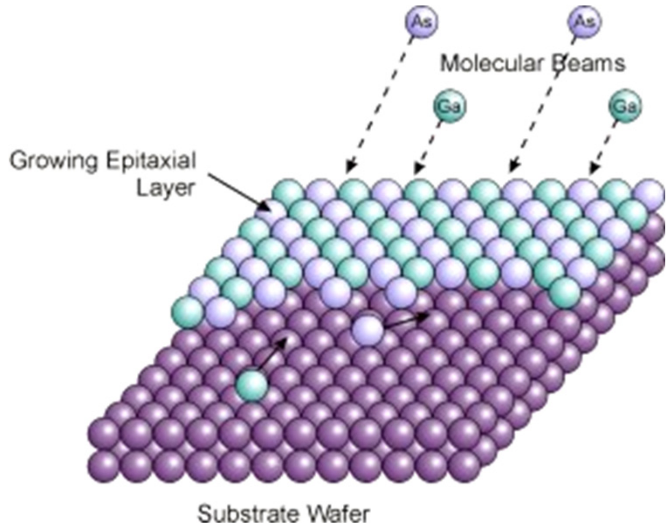


The lattice parameters of semiconductors are almost never the same

$\Rightarrow$ Strain induced in the semiconductor layers

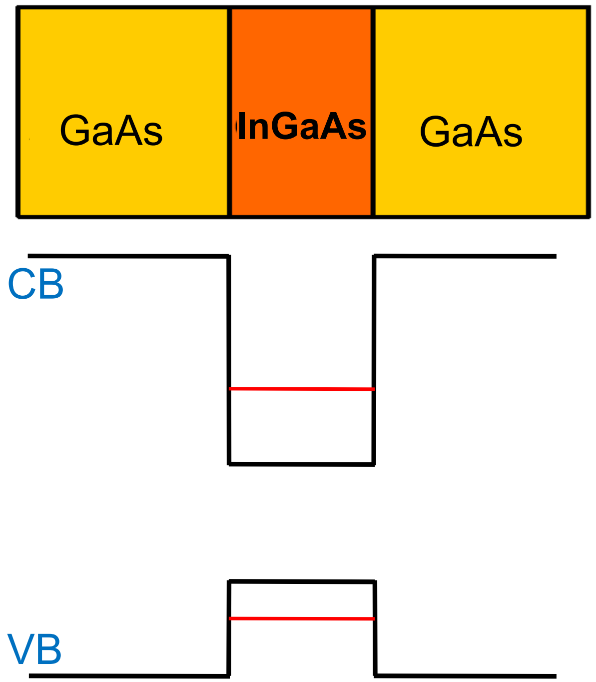
Epitaxial growth

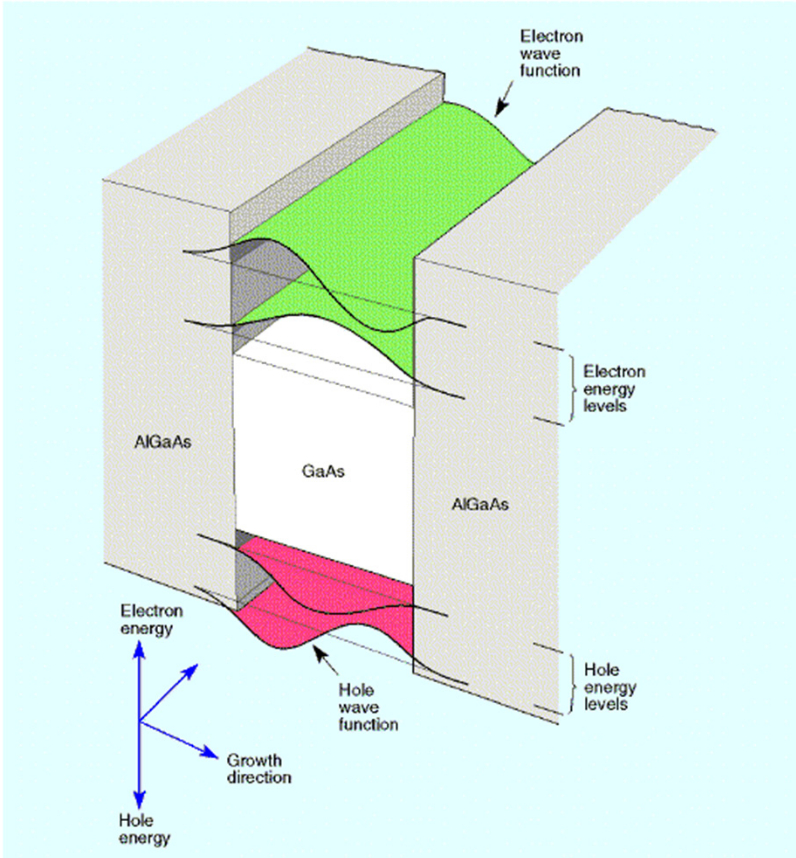




Epitaxy: crystal growth proceeds layer-by-layer and the layer structure complies with the substrate lattice

2D nanostructures: quantum wells

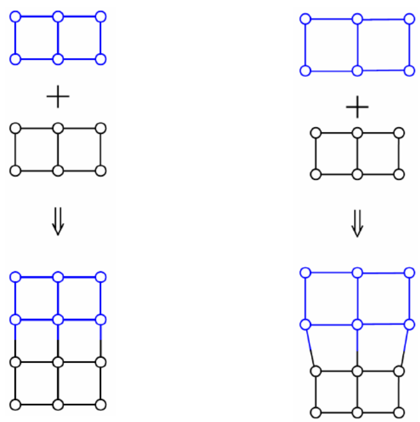


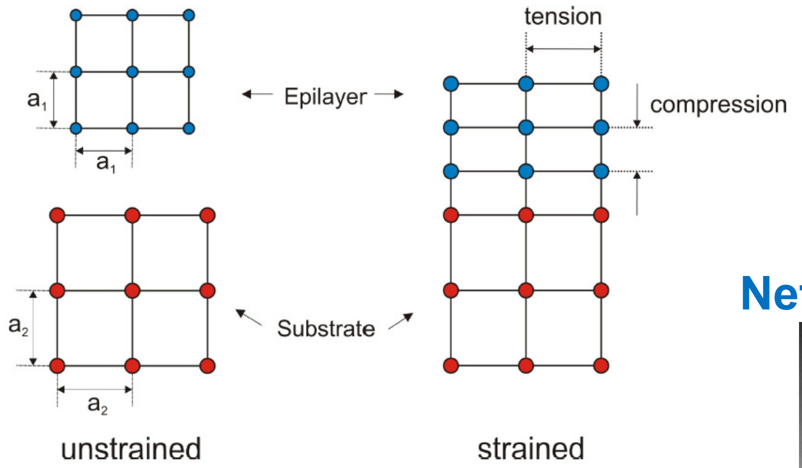


Epitaxial growth: case of heteroepitaxy

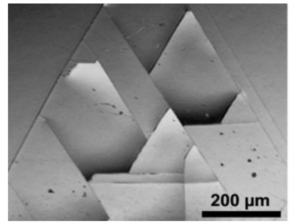
Epitaxial growth – Basic principle and problems

Lattice matched Pseudomorphic



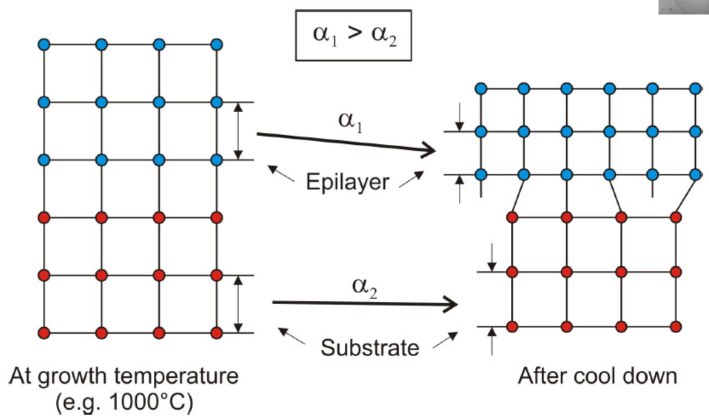


Network of cracks



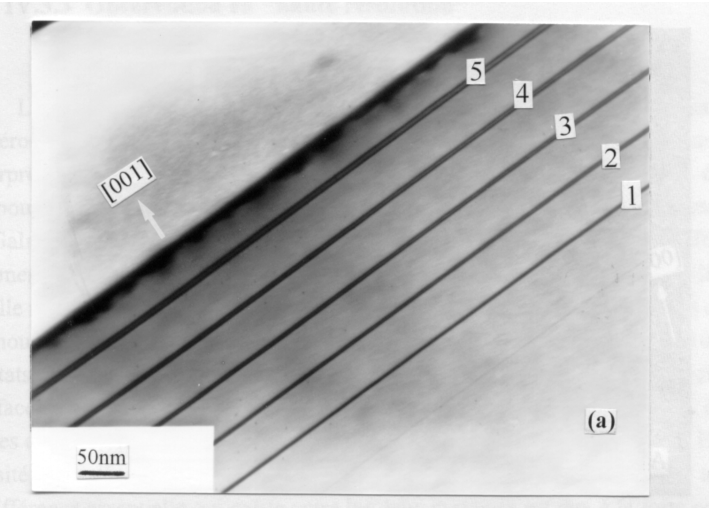
Thermal expansion coefficient (TEC), α

→ different TECs lead to strain in the lattice



Heteroepitaxy: case of InGaAs/GaAs multiple quantum wells

No dislocation

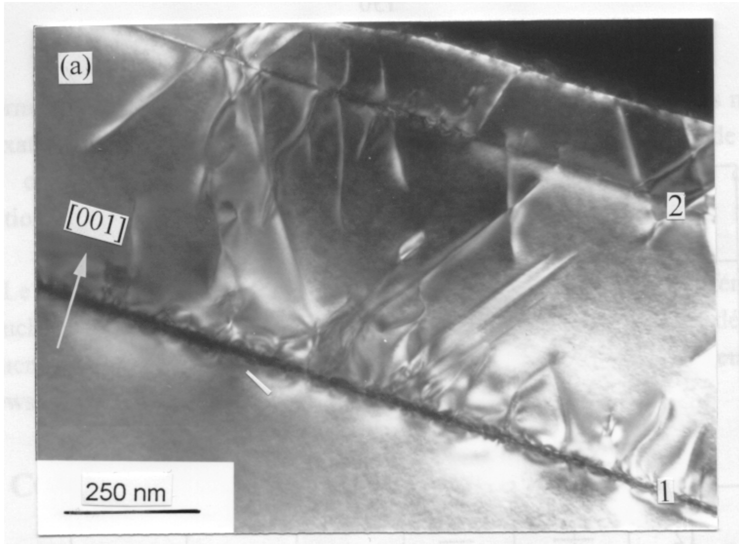


Elastic deformation

(Coherent growth)

TEM

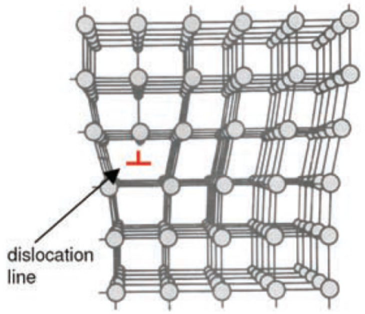
Dislocations

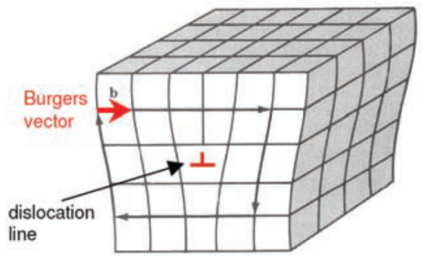


Plastic deformation

Extended defects: threading dislocations

Burgers vector ⇒ It represents the magnitude and direction of the lattice distortion caused by a dislocation in a crystal lattice

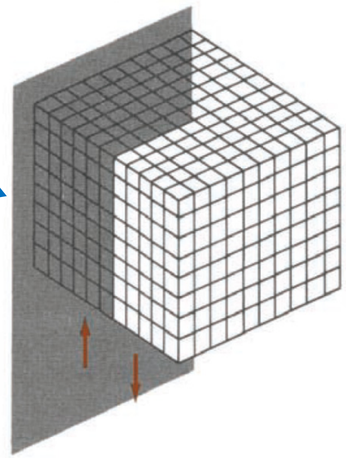


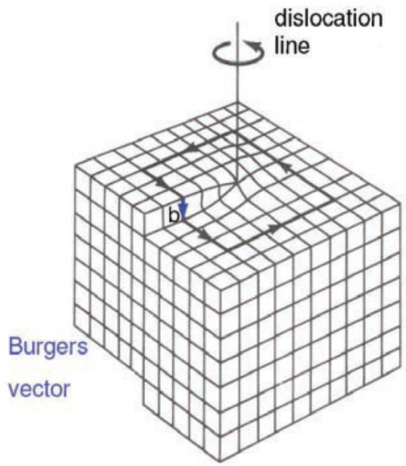


- Edge type dislocation:

The Burgers vector and the dislocation line are at right angles to one another

Gliding plane



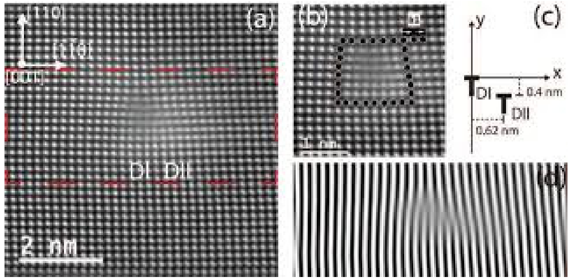


- Screw type dislocation:

The Burgers vector and the dislocation line are parallel

Dislocation usually associated with spiral growth

Imaging dislocations using microscopy techniques

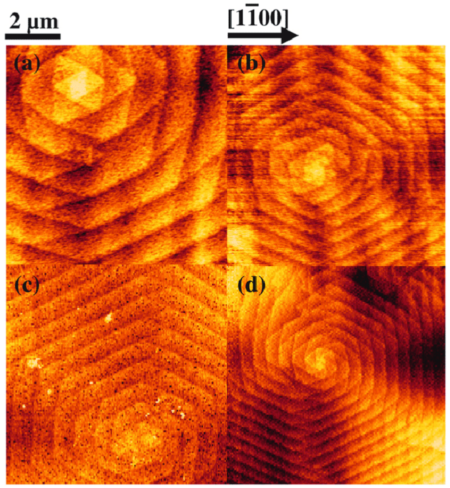


APL **107**, 093501 (2015)

Parallel edge threading dislocations in Ge crystals grown on Si (001) substrate

- Edge type dislocation:

The Burgers vector and the dislocation line are at right angles to one another



N-face GaN (000-1)

APEX **6**, 035503 (2013)

- Screw type dislocation:

The Burgers vector and the dislocation line are parallel

Dislocation usually associated with spiral growth

Critical thickness for plastic relaxation of a 2D layer

Minimizing the total energy density with respect to the dislocation line density yields the critical thickness h_c

h_c can be a macroscopic quantity (> 1 µm)!

$$\boxed{h_c = \frac{Kb^2}{4\pi B f_i b_{,\mathrm{edge}}} \cdot \ln\left(h_c\, \alpha / b\right)}$$

Transcendental equation!

b ($b_{//}$): Burgers vector (edge component)
α: numerical factor accounting for the energy of the dislocation core

$B = 2\mu(1+\nu)/(1-\nu)$ Bulk modulus (infinitesimal pressure increase to relative volume decrease)
$K = \mu/(1-\nu)$ is the dislocation energy coefficient

f_i: misfit between substrate and growing layer
μ: shear modulus (pressure unit)
ν: Poisson's ratio (dimensionless parameter, usually > 0, negative ratio of transverse to axial strain)

F. C. Frank and J. H. van der Merwe, Proc. R. Soc. London, Ser. A **198**, 205 (1949); > 1600 citations
J. H. van der Merwe, Crit. Rev. Solid State Mater. Sci. **17**, 187 (1991).

Strain and heteroepitaxy

Lattice-mismatch: $\Delta a/a = (a_l - a_s)/a_s$

a_s: in-plane lattice parameter of the *substrate*

Strain: $\varepsilon_{//} = (a_s - a_l)/a_l$

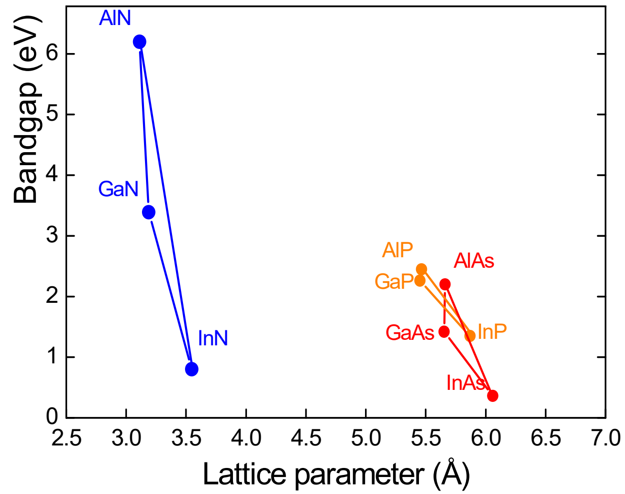
a_l: relaxed value of the in-plane lattice parameter of the *deposited layer*

Example: AlN/GaN combination

$a_{GaN} = 3.189$ Å *and* $a_{AlN} = 3.112$ Å

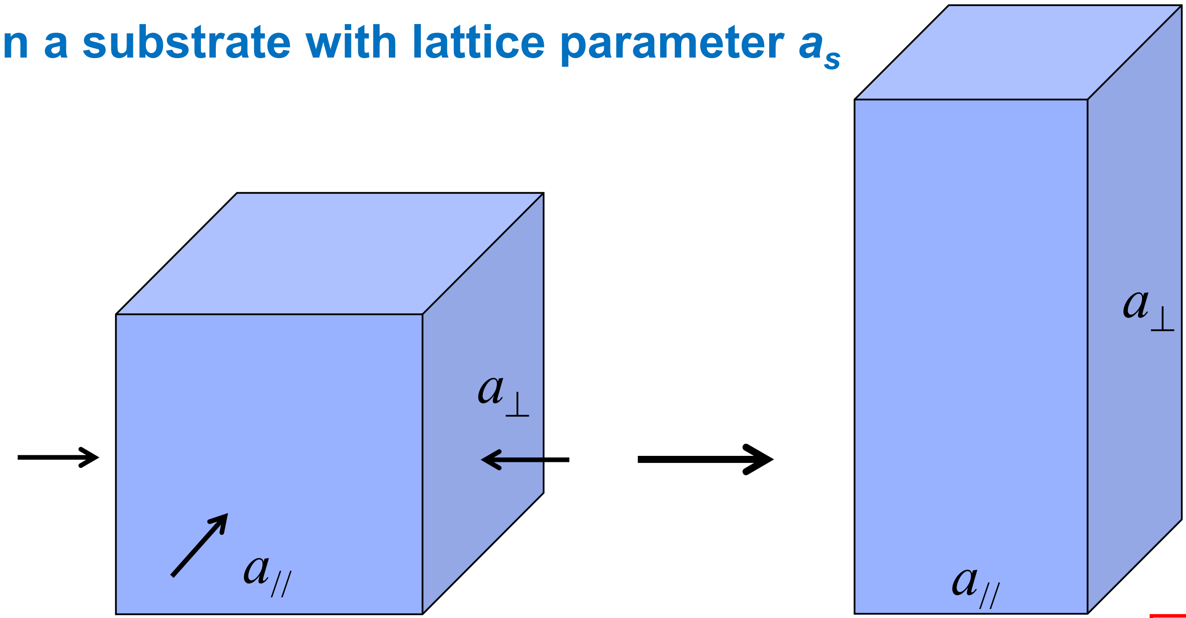
GaN on AlN: $\Delta a/a = 2.47\%$ and $\varepsilon_{//} = -2.42\%$

$\varepsilon_{//} < 0$	compressive strain
$\varepsilon_{//} > 0$	tensile strain



Biaxial strain (compression)

Growth on a substrate with lattice parameter a_s



$\varepsilon_{//} = (a_s - a_l)/a_l$

$a_{//} = a_\perp = a_l$

$a_{//} = a_s$

Deformation at the level of a single monolayer!

$$\boxed{a_\perp = (1 + \varepsilon_\perp)\, a_l}$$

h_c linked to the lattice deformation along the growth axis $a_\perp$

$\Rightarrow$ necessity to determine $\varepsilon_\perp$ to deduce the growth time or the number of monolayers before plastic relaxation occurs $\Rightarrow$ h_c should be an "integer" multiple of $a_\perp$

Elasticity theory

Overview

Elastic deformation:

dimensionless $\equiv$ pressure

Hooke's law: relation between the tensors of deformations ε_{ij}, stress σ_{ij}, and elastic constants C_{ijkl}: $\sigma_{kl} = C_{ijkl}\,\varepsilon_{ij}$ (use of Einstein summation notation (i.e., summation takes place when an index variable appears twice in a single term))

For cubic crystals defined by the crystallographic axes [100], [010] and [001]:

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \times \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

Elasticity theory

Overview

A few words on Voigt notations:

Indices: $\sigma_1 = \sigma_{xx} = \sigma_{11}$, equivalently 2 = y and 3 = z

$\sigma_4 = \sigma_{yz}$, $\sigma_5 = \sigma_{zx}$ and $\sigma_6 = \sigma_{xy}$

The same statement for indices holds for the components of the tensor of deformations $\varepsilon_{i\,=\,1\text{ to }6}$

Elasticity theory

During growth, the surface is stress-free and can freely move along the growth axis (usually coinciding with *z*). Thus, it leads to:

$$\sigma_{13} = 0$$

$$\sigma_{23} = 0$$

$$\sigma_{33} = 0$$

Extra note: The boundary conditions are such that such an epilayer (i.e., a 2D layer heteroepitaxially grown on a substrate) undergoes zero stress in the *z* direction, <u>zero shear stresses</u>, and it has <u>in-plane symmetry of *x* and *y* directions</u>.

In the layer plane, the deformations are identical:

$$\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{//}$$

$$\varepsilon_{12} = 0$$

Let us write (cf. slide 13) $\varepsilon_{\perp} = \varepsilon_{33}$ and $\varepsilon_{//} = (a_l - a_l^0)/a_l^0$

Relaxed value of the in-plane lattice parameter

Elasticity theory: case of epitaxial growth system

[*hkl*] = [001]: **Orientation at play for the CMOS technology (but not only)!**

$$\varepsilon_{13} = 0$$

$$\sigma_{11} = \sigma_{22} = \varepsilon_{//} (C_{11}+2C_{12})(C_{11}-C_{12})/C_{11}$$

$$\boxed{\varepsilon_{\perp} = -2\, C_{12}/C_{11}\, \varepsilon_{//}}$$

Relationship deduced from Hooke's law: a tensile in-plane strain leads to a compressive out-of-plane deformation and vice versa!

Cf. sketch on top of slide 7!

[*hkl*] = [111]:

$$\varepsilon_{13} = 0$$

$$\sigma_{11} = \sigma_{22} = \varepsilon_{//}\, 6C_{44}(C_{11}+2C_{12})/(C_{11}+2C_{12}+4C_{44})$$

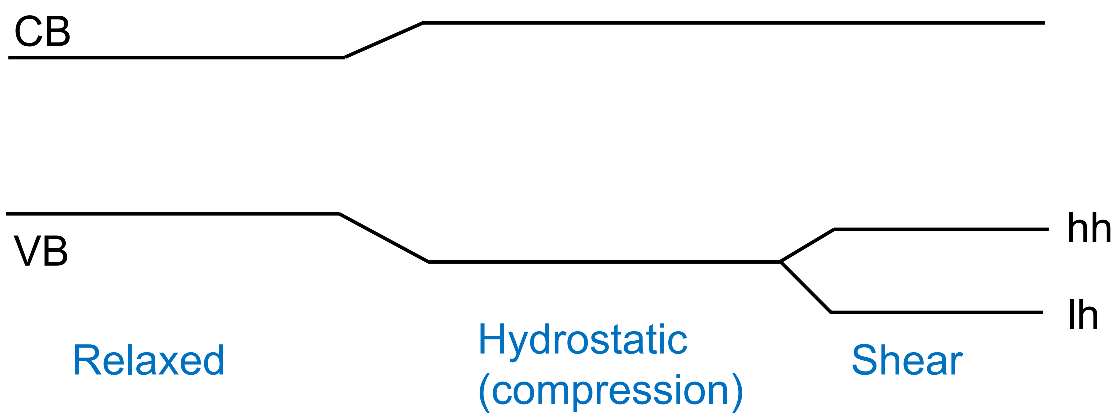
$$\varepsilon_{\perp} = -2\, (C_{11}+2C_{12}-2C_{44})/(C_{11}+2C_{12}+4C_{44})\, \varepsilon_{//}$$

Strain effect on the band structure

The crystal symmetry is changed and thereby the band structure

The strain Hamiltonian can be written as the sum of two components: a purely hydrostatic term H_H and a shear strain term H_S.

$$H = H_H + H_S$$



Case of a cubic semiconductor

Strain effect on the band structure

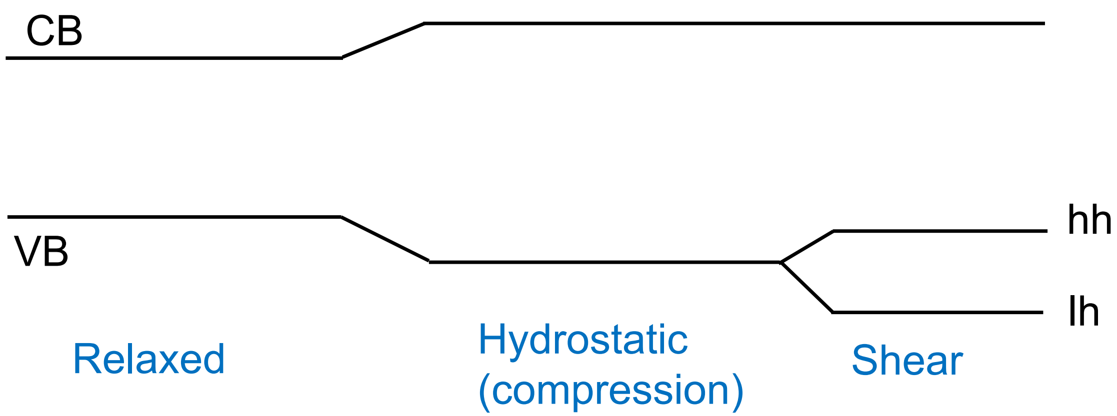
The band structure is affected in different ways by deformations:

1. A volume dilatation (described by LA-phonons at the microscopic scale) does not change the crystal symmetry but the e^--LA phonon interaction is responsible for a change in bandgap (e.g., an increase for hydrostatic pressure)

2. TA-phonons contain shear waves (*shear component LA-phonons less important*) ⇒ shear strain:

(i) does not affect (to 1st order) the energy of a nondegenerate band in a cubic crystal,

(ii) does lift some of the degeneracy of energy bands at high-symmetry points of the 1st Brillouin zone (*Matrix-element theorem + crystal symmetry*)



Cf. Chap. 3
Yu-Cardona

Strain effect on the band structure

$\Sigma_H = 2\,(1 - C_{12}/C_{11})\varepsilon_{//}$ *Hydrostatic deformation*

$\Sigma_S = -2\,(1 + 2C_{12}/C_{11})\varepsilon_{//}$ *Shear deformation*

Cubic semiconductor

"Hydrostatic" term

1. **Conduction band**

   Due to symmetry reasons, only the hydrostatic component plays a role on the CB and E_C changes by $\delta E_C = a_c \Sigma_H$ where a_c is the CB potential of deformation

   Dimensionality: energy

2. **Valence band**

   The hydrostatic component modifies the VB edge E_v by $\delta E_V = a_v \Sigma_H$ where a_v is the VB potential of deformation

Strain effect on the band structure

"Shear" term

The shear strain deeply affects the ordering of the valence band levels (hh, lh, and spin-orbit). Given b_v the potential of deformation due to shear strain and Δ_{SO} the spin-orbit splitting, the energy shifts of hh and lh write

$$\delta E_{hh} = -b_v \Sigma_S$$

$$\delta E_{lh} = -\frac{\Delta_{SO} - b_v \Sigma_S - \sqrt{\left(\Delta_{SO} + b_v \Sigma_S\right)^2 + 8\left(b_v \Sigma_S\right)^2}}{2}$$

Case of zinc-blende SCs

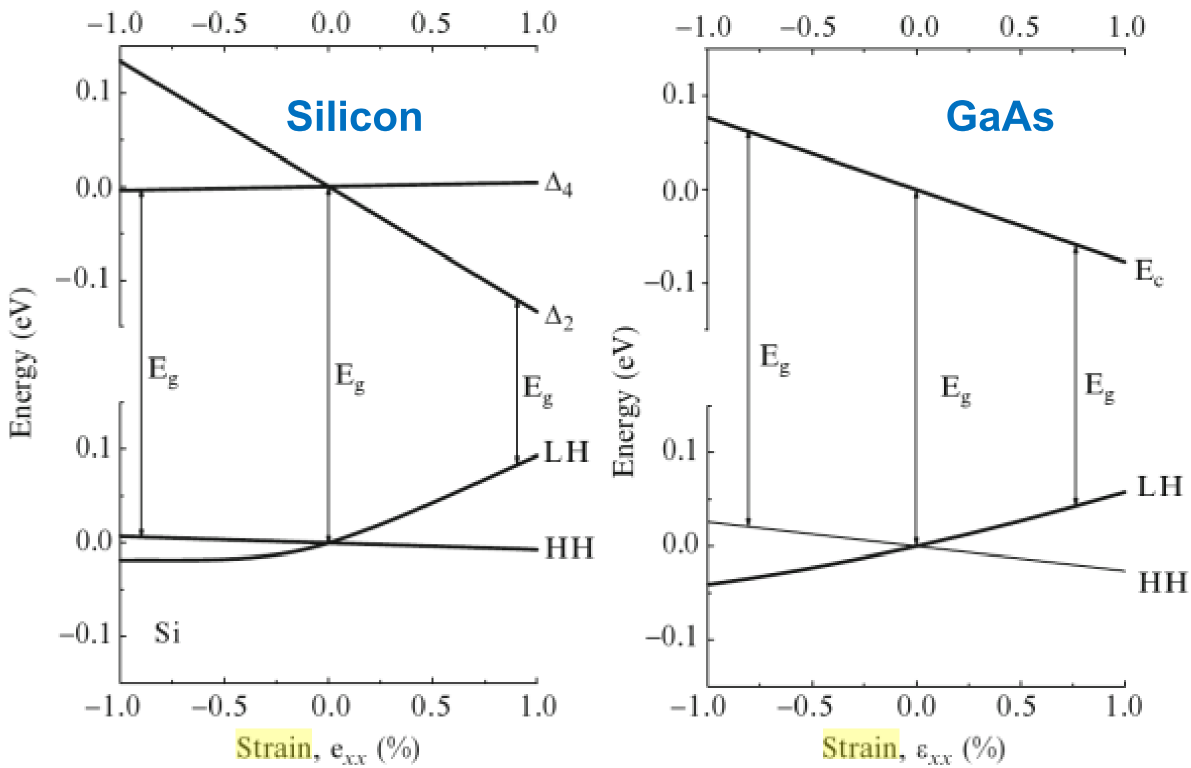
In summary, we have (at the Γ-point):

$$\boxed{\begin{aligned} E_e &= E_V + E_g + a_c \Sigma_H \\ E_{hh} &= E_V + a_v \Sigma_H - b_v \Sigma_S \\ E_{lh} &= E_V + a_v \Sigma_H - \frac{\Delta_{SO} - b_v \Sigma_S - \sqrt{\left(\Delta_{SO} + b_v \Sigma_S\right)^2 + 8\left(b_v \Sigma_S\right)^2}}{2} \end{aligned}}$$

Numerical example using the band structure parameters of GaAs

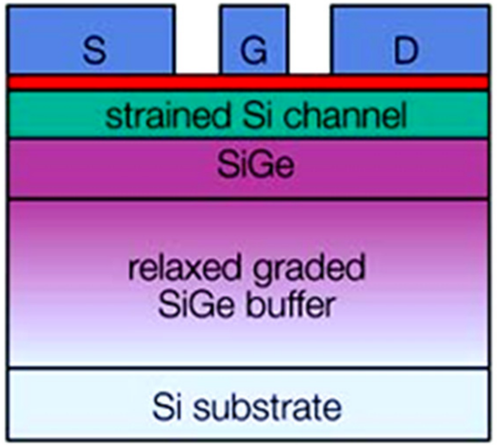
Δ_{SO} (eV)	C_{11} (GPa)	C_{12} (GPa)	a_c (eV)	a_v (eV)	b_v (eV)
0.341	1221	566	-7.17	1.16	-2.0

Strain effect on the band structure

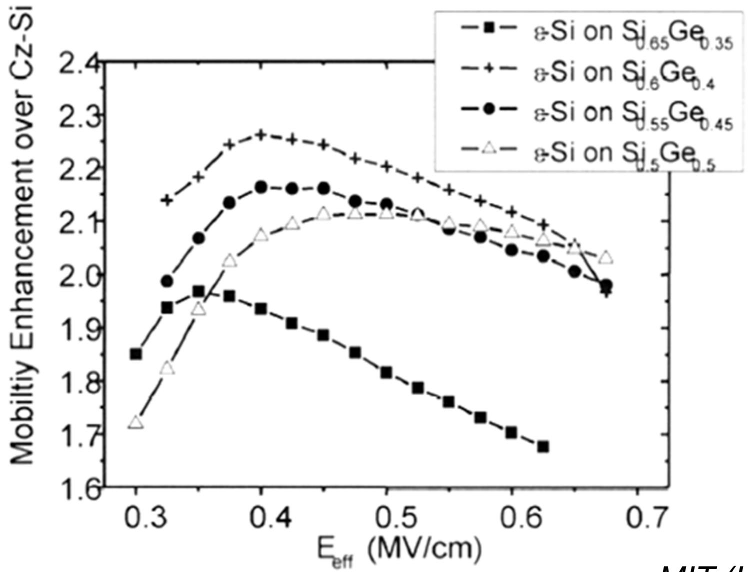


Strain Effect in Semiconductors: Theory and Device Applications
Yongke Sun, Scott Thompson,Toshikazu Nishida

Si/SiGe MOSFET



(a) surface-channel MOSFET



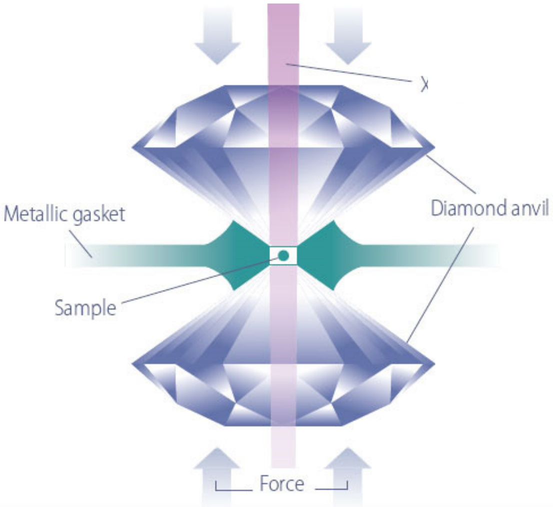
MIT (US) 2003

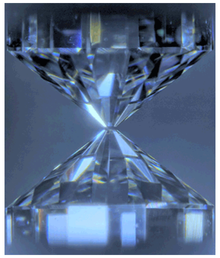
Figure 1. The mobility enhancement of holes vs. vertical field under the gate in PMOSFETs in strained Si for different Ge concentrations in the relaxed $Si_{1-x}Ge_x$ buffer.

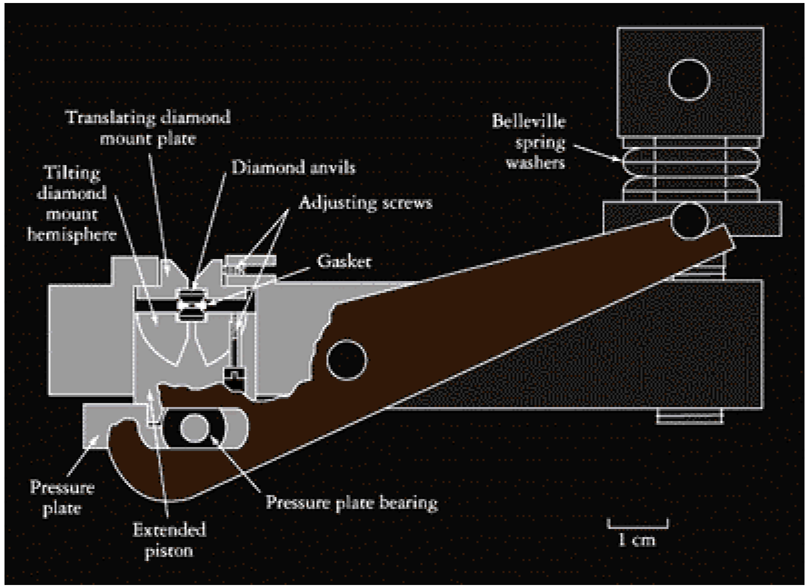
Origin of this MOSFET transistor performance enhancement?

Strain effect on the band structure

- **Hydrostatic strain**
  - Equivalent strain along *x*, *y*, and *z*







- **Biaxial strain**
  - Strain along 2 directions: strained semiconductor epilayers