Chapter

1

STRUCTURAL PROPERTIES OF SEMICONDUCTORS

X-RAY DIFFRACTION

Classical particles such as electrons, neutrons, and classical waves such as X-rays can be used to map out the crystal structure.

Optical path difference between waves reflected from adjacent planes is $2d \sin \theta$.

Constructive interference \rightarrow bright spots



(a) Wavelength versus energy for photons and electrons. (b) Geometry used to derive Bragg's law.

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STRUCTURAL ISSUES: HETEROSTRUCTURES Semiconductor devices (and test structures) are fabricated on a substrate which is sliced from a "boule." The boule is a large crystal (as large as 1 meter long, 30 cm diameter for silicon) grown by bulk crystal growth.



There are very few materials which can be grown as large as single crystals by bulk crystal growth. As a result, there are only a few available substrates. Here are some important substrates:

Si: lattice constant 5.431 Å	; large wafers are available
GaAs: lattice constant 5.653Å	(up to 30 cm). ; high quality wafers up to
InP: lattice constant	 is cm are available. is high quality wafers ~10 is are available.
Quartz; Sapphire	; wafers of ~2-3 cm are available
Ge: lattice constant 5.658Å.	
SiC: lattice constant 4.36 Å	; small substrates are available

GaN: work in progress with great potential payoff.

HETEROEPITAXY

Most semiconductor devices involve growth of a thin (~ microns) of a semiconductor layer on top of a substrate. In general, the overlayer and substrate will have different lattice constants: a_L and a_S , respectively.

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



CRITICAL THICKNESS AND PSUEDOMORPHIC GROWTH In general the initial growth of the overlayer occurs so that the overlayer "fits" to the lattice constant of the substrate. For example, if: $a_L > a_S$, there is a compression in the plane of the growth and an expansion in the growth direction. Once the overlayer thickness exceeds a critical thickness : $d_c \left(\sim \frac{a_L}{2\epsilon} \right)$ dislocations are generated.



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STRAIN TENSOR (ε_{ij}) : THEORY What is the nature of the strain tensor in an epitaxial film?



Undistorted structure axes

$$\mathbf{x'} = (1 + \varepsilon_{xx}) \mathbf{x} + \varepsilon_{xy} \mathbf{y} + \varepsilon_{xz} \mathbf{z}$$
$$\mathbf{y'} = \varepsilon_{yx} \mathbf{x} + \varepsilon_{yy} \mathbf{y} + \varepsilon_{zz} \mathbf{z}$$
$$\mathbf{z'} = \varepsilon_{zx} \mathbf{x} + \varepsilon_{zy} \mathbf{y} + \varepsilon_{zz} \mathbf{z}$$

Distortion
$$\mathbf{R} = \mathbf{r'} - \mathbf{r} = (x \ \varepsilon_{xx} + y \ \varepsilon_{yx} + z \ \varepsilon_{zx}) \mathbf{x}$$

$$= (x \ \varepsilon_{xy} + y \ \varepsilon_{yy} + z \ \varepsilon_{zy}) \mathbf{y}$$

$$= (x \ \varepsilon_{xz} + y \ \varepsilon_{yz} + z \ \varepsilon_{zz}) \mathbf{z}$$

$$\equiv u(r) \mathbf{x} + v(r) \mathbf{y} + w(r) \mathbf{z}$$

$$\varepsilon_{xx} = \frac{\partial u}{\partial x}; \ \varepsilon_{yy} = \frac{\partial v}{\partial y}; \ \varepsilon_{zz} = \frac{\partial w}{\partial z}$$

$$e_{xy} = x' \cdot y' \approx \varepsilon_{yx} + \varepsilon_{xy} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial x}$$

$$e_{yz} = y' \cdot z' \approx \varepsilon_{zy} + \varepsilon_{yz} = \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y}$$

$$e_{zx} = z' \cdot x' \approx \varepsilon_{zx} + \varepsilon_{xz} = \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x}$$
Dilation = $\mathbf{x'} \cdot (\mathbf{y'} \times \mathbf{z'}) - \mathbf{x} \cdot (\mathbf{y} \times \mathbf{z}) \approx \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}$

erms arise listortion.

STRAIN-STRESS RELATIONS



For cubic systems: $(e \equiv \varepsilon)$

	<i>e</i>	<i>e</i>	<i>e</i>	<i>e</i>	<i>e</i>	<i>e</i>
	- XX	Зуу	- 22	- <i>yz</i>	- ZX	- xy
X_{x}	c ₁₁	c ₁₂	c ₁₂	0	0	0
Y_{y}	c ₁₂	c ₁₁	c ₁₂	0	0	0
$\dot{Z_z}$	c ₁₂	c ₁₂	c ₁₁	0	0	0
Y_{z}	0	0	0	c ₄₄	0	0
Z_{x}	0	0	0	0	c ₄₄	0
X_y	0	0	0	0	0	c ₄₄

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$$U = \frac{1}{2}c_{11}(e_{xx}^{2} + e_{yy}^{2} + e_{zz}^{2}) + \frac{1}{2}c_{44}(e_{yz}^{2} + e_{zx}^{2} + e_{xy}^{2}) + c_{12}(e_{yy}e_{zz} + e_{zz}e_{xx} + e_{xx}e_{yy})$$

Bulk modulus, Compressibility
For uniform dilation, δ
 $e_{xx} = e_{yy} = e_{zz} = \frac{1}{3}\delta$
 $U = \frac{1}{6}(c_{11} + 2c_{12})\delta^{2}$

 $= \frac{1}{2}B \,\delta^2$ where *B* is the bulk modules $B = \frac{1}{3}(c_{11} + 2c_{12})$

Compressibility: $K = \frac{1}{B}$

Elastic constants (10¹¹ N/m² or 10¹² dynes/cm²)

Material	c ₁₁	c ₁₂	c ₄₄
Si	1.66	0.639	0.796
Ge	1.285	0.483	0.668
GaAs	1.188	0.538	0.594
С	10.76	1.25	5.76
InSb	0.672	0.367	0.302

STRAIN TENSOR IN AN EPITAXIALLY GROWN ATOMICALLY SMOOTH FILM $\varepsilon_{\parallel} = \frac{a_L}{a_S} - 1$ Coherent growth Compressive strain Tensile strain in the plane in the plane Substrate plane (001) Substrate plane (111) Poisson ratio $\sigma = \frac{c_{11}}{2c_{12}}$ $\sigma = \frac{c_{11} + 2c_{12} + 4c_{44}}{2c_{11} + 4c_{12} - 4c_{44}}$ $\mathbf{\varepsilon}_{xx} = \mathbf{\varepsilon}_{//}$ $\boldsymbol{\varepsilon}_{xx} = \left[\frac{2}{3} - \frac{1}{3} \left(\frac{2c_{11} + 4c_{12} - 4c_{44}}{c_{11} + 2c_{12} + 4c_{44}}\right)\right] \boldsymbol{\varepsilon}_{//}$ $\varepsilon_{yy} = \varepsilon_{xx}$ $\varepsilon_{yy} = \varepsilon_{xx}$ $\mathbf{\epsilon}_{zz} = \frac{-2\mathbf{c}_{12}}{\mathbf{c}_{11}} \mathbf{\epsilon}_{//} \quad \mathbf{\epsilon}_{zz} = \mathbf{\epsilon}_{xx}$ $\varepsilon_{xy} = \left[\frac{-1}{3} - \frac{1}{3} \left(\frac{2c_{11} + 4c_{12} - 4c_{44}}{c_{11} + 2c_{12} + 4c_{44}} \right) \right] \varepsilon_{//}$ $\varepsilon_{xy} = 0$ $\begin{aligned} \mathbf{\varepsilon}_{yz} &= \mathbf{0} \\ \mathbf{\varepsilon}_{zx} &= \mathbf{0} \end{aligned}$ $\varepsilon_{yz} = \varepsilon_{xy}$ $\varepsilon_{7x} = \varepsilon_{y7}$

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HIGH STRAIN EPITAXY: RECIPE FOR "SELF-ASSEMBLED" DOTS A very interesting effect occurs as strain is increased.



Lateral feature sizes can be controlled from 100 Å-1000 Å $\implies 10^{12}$ features per wafer can be produced without lithography.

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STRAIN EFFECTS AND PIEZOELECTRIC EFFECT

Strain induced distortion of atomic positions can lead to a net dipole moment and generate polarization in a material. This effect is called the piezoelectric effect and can be exploited for strain sensors, built-in electric field and/or charge generation in devices, etc.

Piezoelectric effect is strong in a variety of materials, such as quartz, $BaTiO_3$, lead zinconate titanate (PZT). It is also significant in a variety of semiconductors, such as GaN, AlN, GaAs, etc.



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POLARIZATION, ELECTRIC FIELD, AND STRAIN

Polarization and strain tensor is related by piezoelectric coefficients:

ZINC BL	ENDE STRUCTURE) (W	URTZITE		
$P_{x} = e_{14}$	ε _{yz}	Growth along <i>c</i> -axis			
$P_{y} = e_{14}$	ϵ_{xz}	ϵ_{xx}	$= \mathbf{\epsilon}_{yy} = \frac{a_S}{a_L} -$	1	
$P_{z} = e_{14}$	ϵ_{xy}	٤ _{٢٢} =	$=\frac{-2C_{13}}{C_{33}}\left(\frac{a_S}{a_L}-1\right)$	l)	
• For a strained film grown on (001) substrate $P_{pz} = 0$		$P_{pz} = e_{33} \varepsilon_{zz} + e_{31} (\varepsilon_{xx} + \varepsilon_{yy})$			
		$F_{pz} = -\frac{1}{\varepsilon_s} \left[e_{33} \varepsilon_{zz} + e_{31} \left(\varepsilon_{xx} + \varepsilon_{yy} \right) \right]$			
• For a strained film grown on		For InGaN system			
(111) substrate $P_x = P_y = P_z = e_{14} \varepsilon_{xy}$		$\frac{C_{12}}{C_{22}} = \frac{1.09 \times 10^{12} \text{ N/m}^2}{3.55 \times 10^{12} \text{ N/m}^2}$			
$ P_{pz}(111) $	$ =\sqrt{3} e_{14} \varepsilon_{xy}$	$\varepsilon_s = 10.2 \varepsilon_o$			
Electric	field $F_{pz} = \frac{-\sqrt{3} e_{14} \varepsilon_x}{\varepsilon_s}$	Σ <u>Υ</u>			
ZINC BLENDE		WURTZITE (<i>c</i> -axis growth)			
Material	e_{14} (C/m ²)	Material	e_{31} (C/m ²)	e_{33} (C/m ²)	
AlAs	-0.23	AlAs	-0.6	1.46	
GaAs	-0.16	GaN	-0.49	0.73	
GaSb	-0.13	InN	-0.57	0.97	
GaP	-0.10				

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-0.05

-0.04

InAs

InP

RANGE OF ELECTRIC FIELD PRODUCED BY PIEZOELECTRIC EFFECTS

Nitride system:	MATERIAL	<i>a</i> (Å)	<i>a</i> (Å)	c/a		
<i>c</i> -axis growth	InN	3.54	5.70	1.61		
	GaN	3.189	5.185	1.625		
	AlN	3.11	4.98	1.601		
Al _x Ga _{1-x} N grown on GaN: $P_{pz} = (-3.2x - 1.9x^{2}) \ 10^{-6} \text{ C cm}^{-2}$ $F_{pz} = (-3.5x - 2.1x^{2}) \text{ MV/cm}$ Interface charge: $(2.0x + 1.19x^{2}) \ 10^{13} \text{ e/cm}^{2}$ In _x Ga _{1-x} N on GaN: $P_{pz} = (14.1x + 4.9x^{2}) \ 10^{-6} \text{ C cm}^{-2}$ $F_{pz} = (15.7x + 5.5x^{2}) \text{ MV/cm}$ Interface charge: $(8.8x + 3.06x^{2}) \ 10^{13} \text{ e/cm}^{2}$						

In_xGa_{1-x}As on GaAs: (111) Growth $P_{pz} = (-0.89x + 0.61x^2) \ 10^{-6} \text{ C cm}^{-2}$ $F_{pz} \cong (-0.7x + 0.5x^2) \text{ MV/cm}$ Interface charge: $(-5.56x + 3.8x^2) \ 10^{12} \text{ e/cm}^2$

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SPONTANEOUS POLARIZATION

In many materials there is a displacement of the cation sublattice with respect to the anion sublattice resulting in a net polarization along the displacement. In ferroelectric materials this displacement can be altered by an external field. However, in materials like InN, GaN, AlN, the polarization is not tailorable by an external field.

NITRIDES IN WURTZITE STRUCTURES:



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EFFECTS OF SPONTANEOUS POLARIZATION AND PIEZOELECTRIC EFFECT INDUCED POLARIZATION

At heterointerfaces of two semiconductors with polarization P_1 and P_2 , a net charge density $\frac{P_1 - P_2}{e}$ is produced can be exploited to induce free charge in electronic

 \Rightarrow devices or to introduce built-in electric fields.

In strained materials with spontaneous polarization the polarization from the two effects add vectorially.

Example: AlGaN grown on GaN



Eg., for Ga-face AlGaN containing 30% Al, the positive sheet charge induced by *SP* and *PE* at the interface is 1.7×10^{13} e/cm².

How can piezoelectric effect and spontaneous polarization be exploited in devices?



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FERROELECTRIC MATERIALS: SPONTANEOUS POLARIZATION

Relative movement of cations and anions



(a) The structure of a typical perovskite crystal illustrated by examing barium titanate. (b) The ferroelectric effect is produced by a net displacement of the positive ions with respect to the negative ions.

FERROELECTRIC EFFECT

Polarization in the material changes as a function of external field.



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