Lecture contents

• Stress and strain
• Deformation potential
Few concepts from linear elasticity theory: Stress and Strain

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

Stresses applied to a infinitely small volume:

**Strain** = Δdisplacement/ Δcoordinate (3x3 symmetric tensor!)
\[ \varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

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):

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

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

For cubic crystals, only 3 constants are independent:

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

\[
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{12} \\
\sigma_{13} \\
\sigma_{23}
\end{bmatrix} =
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\varepsilon_{12} \\
\varepsilon_{13} \\
\varepsilon_{23}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
\varepsilon_{12} \\
\varepsilon_{13} \\
\varepsilon_{23}
\end{bmatrix} =
\begin{bmatrix}
\sigma_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
\sigma_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
\sigma_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\
\sigma_{11} & \sigma_{12} & \sigma_{12} & \sigma_{11} & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{bmatrix}
\]

\[
\begin{align*}
\sigma_{11} &= c_{11}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{12}\varepsilon_{33}; \\
\sigma_{22} &= c_{12}\varepsilon_{11} + c_{11}\varepsilon_{22} + c_{12}\varepsilon_{33}; \\
\sigma_{33} &= c_{12}\varepsilon_{11} + c_{12}\varepsilon_{22} + c_{11}\varepsilon_{33}; \\
\sigma_{12} &= 2c_{44}\varepsilon_{23}; \\
\sigma_{31} &= 2c_{44}\varepsilon_{31}; \\
\sigma_{12} &= 2c_{44}\varepsilon_{12}.
\end{align*}
\]
Effects of crystal symmetry on elastic constants
Definitions for other elastic constants

For cubic crystal (3 constants are independent):

Anisotropy ratio \( A = \frac{2c_{44}}{c_{11} - c_{12}} \)

For isotropic material, \( A=1 \), only two elastic constants are independent

Lamé coefficient \( \lambda \) and shear modulus \( \mu \):

\[
\begin{align*}
\sigma_{11} &= c_{11} \varepsilon_{11} + c_{12} \varepsilon_{22} + c_{12} \varepsilon_{33}; \\
\sigma_{22} &= c_{12} \varepsilon_{11} + c_{11} \varepsilon_{22} + c_{12} \varepsilon_{33}; \\
\sigma_{33} &= c_{12} \varepsilon_{11} + c_{12} \varepsilon_{22} + c_{11} \varepsilon_{33}; \\
\sigma_{23} &= 2c_{44} \varepsilon_{23}; \\
\sigma_{31} &= 2c_{44} \varepsilon_{31}; \\
\sigma_{12} &= 2c_{44} \varepsilon_{12}. \\
2c_{44} &= c_{11} - c_{12}
\end{align*}
\]

\[
\begin{align*}
\sigma_{11} &= (\lambda + 2\mu) \varepsilon_{11} + \lambda \varepsilon_{22} + \lambda \varepsilon_{33}; \\
\sigma_{22} &= \lambda \varepsilon_{11} + (\lambda + 2\mu) \varepsilon_{22} + \lambda \varepsilon_{33}; \\
\sigma_{33} &= \lambda \varepsilon_{11} + \lambda \varepsilon_{22} + (\lambda + 2\mu) \varepsilon_{33}; \\
\sigma_{23} &= 2\mu \varepsilon_{23}; \\
\sigma_{31} &= 2\mu \varepsilon_{31}; \\
\sigma_{12} &= 2\mu \varepsilon_{12};
\end{align*}
\]

Fractional change of crystal volume under uniform deformation

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

From Singh, 2003
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 isotropic 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: \[ \varepsilon = \frac{a_S - a_L}{a_L} \]

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.
Stress in pseudomorphic epitaxial films

\[ \epsilon_{||} = \frac{a_S}{a_L} - 1 = \epsilon \]

Biaxial strain.
No stress along the growth direction!

For strained growth on (001) substrate & fcc lattice

\[
\begin{align*}
\epsilon_{xx} &= \epsilon_{||} \\
\epsilon_{yy} &= \epsilon_{xx} \\
\epsilon_{zz} &= -\frac{2c_{12}}{c_{11}}\epsilon_{||} \\
\epsilon_{xy} &= 0 \\
\epsilon_{yz} &= 0 \\
\epsilon_{zx} &= 0
\end{align*}
\]

For strained growth on (111) substrate & fcc lattice

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

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

Interatomic spacing
Deformation potential

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

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

- Number of independent non-zero $D_{ij}^{\alpha}$ depends on symmetry of the state $\alpha$

- 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 reduces the electron effective masses

- Strain induces piezoelectric field in polar semiconductor structures

Effect of strain on direct band-edges

$\varepsilon > 0$

- Tensile strain in growth plane

$\varepsilon < 0$

- Compressive strain in growth plane

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

From Singh, 2003
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 $\Gamma_{1c}$ conduction band minimum or the highest energy $\Gamma_{15v}$ valence band maximum (zinc-blende notation). $b$ and $d$ are the shear deformation potentials for the $\Gamma_{15v}$ valence band maximum. $\Xi_d$ and $\Xi_u$ denote deformation potentials at zone boundaries. Most of the data are taken from [3.30]

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

$^a$[100] valleys;


Volume DP for the bandgap

From Yu and Cordona, 2003
Strained $\text{Si}_{1-x}\text{Ge}_x$ / Si

Effect of strain on indirect band-edges

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

From Singh, 2003
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.

**Effect of biaxial tensile strain and quantum confinement on band edges**

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
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