Importance of strains in semiconductors and 
Effect of strain on valence band

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1 Importance of strains in semiconductors

This lecture provides you about the strained layer and the mathematical representation of it in low dimensional semiconductor

In the late 1980s, it was believed that laser devices could only be made reliably from lattice-matched epitaxial materials. By 1999, low cost diode pumped laser were fabricated from the strained-layer. The presence of strains within atoms in a lattice will changes the physical properties and the device obtained from those materials will have enhanced performance. For e.g., strained silicon is a layer of silicon in which the silicon atoms are stretched beyond their normal interatomic distance. This can be done by deposited thin film of silicon over a substrate of silicon germanium (SiGe). As the atoms in the silicon layer align with the atoms of the underlying silicon germanium layer, the bonds between the silicon atoms become stretched - thereby leading to strained silicon. This reduces the atomic forces that interfere with the movement of electrons and can move faster with better mobility. Also allowing strained based silicon transistors to switch faster.

1.1 Strained Layers

In general, the quality of an interface between two materials depends greatly on the relative size of the lattice constants. If the lattice constants are very similar, as in the case of the Al\(_x\)Ga\(_{1-x}\)As and GaAs heterojunctions, for which the lattice constant varies less than 0.2\% for the whole range of \(x\), and the thermal expansion coefficients are similar, no stresses are introduced at the interface. However, in other cases, heterojunctions with differences in lattice constants up to 6\% are fabricated (for instance, In\(_x\)Ga\(_{1-x}\)As and GaAs). In this case strong stresses appear at the interface and only very thin films of a few monolayers can be grown on a given substrate.

These strained layers show new effects that are exploited in various optoelectronic applications, especially in quantum well lasers and electro-optic modulators due to reduced or change in atomic force between atoms in the lattice.

Suppose a layer of lattice constant \(a_L\) is grown on a substrate of lattice constant \(a_S\). The strain \(\varepsilon\) of the layer is define as:

\[
\varepsilon = \frac{a_L - a_S}{a_S}
\]  

(1)

Fig. 1 shows the case of In\(_x\)Ga\(_{1-x}\)As grown on GaAs for which \(a_L > a_S\). In Fig. 1, the situation of the separate layer and substrate is depicted. If the epilayer is not too thick, the atoms of the layer match those of the substrate. Therefore, the layer is subjected to a compressive stress in the plane of the interface and the interplanar vertical (or on the
As a consequence of the distortion of the InGaAs lattice, elastic energy is stored in the system, which increases with layer thickness. Therefore, if the thickness of the film is larger than the so-called critical thickness, the system relaxes and the appearance of dislocations in the plane of the interface is energetically favourable (Fig. 1(c)).

**1.2 Effect of strain on valence bands**

- Electrons in a semiconductor experience the periodic potential of the crystal lattice. This potential leads to the formation of energy bands. The electronic band structure of a semiconductor describes the energy states that an electron is allowed or forbidden.

- Band structure is altered by the application of stress and strain. Both are tensor quantities and are related through Hook's law. To know about the effect of stress/strain on band structure, let we go through the fundamental theory of elasticity of it.

**1.3 Elasticity**

The property of solid materials to deform under the application of an external force and to regain their original shape after the force is removed is referred to as its elasticity. The external force applied on a specified area is known as stress, while the amount of deformation is called the strain. Imagine an object oriented in the cartesian coordinate system with a number of forces acting on it, such that the vector sum of all the forces is zero. Take a slice orthogonal to the -direction and define a small area on this slice as \( \Delta A_x \). Let the total force acting on this small area be...
\[ \Delta F = \Delta F_x \hat{i} + \Delta F_y \hat{j} + \Delta F_z \hat{k} \]  

(2)

We can define the following scalar quantities

\[
T_{xx} = \lim_{
\begin{align*}
\Delta A_{x} \to 0
\end{align*}
}
\frac{\Delta F_x}{\Delta A_x} ,
T_{xy} = \lim_{
\begin{align*}
\Delta A_{y} \to 0
\end{align*}
}
\frac{\Delta F_y}{\Delta A_y} ,
T_{xz} = \lim_{
\begin{align*}
\Delta A_{z} \to 0
\end{align*}
}
\frac{\Delta F_z}{\Delta A_z} 
\]

The subscript \( i \) and \( j \) in \( T_{ij} \) refer to the plane and the force direction, respectively. Similarly considering slices orthogonal to the \( y \) and \( z \)-direction, we obtain

\[
T_{yx} = \lim_{
\begin{align*}
\Delta A_{x} \to 0
\end{align*}
}
\frac{\Delta F_x}{\Delta A_x} ,
T_{yy} = \lim_{
\begin{align*}
\Delta A_{y} \to 0
\end{align*}
}
\frac{\Delta F_y}{\Delta A_y} ,
T_{yz} = \lim_{
\begin{align*}
\Delta A_{z} \to 0
\end{align*}
}
\frac{\Delta F_z}{\Delta A_z} 
\]

\[
T_{zx} = \lim_{
\begin{align*}
\Delta A_{x} \to 0
\end{align*}
}
\frac{\Delta F_x}{\Delta A_x} ,
T_{zy} = \lim_{
\begin{align*}
\Delta A_{y} \to 0
\end{align*}
}
\frac{\Delta F_y}{\Delta A_y} ,
T_{zz} = \lim_{
\begin{align*}
\Delta A_{z} \to 0
\end{align*}
}
\frac{\Delta F_z}{\Delta A_z} 
\]

The scalar quantity can be arranged in a matrix form to yield the stress tensor and the various components are shown in Fig. 2.

\[
T = \begin{pmatrix}
T_{xx} & T_{xy} & T_{xz} \\
T_{yx} & T_{yy} & T_{yz} \\
T_{zx} & T_{zy} & T_{zz}
\end{pmatrix}
\]  

(3)

The condition of static equilibrium implies

\[ T_{ij} = T_{ji} \]  

(4)

Fig. 2. Component of the stress sensor
A body under elastic deformation experiences an internal restoring force. The amount of deformation caused is called strain. Similar to stress, the tensor strain component can be given as

\[
\varepsilon = \begin{pmatrix}
\varepsilon_{xx} & \varepsilon_{xy} & \varepsilon_{xz} \\
\varepsilon_{yx} & \varepsilon_{yy} & \varepsilon_{yz} \\
\varepsilon_{zx} & \varepsilon_{zy} & \varepsilon_{zz}
\end{pmatrix}
\]  

(5)

Such that

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

(6)

The sign convention adopted for stress is that tensile stress causes an expansion, whereas compressive stress causes a contraction.

The relation between stress and strain was given by Hooke's law and it states that the amount by which a material body is deformed (the strain) is linearly related to the force causing the deformation (the stress). The most general relationship between stress and strain can be mathematically written as

\[
\varepsilon_{ij} = S_{ijkl} T_{kl}
\]

(9)

Here, \( S_{ijkl} \) is a fourth order elastic stiffness tensor comprising 81 coefficients. However, depending on the symmetry of the crystal, the number of coefficients can be reduced. For cubic crystals such as Si and Ge, only three unique coefficients, \( C_{11}, C_{12} \), and \( C_{44} \), exist. These coefficients are known as the stiffness constants. The generalized Hooke’s law in matrix form is given as

\[
\begin{pmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6
\end{pmatrix}
= \begin{pmatrix}
c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\
c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & c_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & c_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & c_{44}
\end{pmatrix}
\begin{pmatrix}
\varepsilon_1 \\
\varepsilon_2 \\
\varepsilon_3 \\
\varepsilon_4 \\
\varepsilon_5 \\
\varepsilon_6
\end{pmatrix}
\]

(10)
Of practical interest is the strain arising from a certain stress condition. The strain components can be obtained by inverting Hook's law and utilizing the compliance coefficients $S_{ijkl}$

$$\varepsilon_{ij} = S_{ijkl} T_{lj}$$  \hspace{1cm} (9)

The stiffness and compliance tensors are linked through the relation $S = C^{-1}$. Using this relation, the three independent compliance coefficients can be calculated as

$$s_{11} = \frac{c_{11} + c_{12}}{c_{11}^2 + c_{11} c_{12} - 2c_{12}^2},$$

$$s_{12} = -\frac{c_{11} + c_{12}}{c_{11}^2 + c_{11} c_{12} - 2c_{12}^2},$$

$$s_{44} = \frac{1}{c_{44}}.$$  \hspace{1cm} (10)

It is often required to know the stress in the crystallographic coordinate system for a stress applied along a general direction. Consider a generalized direction $[x', y', z']$ in which the stress is applied. The stress in the crystallographic coordinate system $[x, y, z]$ can be calculated using the transformation matrix $U$.

$$U(\theta, \phi) = \begin{pmatrix} 
\cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\
-\sin \phi & \cos \phi & 0 \\
\sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta 
\end{pmatrix}$$ \hspace{1cm} (11)

Here $\theta$ denotes the polar and $\phi$ the azimuthal angle of the stress direction relative to the crystallographic coordinate system, as shown in Fig.3. The stress in the crystallographic coordinate system is then given by

$$T_{\text{cryst}} = U.T.U^T$$
Applying a non-zero stress of magnitude applied along the [100], [110] and [111] directions, the stress tensors in the principal coordinate system read, respectively

\[
T_{[100]} = \begin{bmatrix} P & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad T_{[110]} = \begin{bmatrix} P/2 & P/2 & 0 \\ P/2 & P/2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad T_{[111]} = \begin{bmatrix} P/3 & P/3 & P/3 \\ P/3 & P/3 & P/3 \\ P/3 & P/3 & P/3 \end{bmatrix}
\]

The corresponding strain tensors are:

\[
\begin{align*}
\varepsilon_{[100]} &= \begin{bmatrix} s_{11}.P & 0 & 0 \\ 0 & s_{12}.P & 0 \\ 0 & 0 & s_{12}.P \end{bmatrix} \\
\varepsilon_{[110]} &= \begin{bmatrix} (s_{11} + s_{12}).P/2 & s_{44}.P/4 & 0 \\ s_{44}.P/4 & (s_{11} + s_{12}).P/2 & 0 \\ 0 & 0 & s_{12}.P \end{bmatrix} \\
\varepsilon_{[111]} &= \begin{bmatrix} (s_{11} + 2s_{12}).P/3 & s_{44}.P/6 & s_{44}.P/6 \\ s_{44}.P/6 & (s_{11} + 2s_{12}).P/3 & s_{44}.P/6 \\ s_{44}.P/6 & s_{44}.P/6 & (s_{11} + 2s_{12}).P/3 \end{bmatrix}
\end{align*}
\]

For the case of epitaxially grown Si on SiGe, the in-plane strain \( \varepsilon_{||} \) is given by Eqn. 1. Consider an interface (primed) coordinate system, the \(-\) axis of which is perpendicular to the Si/SiGe interface. The strain tensor in this coordinate system can be written as

\[
\varepsilon' = \begin{bmatrix} \varepsilon_{11}' & \varepsilon_{12}' & \varepsilon_{13}' \\ \varepsilon_{21}' & \varepsilon_{22}' & \varepsilon_{23}' \\ \varepsilon_{31}' & \varepsilon_{32}' & \varepsilon_{33}' \end{bmatrix}
\]

with \( \varepsilon_{11}' = \varepsilon_{22}' = \varepsilon_{1} \). Since epitaxial growth does not produce any in-plane shear strain in the interface coordinate system, we have \( \varepsilon_{12}' = \varepsilon_{21}' = 0 \)

Other strain components can be determined by considering all the external stress components in the vertical direction vanish i.e. \( T_{13}=T_{23}=T_{33}=0 \) and using Hooke’s law.
Expanding above equation,

\[ 2C_{ij}^{33} \varepsilon_{ij} + 2C_{ij}^{23} \varepsilon_{ij} + 2C_{ij}^{13} \varepsilon_{ij} = - (C_{ij}^{11} + C_{ij}^{12}) \varepsilon_{ij} \]

This can be expressed in matrix form as

\[
\begin{pmatrix}
C_{3333} & C_{3233} & C_{3331} \\
C_{3233} & C_{2333} & C_{2331} \\
C_{3133} & C_{3123} & C_{3131}
\end{pmatrix}
\begin{pmatrix}
\varepsilon_{33}/2 \\
\varepsilon_{23} \\
\varepsilon_{31}
\end{pmatrix}
= - \frac{\varepsilon_{ij}}{2}
\begin{pmatrix}
C_{3311} + C_{3131} \\
C_{2311} + C_{3232} \\
C_{3111} + C_{3122}
\end{pmatrix}
\]

where \( U \) denotes the transformation matrix. Once the matrix elements are known, the matrix can be inverted to determine the \( \varepsilon_{ii} \). Having determined the strain tensor in the interface coordinate system, the tensor can be transformed to the principal coordinate system using

\[ \varepsilon_{ii} = U_{ai}U_{bj} \varepsilon_{ij} \]

Equation A and B can be solved to obtain the strain tensor. Above table lists the expressions for the strain tensor components for the high-symmetry (100), (110) and (111) oriented SiGe substrates. Table 1 summarizes these symmetry points and directions. These points and directions are of importance for interpreting the band structure plots.

<table>
<thead>
<tr>
<th>Substrate orientation</th>
<th>[100]</th>
<th>[110]</th>
<th>[111]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varepsilon_{11} )</td>
<td>( \varepsilon_{1} )</td>
<td>( \varepsilon_{1} )</td>
<td>( \varepsilon_{1} )</td>
</tr>
<tr>
<td>( \varepsilon_{22} )</td>
<td>( \varepsilon_{2} )</td>
<td>( \varepsilon_{2} )</td>
<td>( \varepsilon_{2} )</td>
</tr>
<tr>
<td>( \varepsilon_{33} )</td>
<td>( -\frac{2c_{12}}{c_{11}} )</td>
<td>( \varepsilon_{1} )</td>
<td>( \frac{4c_{44}}{c_{11} + 2c_{12} + 4c_{44}} )</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>( \varepsilon_{12} )</td>
<td>0</td>
<td>( -\varepsilon_{1} \frac{c_{11} + 2c_{12}}{c_{11} + c_{12} + 2c_{44}} )</td>
<td>( -\varepsilon_{1} \frac{c_{11} + 2c_{12}}{c_{11} + c_{12} + 2c_{44}} )</td>
</tr>
<tr>
<td>( \varepsilon_{13} )</td>
<td>0</td>
<td>0</td>
<td>( -\varepsilon_{1} \frac{c_{11} + 2c_{12}}{c_{11} + c_{12} + 2c_{44}} )</td>
</tr>
<tr>
<td>( \varepsilon_{23} )</td>
<td>0</td>
<td>0</td>
<td>( -\varepsilon_{1} \frac{c_{11} + 2c_{12}}{c_{11} + c_{12} + 2c_{44}} )</td>
</tr>
</tbody>
</table>

Fig. 4. (a) Structure of Si crystal lattice (b) Brillouin zone

<table>
<thead>
<tr>
<th>Symmetric points</th>
<th>Direction</th>
<th>Coordinate</th>
<th>Remark</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( \Gamma )</td>
<td>(0,0,0)</td>
<td>Origin of ( k ) space</td>
</tr>
<tr>
<td></td>
<td>( X )</td>
<td>(1,0,0)</td>
<td>Middle of square faces</td>
</tr>
<tr>
<td></td>
<td>( L )</td>
<td>( \left( \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) )</td>
<td>Middle of hexagonal faces</td>
</tr>
<tr>
<td></td>
<td>( K )</td>
<td>( \left( \frac{3}{4}, \frac{3}{4}, \frac{3}{4} \right) )</td>
<td>Middle of edge shared by two hexagons</td>
</tr>
<tr>
<td></td>
<td>( U )</td>
<td></td>
<td>Middle of edge shared by</td>
</tr>
<tr>
<td></td>
<td>hexagons and square</td>
<td></td>
<td></td>
</tr>
<tr>
<td>----</td>
<td>---------------------------------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$W$</td>
<td>Middle of edge shared by two hexagons and square</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Delta$</td>
<td>$\langle 1,0,0 \rangle$ Directed from $\Gamma$ and $X$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Lambda$</td>
<td>$\langle 1,1,1 \rangle$ Directed from $\Gamma$ and $L$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\Sigma$</td>
<td>$\langle 1,1,0 \rangle$ Directed from $\Gamma$ and $K$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

2 Effect of strain on valence band

This lecture deals about the change in band structure in strained layers of semiconducting materials

Several symmetry operations can be performed on the diamond structure which leave the structure unchanged. Apart from translation, such operations can be categorized as rotation or inversion, or a combination, and are collectively known as symmetry operations. Due to the fcc lattice of the diamond structure there exist a total of 48 such independent symmetry operations. This symmetry of the lattice in real space is also reflected in the first Brillouin zone. The lowering of symmetry of the fcc structure due to strain can distort it to some of the 14 Bravais lattice forms, such as the tetragonal, orthorhombic or trigonal lattice. The new lattice structure formed has different symmetry properties which can have pronounced consequences on the band structure. Numerical methods for calculating the band structure allow the prediction of several important electronic and optical properties.
At T=0K, the highest energy band that is completely filled is denoted as the valence band. The next higher band is completely empty at and called the conduction band. The two bands are separated by a forbidden energy gap, known as the bandgap $E_g$.

The principal conduction band minima of Si are located along the [100], [010] and [001] directions at a distance of about 85% from the -point to the X-points. The minima of the second conduction band touch the first conduction band at the X-points. This degeneracy of the two conduction bands can produce interesting effects on applying shear strain we discussed earlier. Close to the principal minima the band structure can be represented by ellipsoidal constant energy surfaces by assuming a parabolic energy dispersion relation. For valleys located along the [100] direction, the energy dispersion reads

$$\varepsilon(k) = \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_i} + \frac{k_y^2}{m_i} + \frac{k_z^2}{m_i} \right)$$

where the wave vector $k = (k_x, k_y, k_z)$. The constant energy surfaces are described by a longitudinal mass, $m_i = 0.91 \cdot m_o$, and a transversal mass $m_i = 0.19 \cdot m_o$. This anisotropy in the masses makes the transport in each valley anisotropic. The 6-fold degeneracy of the valleys arise due to the symmetry of the lattice along the [100], [010] and [001]
directions. At low values of the electric field, the electrons occupy all the 6 valleys equally and thus the transport is isotropic.

Unlike the conduction band, the valence band structure looks highly anisotropic even in the unstrained case. The valence band maximum in Si is located at the $\Gamma$ point. Due to the degeneracy of the bands at the $\Gamma$ point, the energy surfaces develop into quadratic surfaces of the form

$$
\varepsilon_{hh}(k) = -Ak^2 - \sqrt{B^2 k^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)}
$$

$$
\varepsilon_{lh}(k) = -Ak^2 + \sqrt{B^2 k^4 + C^2 (k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2)}
$$

Here $\varepsilon_{hh}(k)$ and $\varepsilon_{lh}(k)$ denote the energies of the two degenerate bands and the parameters A, B and C denote the inverse band parameters. Due to the smaller energy values of the $\varepsilon_{hh}(k)$ bands in comparison to the $\varepsilon_{lh}(k)$, the effective masses for the $\varepsilon_{hh}(k)$ band is larger. Therefore, this band is referred to as the heavy hole (HH) band and the $\varepsilon_{lh}(k)$ band as the light hole (LH) band. The shape of the constant energy surface for the LH and HH bands is warped or fluted. There is also a third band, the so called split-off band located about 44 meV below the HH/LH bands. A schematic plot of the constant energy surface for the HH band is shown in Fig. 4(b)

### 2.1 Band structure in quantum well and exciton effect

Quantum wells are formed in semiconductors by having a material, like gallium arsenide sandwiched between two layers of a material with a wider bandgap, like aluminium arsenide. Because of their quasi-two dimensional nature, electrons in quantum wells have a density of states as a function of energy that has distinct steps, versus a smooth square root dependence that is found in bulk materials. Additionally, the effective mass of holes in the valence band is changed to more closely match that of electrons in the conduction band. The optical properties of quantum well strongly depend upon band structure. For example, in multiple quantum well of GaAs-AlGaAs, the optical spectrum follows in general the steps of the density of state curve in two dimensional
semiconductors. At the edge of each step there will be a sharp maximum and is attributed to excitonic effects.

In the case of confined systems for electrons and holes, such as quantum wells, wires, and dots, the excitonic effects are much more important than in bulk solids. In effect, the binding energy of the electron–hole system forming an exciton is much higher in quantum confined systems than in the case of solids, and, therefore, the excitonic transitions can be observed even at temperatures close to room temperature, as opposed to the bulk case for which low temperatures are needed. This makes the role played by excitons in many modern optoelectronic devices very important. Qualitatively, it is easy to understand the reason by which the binding energies of excitons $E_B$ in quantum confined systems are much higher than in the bulk. For instance, in the case of bulk GaAs the binding energy of excitons is only $E_B = 0.2 \text{meV}$ and the Bohr radius has a fairly large value of about $a_B = 150\text{Å}$. In the figure, the exciton is represented in two situations, the one in (a), in which the Bohr radius of the exciton is much smaller than the quantum well width, and the one in (b), for which the width of the well is smaller than $a_B$. In this case, the separation between the electron and the hole is limited by the width of the well and therefore the exciton becomes squeezed, thus increasing the Coulomb attractive force. For a two-dimensional hydrogenic atom, a simple calculation shows that $E_B$ is about four times larger in the 2D case than for 3D solid. Another consequence of their high value of $E_B$ is that excitons can survive very high electric fields in quantum wells which will find many applications in electro-optic modulators.
3 Quiz and Assignment

1. For an isotropic material with \( E = 100 \text{GPa} \) and \( \nu = 0.25 \). Find the stress tensor and strain energy density at a point in a body if the components of the strain tensor are given by

\[
\varepsilon_{ij} = \begin{bmatrix} 200 & 100 & 0 \\ 100 & 200 & 100 \\ 0 & 100 & 0 \end{bmatrix} \times 10^{-6}
\]

2. A solid is subjected to stresses as shown by the arrows in the figure below. Indicate the indices for each of the stress components, and whether the stresses should be positive or negative.

3. Suppose that the stress tensor field in a body is given by

\[
\sigma_{ij} = \begin{bmatrix} x_1^2 + x_2 & -2x_3^2 & x_1^2 + x_2 \\ 2x_3^2 & x_1 + x_3 & -x_3^2 + x_2 \\ x_1^2 + x_2 & -x_3^2 + x_2 & x_1^2 + x_2 \end{bmatrix} \text{MPa}
\]

Find the body force distribution required to maintain equilibrium. (\(x_1, x_2, \text{and} x_3\) are in meters). Show units.

4. Find the surface tractions at the internal point \( r = (1,-1,2) \) in the body on an internal surface with a surface normal \( \hat{n} = (-1,-1,1) \).

5. Find the hydrostatic and deviatoric stress at the point \( r = (1,-1,2) \). Find the principal stresses at this point.

6. Diamond structure has the \( \text{___________} \) lattice and exist a \( \text{_____} \) Symmetry operations.

7. The principal conduction band minima of Si are located along the \( \text{___________} \) directions.

8. The band present in between the light and heavy hole band is called as \( \text{_______} \)

9. How Quantum well is formed?

10. The optical properties of quantum well strongly depend upon \( \text{___________} \)
3.1 Solutions

1. The shear modulus (μ) is given by,

\[ \mu = \frac{E}{2(1 + \nu)} = \frac{100}{2.5} = 40 \text{GPa} = 40 \times 10^6 \text{ KPa} \]

The Lamé modulus (λ) is given by

\[ \lambda = \frac{E \nu}{(1 + \nu)(1 - 2\nu)} = \frac{25}{(1.25)(0.5)} = 40 \text{GPa} = 40 \times 10^6 \text{ KPa} \]

The stress-strain relation for isotropic materials is

\[ \sigma_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij}\]

Therefore, (after converting and into KPa so that the 10^{-6} term in the strain cancels out),

\[ \sigma_{11} = 40[2\varepsilon_{11} + \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}] = 40[(3)(200) + 200 + 0] = (40)(800) = 32000 \]
\[ \sigma_{22} = 40[2\varepsilon_{22} + \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}] = 40[(3)(200) + 200 + 0] = (40)(800) = 32000 \]
\[ \sigma_{33} = 40[2\varepsilon_{33} + \varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33}] = 40[(3)(0) + 200 + 200] = (40)(400) = 16000 \]
\[ \sigma_{23} = 40[2\varepsilon_{23}] = (40)(200) = 8000 \]
\[ \sigma_{31} = 40[2\varepsilon_{31}] = (40)(0) = 0 \]
\[ \sigma_{12} = 40[2\varepsilon_{12}] = (40)(200) = 8000 \]

In 3 x 3 matrix form (after converting into MPa from KPa)

\[ \sigma_{ij} = \begin{bmatrix} 32 & 8 & 0 \\ 8 & 32 & 8 \\ 0 & 8 & 16 \end{bmatrix} \text{ MPa} \]

The strain energy density is given by

\[ U(\varepsilon) = \frac{1}{2} \sigma_{ij} \varepsilon_{ij} \]
Therefore,

\[ U(\varepsilon) = \frac{1}{2} \left[ \sigma_{11} \varepsilon_{11} + \sigma_{22} \varepsilon_{22} + \sigma_{33} \varepsilon_{33} + \sigma_{23} \varepsilon_{23} + \sigma_{31} \varepsilon_{31} + \sigma_{12} \varepsilon_{12} \right] \]

\[ = \frac{1}{2} \left[ (32)(200) + (32)(200) + (16)(0) + (2)(8)(0) + (2)(0)(0) + (2)(8)(100) \right] Pa \]

\[ = \frac{1}{2} [6400 + 6400 + 1600 + 1600] Pa \]

\[ = 8000 Pa = 8KPa \]

The strain energy density is \( U = 8KPa \)

2.

3. The equation of equilibrium is

\[ \nabla \cdot \sigma + b = 0 \] or \( \sigma_{ij} + b_j = 0 \)

Therefore,
\[
\begin{align*}
&\frac{\partial}{\partial x_1}(x_1^2 + x_2) + \frac{\partial}{\partial x_2}(-2x_1^2) + \frac{\partial}{\partial x_3}(x_1^2 + x_2) + b_1 = 0 \\
&\frac{\partial}{\partial x_1}(-2x_3^2) + \frac{\partial}{\partial x_2}(x_1^2 + x_2) + \frac{\partial}{\partial x_3}(-x_3^2 + x_2) + b_2 = 0 \\
&\frac{\partial}{\partial x_1}(x_2^2 + x_2) + \frac{\partial}{\partial x_2}(-x_3^2 + x_2) + \frac{\partial}{\partial x_3}(x_1^2 + x_2) + b_3 = 0
\end{align*}
\]

(or)

\[
\begin{align*}
2x_1 + 0 + 0 + b_1 &= 0 \\
0 + 0 - 2x_3 + b_2 &= 0 \\
2x_1 + 1 + 0 + b_3 &= 0
\end{align*}
\]

The required body forces are (in MN/m\(^3\))
\[
b_1 = -2x_1; b_2 = 2x_3; b_3 = -(1 + 2x_1)
\]

4. The surface traction is given by
\[
t = \hat{n} \cdot \sigma \quad \text{or} \quad t_j = n_i \sigma_{ij}
\]

The stress at point \( r \) is
\[
[\sigma] = \begin{bmatrix}
0 & -8 & 0 \\
-8 & 3 & -5 \\
0 & -5 & 0
\end{bmatrix} \text{MPa}
\]

Therefore
\[
\begin{align*}
t_1 &= n_1 \sigma_{11} + n_2 \sigma_{21} + n_3 \sigma_{31} \\
&= (-1)(0) + (-1)(-8) + (1)(0) = 8 \text{MPa}
\end{align*}
\]
\[
\begin{align*}
t_1 &= n_1 \sigma_{12} + n_2 \sigma_{22} + n_3 \sigma_{32} \\
&= (-1)(-8) + (-1)(3) + (1)(-5) = 0 \text{MPa}
\end{align*}
\]
\[
\begin{align*}
t_1 &= n_1 \sigma_{13} + n_2 \sigma_{23} + n_3 \sigma_{33} \\
&= (-1)(0) + (-1)(-5) + (1)(0) = 5 \text{MPa}
\end{align*}
\]

The traction vector is (after converting \( n^\wedge \) into a unit normal)
\[
t = \left(\frac{1}{\sqrt{3}}\right)(8,0,5) \text{MPa}
\]

5. The hydrostatic stress is given by
\[
\sigma_h = \frac{t \cdot r \cdot \sigma}{3} I
\]
In this case
\[ t \cdot r \cdot \sigma = \sigma_{11} + \sigma_{22} + \sigma_{33} = 0 + 3 + 3 = 3 \]
Therefore,
\[
\sigma_h = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\end{bmatrix} \text{ MPa}
\]
The deviatoric stress is given by
\[ \sigma_d = \sigma - \sigma_h \]
Therefore,
\[
\sigma_d = \begin{bmatrix}
-1 & -8 & 0 \\
-8 & 2 & -5 \\
0 & -5 & -1 \\
\end{bmatrix} \text{ MPa}
\]
The principal stresses can be found using the equation
\[ \det(\sigma - \lambda I) = 0 \]
where is a principal stress. In expanded form,
\[
\det \begin{bmatrix}
\sigma_{11} - \lambda & \sigma_{12} & \sigma_{13} \\
\sigma_{12} & \sigma_{22} - \lambda & \sigma_{23} \\
\sigma_{13} & \sigma_{23} & \sigma_{33} - \lambda \\
\end{bmatrix} = 0
\]
Substituting the values of stress into the above equation,
\[
\det \begin{bmatrix}
-\lambda & -8 & 0 \\
-8 & 3-\lambda & -5 \\
0 & -5 & -\lambda \\
\end{bmatrix} = 0
\]
Expanding out,
\[
-\lambda\left[(3-\lambda)(-\lambda) - (-5)(-5)\right] - (-8)\left[(-8)(-\lambda) - (-5)(0)\right] = 0
-\lambda(-3\lambda + \lambda^2 - 25) + 8(8\lambda) = 0
3\lambda^2 - \lambda^3 + 25\lambda + 64\lambda = 0
\lambda^3 - 3\lambda^2 - 89\lambda = 0
\]
Thus, the first possible value of \( \lambda = 0 \) MPa.
Also
\[ \lambda^2 - 3\lambda - 89 = 0 \]

Therefore,

\[ \lambda = \frac{3 \pm \sqrt{9 + 356}}{2} = (11.05, -8.05) \text{MPa} \]

The principal stresses are (in MPa)

\[ \sigma_1 = 11.05; \quad \sigma_2 = 0; \quad \sigma_3 = -8.05; \]

6. fcc, 48
7. [100], [010] and [001]
8. Split off band.
9. Quantum wells are formed as low band gap semiconductors material is
   sandwiched between two layers of a wider band gap material.
10. Band structure

5 References

[1] L.O. Lokot, Strain effect on the valence band structure, optical transitions, and
    light gain spectra in zinc-blende GaN quantum wells, Semiconductor Physics,
    First-principles investigation of strain effect on the energy gaps in silicon