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Physics

Physics at Nanoscale – IV

Strain and stress at heterointerface

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Description of Module	
Subject Name	Physics
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4.3 Stress and strain in heterostructure

4.3.1 Heterstructure with mismatched lattice

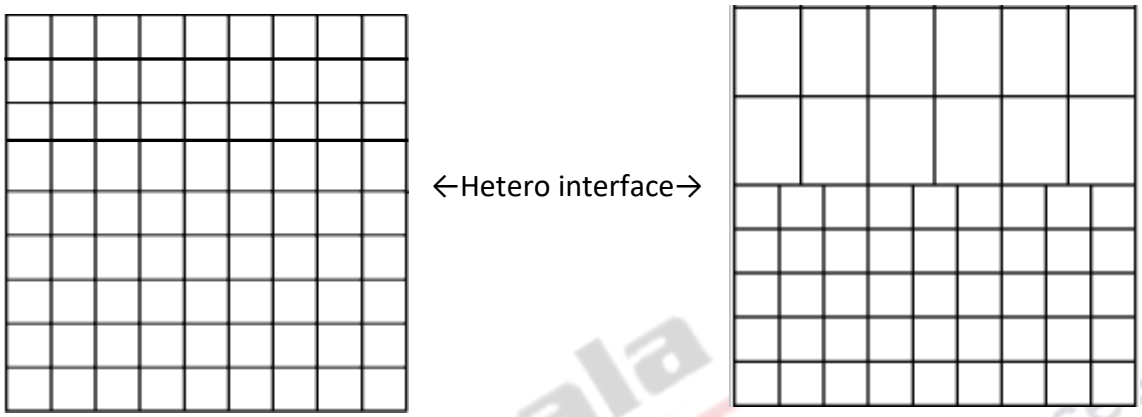

Figure 4.9 *Hetero structure with two participating semiconductors having (a) same, (b) different lattice constants.*

When a thin layer of material is grown on a different semiconductor, there arises two different situation, (a) lattice matching: if the lattice constants of both semiconductors are same, (b) lattice mismatching: if the lattice constants of both semiconductors are different, as shown in Figure 4.9.

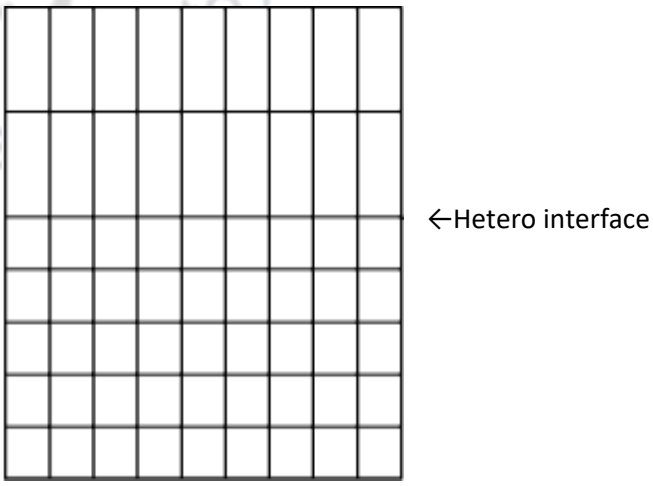

Figure 4.10 *Top thin epitaxial layer strained to adjust its lattice constant to the underlying semiconductor layer.*

In case of lattice mismatched hetero-structure, the epitaxial layer that has a significantly different lattice constant, will be forced to adjust its lattice constant of the bottom layer if the lattice mismatch is less than about 10%. When the top epitaxial layer adopts the lattice constant of the bottom layer, it becomes strained, i.e., it is either compressed or expanded from its usual lattice structure in bulk. There exists a maximum thickness of the thin layer below which the lattice mismatch can be accommodated through strain, as shown in Figure 4.10. For layer thickness above the critical thickness, the lattice mismatch cannot be accommodated through strain resulting dislocations at the hetero interface. When the thickness of the top layer is less than critical thickness, the strained layer can be in either compressive or tensile strain which is homogenous within the layer. If the lattice constant of the top layer is less than that of the underlying layer the hetero structure will be in tensile strain and if the lattice constant of the strained layer is greater than that of the underlying layer, the hetero structure will be in compressive strain.

4.3.2 Stress Tensor

Strain is a measure of the change in length due to small deformations caused by an applied force per unit area, known as stress. The stress and strain are tensor quantities which have nine components that describe the relative stress and strain along the principal directions of the crystal. The stress vector P_n acting at a point P on a surface with unit normal vector **n** is defined as

$$\boldsymbol{P_n} = \lim_{A \to 0} \frac{F}{A} \qquad (4.20)$$

Where F is the force and A is the area of the surface. The stress vector can be written as

$$\boldsymbol{P_n} = \sigma \boldsymbol{n} \qquad (4.21)$$

Where σ is the stress tensor and **n** the normal vector. Expanding Eq. 4.21 yields

$$\begin{aligned} \boldsymbol{P_1} &= \sigma_{11}\widehat{\boldsymbol{e_1}} + \sigma_{12}\widehat{\boldsymbol{e_2}} + \sigma_{13}\widehat{\boldsymbol{e_3}} \\ \boldsymbol{P_2} &= \sigma_{21}\widehat{\boldsymbol{e_1}} + \sigma_{22}\widehat{\boldsymbol{e_2}} + \sigma_{23}\widehat{\boldsymbol{e_3}} \qquad (4.22) \\ \boldsymbol{P_3} &= \sigma_{31}\widehat{\boldsymbol{e_1}} + \sigma_{32}\widehat{\boldsymbol{e_2}} + \sigma_{33}\widehat{\boldsymbol{e_3}} \end{aligned}$$

Where e_1,e_2 and e_3 are the three normal vectors to the ordinate planes. In case of cubic symmetry, general coordinates e_1,e_2 and e_3 are vectors along x, y, and z directions. P_1 represents the stress vector acting on the surface whose outward normal vector is e_1 and P_1 has three components, σ_{11}, σ_{12} , and σ_{13}. σ_{11} is the normal component, and σ_{12} and σ_{13} are the tangential components of the stress vector. Here, σ_{12} is the stress is along the $\mathbf{e}_1$ direction acting on the plane with a normal vector parallel to the e_2 axis. Therefore, in this case, σ_{12} , the stress is tangential to the surface of the plane and is called a *shear stress*. The stress component σ_{11} is the normal component of the stress on the 23 plane and is called *normal stresses*. If the normal stress is positive, acting outward from the surface, it is called a *tensile stress*. If the normal stress is negative, acting inward toward the surface, it is called a *compressive stress*.

The general relationship between the stress tensor $\sigma_{ij}$and the strain tensor $\varepsilon_{kl}$is then given as

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \qquad (4.23)$$

The index *i* indicates the direction of the component of the force per unit area on a plane whose normal is parallel to the e_j direction. C_{ijkl} is the elasticity tensor which can be simplified by some inherent symmetries that reduce the number of independent components of C. The first simplification arises from the fact that there can be no net torque from external forces on an infinitesimal volume element. Therefore, the stress components must obey

$$\sigma_{ij} = \sigma_{ji} \qquad (4.24)$$

Similarly, $\varepsilon_{kl} = \varepsilon_{lk.}$Therefore, the components of the elasticity tensor must obey

$$C_{ijkl} = C_{jikl} = C_{ijlk} = C_{jilk} \qquad (4.25)$$

The elasticity tensor can be further simplified as follows. The differential work done, dW, when a unit volume element is reversibly deformed by differential strain increments $d\varepsilon_{ij}$ is

$$dW = \sigma_{ij}d\varepsilon_{ij} = C_{ijkl}\varepsilon_{kl}\, d\varepsilon_{ij} \qquad (4.26)$$

For an isothermal system, $dW=dF$, where F is Helmholtz free energy.

$$dF = C_{ijkl}\varepsilon_{kl}\, d\varepsilon_{ij} \qquad (4.27)$$

Taking the second derivative of F with respect to ε, Eq. 4.28 becomes

$$\frac{\partial^2 F}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}} = C_{ijkl} \qquad (4.28)$$

$$\frac{\partial^2 F}{\partial\varepsilon_{kl}\partial\varepsilon_{ij}} = C_{klij} \qquad (4.29)$$

As dF is an exact differential, so

$$\frac{\partial^2 F}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}} = \frac{\partial^2 F}{\partial\varepsilon_{KL}\partial\varepsilon_{ij}} \qquad (4.30)$$

$$C_{ijkl} = C_{klij} \qquad (4.31)$$

Which implies that C is symmetric along the diagonal. It is clear that for the multiplication of C and ε to be valid, the number of elements in the rows of C must match the number of elements in the columns of ε . σ_{ij} and ϵ_{ij} have nine elements each, that C_{ijkl} must then be 9 x 9. The multiplication is then between C, a 9×9 matrix, and ε, a 9×1 matrix to form σ, a 9×1 matrix. The multiplication can now be written in matrix form as

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{31}\\ \sigma_{12}\\ \sigma_{32}\\ \sigma_{13}\\ \sigma_{21}\end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{14} & c_{15} & c_{16}\\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{24} & c_{25} & c_{26}\\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} & c_{34} & c_{35} & c_{36}\\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}\\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56}\\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66}\\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} & c_{44} & c_{45} & c_{46}\\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} & c_{45} & c_{55} & c_{56}\\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} & c_{46} & c_{56} & c_{66}\end{bmatrix} \qquad (4.32)$$

Since ij = kl by Eq. 4.31, we can replace ij by m and kl by n. For a material with cubic symmetry, the system is invariant under a rotation by 90^0 about the cubic axes. As a result, only three independent components remain of the original 81 elements of C for the cubic case. These are c_{11},c_{12} and c_{44}, which are equal to

$$c_{11} = c_{1111} = c_{2222} = c_{3333}$$

$$c_{12} = c_{1122} = c_{1133} = c_{2233} \qquad (4.33)$$

$$c_{44} = c_{1212} = c_{2323} = c_{3131}$$

With these simplifications, the elastic constants matrix C for a cubic material becomes

$$C_{mn} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} \qquad (4.34)$$

Based on this analysis of stress and strain, the origin of strain induced piezoelectricity can be understood in hetero-structures and how these fields can potentially be utilized in hetero-structure based devices. As discussed before, the lattice mismatch between two semiconductor layers can be adjusted either through the formation of misfit dislocations or by strain depending on the thickness of the top epitaxial layer. If the thickness of the top layer is less than critical thickness, the lattice mismatch is adjusted by either tensile or compressive strain which, in turn, results strain-induced polarization fields. In addition to electric filed due to hetero-interface, the strain-induced polarization fields can also alter the carrier concentration at the interface of hetero-structure by changing the local electric field profile. Hence, the carrier concentration at hetero-interface can be modulated without modulation doping.

4.3.3 Stress induced polarization in semiconductor heterostructure

A polarization field can be produced within a material when a stress is applied to it. This is known as the *direct piezoelectric effect* and can be expressed mathematically as

$$P_I = d_{ijk}\sigma_{jk} \qquad (4.35)$$

where the components of d are called the *piezoelectric moduli*. Equatio 4.35 implies that each component of P depends upon all the components of σ. P_1 given by Eq. 4.35 can be expanded out as

$$P_1 = d_{111}\sigma_{11} + d_{112}\sigma_{12} + d_{113}\sigma_{13} + d_{121}\sigma_{21} + d_{122}\sigma_{22} + d_{123}\sigma_{23} + d_{131}\sigma_{31} + d_{132}\sigma_{32} + d_{133}\sigma_{33} \qquad (4.36)$$

Similar equations can be written for P_2 and P_3. Using the repeated index notation, Eq. 4.36 can be written in a much simpler and compact form as

$$P_1 = d_{1jk}\sigma_{jk} \qquad (4.37)$$

where, as is usual, there is an implied sum over both indices j and k on the right-hand side. It is useful to relate the polarization field P to the strain ε using Eqs. 4.24 and 4.37 In matrix form, P can be written as

$$P = d\sigma = d(C\varepsilon) = e\varepsilon \qquad (4.38)$$

which is in component form

$$P_I = d_{ijk}C_{jklm}\varepsilon_{lm} = e_{ilm}\varepsilon_{lm} \qquad (4.39)$$

Depending on the symmetry of the crystal, only some components are nonzero in Eq. 4.39. In this way, an expression for the polarization vector can be obtained from the piezoelectric tensor e and the strain tensor ε. The strain induced polarization is important in group III-nitride semiconductor materials which crystallize in the wurtzite phase, as shown in Figure 4.11 and form highly strained heterostructure and are strongly piezoelectric.

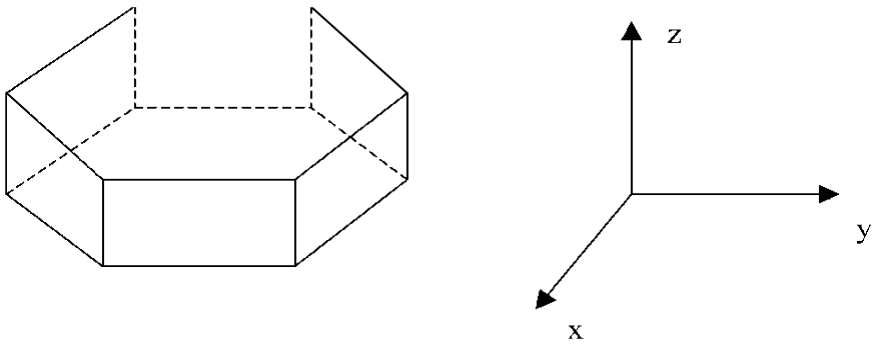

Figure 4.11 *Wurtzite unit cell, showing the hexagonal symmetry of the system. The z axis direction is known as c axis and x-y plane is known as basal plane.*

From the Figure 4.11, it is clear that the properties of the crystal is different along the z axis then along the in-plane axes, x and y. The lattice constants along the z axis, c, and in-plane, a, are generally different. The strains along the z axis and in-plane are defined as

$$\varepsilon_{zz} = \frac{c-c_0}{c_0} \quad \varepsilon_{xx} = \varepsilon_{yy} = \frac{a-a_0}{a_0} \qquad (4.40)$$

where c_0 and a_0 are the lattice constants in the unstrained system and c and a are the lattice constants under strain conditions. The piezoelectrically induced polarization field in the z direction is given as

$$P_z = e_{33}\varepsilon_{zz} + e_{31}(\varepsilon_{xx}+\varepsilon_{yy}) \qquad (4.41)$$

The strain, caused by compression or expansion of the crystalline lattice from its unstrained condition, lead to either ions together or pulls them apart. In either case, the local dipole moments are different, resulting in a change in the macroscopic polarization vector, **P**.

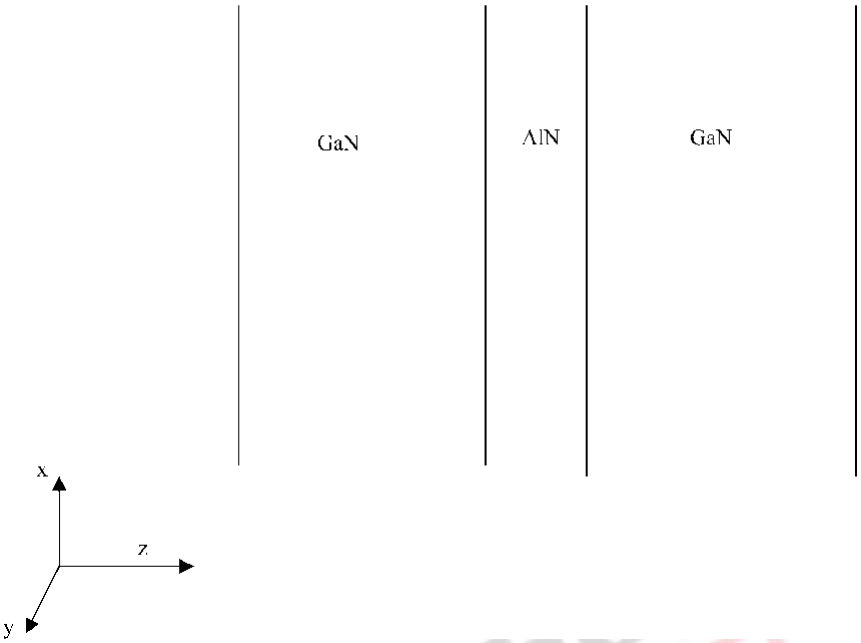

Figure 4.12 *A thin layer of AlN sandwiched between two GaN layers. Due to lattice mismatch between AlN and GaN, the AlN layer is strained, resulting strain-induced polarization fields along the z direction.*

Figure 4.12 shows a three layer system, in which a thin AlN layer is sandwiched between two relatively thick GaN layers. The lattice mismatch of the system is accommodated by straining the thin AlN layer. The thickness of AlN layer should be less than the critical thickness, which for AlN is about 3.0 nm. A polarization field **P** is produced in the along z direction. Now one can define the electric displacement vector **D**, given by

$$D = \epsilon_0 E + P \qquad (4.42)$$

where $\in_0$ is the free-space dielectric constant. **D** can be obtained from Poisson's equation ,

$$\nabla . D = \rho \qquad (4.43)$$

where ρ is the charge concentration. Equation 4.43 can be modified as

$$\nabla . (\epsilon_0 E + P) = \rho \qquad (4.44)$$

Rearranging Eq. 4.44 and defining the polarization charge ρ_{pz} yields

$$\nabla . \in_0 E = \rho - \nabla . P = \rho + \rho_{pz} \qquad (4.45)$$

Now the polarization **P** can be obtained from

$$\nabla . P = -\rho_{pz} \qquad (4.46)$$

As the strain condition changes abruptly at the two hetero interfaces in GaN/AlN/GaN structure, the polarization vector changes across the interface. Eq. 4.46 implies that there exists a polarization charge at the interface. One side of the hetero interface has a positive charge while an equal but opposite negative charge is produced on the other side.

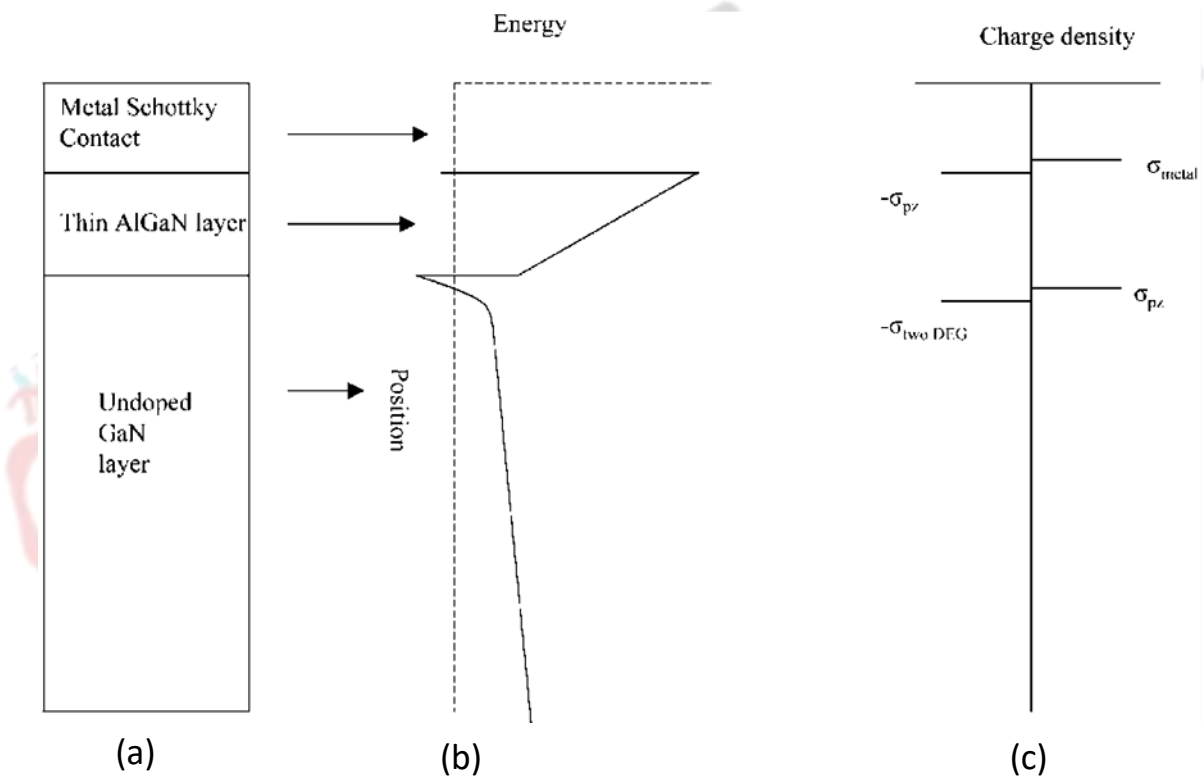

Figure 4.13 *(a) AlGaN/GaN based heterostructure with metallic Schottky contact to AlGaN layer. (b) Energy band profile of the heterostructure with trigular quantum well at GaN/AlGaN interface. (c) Charge density at the interface.*

The strain-induced polarization field can be used to change the local carrier concentration near the hetero interface which is shown in Figure 4.13. In this system a Schottky metal gate contact is formed on top of a thin AlGaN/GaN heterotructure. The thin AlGaN layer is

strained, resulting a polarization field which induces a polarization charge density, σ_{pz}, at both interfaces of AlGaN layer. The polarization charge density at each interface is compensated by charge density in the top metal Schottky barrier and in the bottom GaN layer. The charge density induced in the bottom GaN layer is due to 2DEG free electrons accumulated at the interface. Thus the local electron concentration at the hetero interface within the GaN layer is increased significantly without doping of either GaN or AlGaN layer. This leads to high carrier concentration at low background impurity concentration and absence of strong carrier-impurity scattering leads to high carrier mobility.

Group III nitride semiconductors such as GaN, InN and AlN also exhibit *spontaneous polarization*, which arises even in the absence of strain. Spontaneous polarization arises due to the non ideality of the crystalline structure of materials with wurtzite crystal structures. Usually, in group III semiconductors c/a ratio deviates from its ideal value resulting difference in the bond lengths and a change in the dipole moment. The net effect is that the material exhibits a built-in polarization. The spontaneous and piezoelectric polarizations due to strain can be either aligned or nonaligned, depending on the whether the layer is in tensile or compressive strain. When the spontaneous and piezoelectric polarizations are aligned, the net polarization is given simply as

$$P = P_{pz} + P_{spon} \qquad (4.47)$$

The combined action of the piezoelectric and spontaneous polarization fields can be used to change the free carrier concentration in a hetero layer.

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