1.1.Building block of silicon devices and General band diagram

Goal;

1. To understand the basic building block of silicon technology
2. to understand the energy band diagram (based on Band line up theory) in space including heterojunction

A. Basic building block of silicon device

— Silicon technology is composed of basic building blocks such as

* silicon (with various doping, some of other material for Ge)
* insulator materials(silicon oxide, nitride and High k and low k material)
* interconnect material for transmission of signals with large band width and low loss(Al, Cu, polysilicon and silicide)
* and other special materials for special purpose(photonics, memory and others)

B. Being able to draw the energy band diagram for electrons (hopefully phonon) is the key to predict the device behavior

— A general band diagram in space for three different materials

χ : electron affinity (measurable quantity)
E_g : electrical bandgap

- reference energy level:
  vacuum level(or Fermi Energy) at the point where the ground potential is applied.
- E_L is the vacuum level and $q\Psi$ is the electrostatic energy.
- ΔE_C and ΔE_V are the energy change in the conduction band edge and valence band edge due to material variation

Ex: Draw the energy band diagram for the following case

- Example 1. Energy band diagram in HEMT device (with AlGaAs-GaAs system)
- Example 2. Energy band diagram in MOS system
- Example 3. Energy band diagram in Si-SiGe BJT

— The above band diagram is based on Anderson's theory(1) assuming that the vacuum level is continuous across the heterojunction. However, many detailed phenomena tasking place at the interface make the theory questionable. Among them are; interface orientation, strain, interface states due to point defects. Other factors are the unclearness of the experiments to measure the energy parameters since they are usually performed at the interface which is far from the real interface. Good coverages on these topics are found in the reference.

※ Ref > Chap1. of Heterojunction band discontinuity, North-Holland, 1987.

Ex>
Fill up the table below for the information about the band related parameters.

	Electron Affinity	Band Gap	Work function(for metal only)
Si			
SixGe1-x			
SiC			
SiO2			
Si3N4			
HfO			
Al			
NiSi			
CoSi			
Ti			
W			

C. E-k diagram

— Band calculation is performed for the electron wave function with proper inclusion of the effects of neucleus. The eigenenergy is expressed in the form of E(k) where k is the crystal momentum. The E(k) diagram is important since the equation of motion of carriers can be best described by the

* group velocity and
* crytal momentum
* and the density of states.

– Stationary states in crystals

$$\psi(r) = e^{ik\cdot r}\, u_k(r)$$

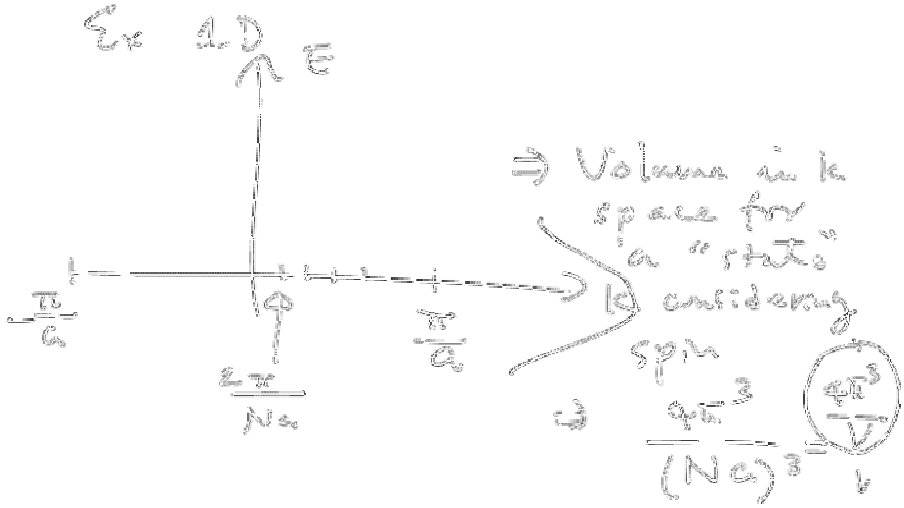
Then $\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi$

becomes

$$\left[-\frac{\hbar^2}{2m}(\nabla + ik)^2 + V(r)\right] u_{nk}(r) = E_n(k)\, u_{nk}(r),$$

which is the reduced problem in a 'single primitive cell'.

Ex 1-D



⇒ Volume in k space for a "state" considering spin

$$\Rightarrow \frac{8\pi^3}{(Na)^3} = \frac{4\pi^3}{V}$$

– Electronic Properties

(1) Group Velocity

$$\langle v \rangle = \frac{1}{\hbar} \nabla_k E_n(k)$$

– This can be verified easily from the 'wave packet argument'

(2) Acceleration theorem

$$\hbar \frac{dk}{dt} = F$$

so that k is called the 'crystal momentum'.

(3) Force acceleration theorem

$$\frac{d}{dt}\langle v \rangle = \frac{1}{\hbar} \frac{d}{dt} \nabla_k E_n(k)$$

$$= \frac{1}{\hbar}\left(\frac{dk}{dt} \cdot \nabla_k\right) \nabla_k E_n(k)$$

Defines $\left(\frac{1}{m_n^*}\right)_{ij} \equiv \frac{1}{\hbar} \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} E_n(k)$

- Density of states [#/ cm³ - eV]

$$D(E) = \sum_k \delta[E - \varepsilon(k)]$$

Using $\sum_k \rightarrow \frac{V}{4\pi^3}$

$$D(E) = \frac{V}{4\pi^3} \int d^3k\, \delta(E - \varepsilon(k))$$

For $\varepsilon(k) = \frac{\hbar^2}{2m} k^2 = \gamma k^2$

$$D(E) = \frac{V}{4\pi^3} 4\pi \int k^2 dk\, \delta(E - \gamma k^2)$$

$$= \frac{V}{4\pi^3} \frac{4\pi}{\gamma} \int k^2 \frac{1}{2k} \delta\left[k - \sqrt{\frac{E}{\gamma}}\right]$$

$$= \frac{V}{4\pi^3} \frac{4\pi}{\gamma} \frac{1}{2} \sqrt{\frac{E}{\gamma}} = a\sqrt{E}$$

-Also, the optical properties, the recombination processes between electrons and holes can be best understood in the E(k) diagram, since the process should satisfy the conservation of 'energy' and 'momentum'.

- Density of states: Also, from E(k) diagram, the density of states can be known from

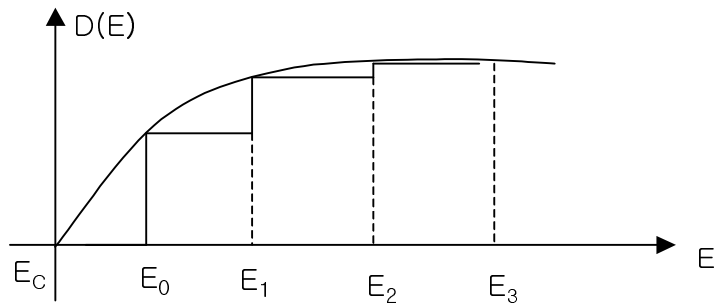
eq. ( ).

- The effects of space scaling: quantization

The electron energy is quantized when the potential well is formed either by the scaling of devices(extremely thin silicon film in SOI, DGFET and silicon nanowire FET, FINFET) or by the inversion layer in MOSFET.

- quantization of MOSFET inversion layer

The electron wave function is quantized in the potential well so that the energy states in the potential well are quantized in the depth direction. The net effect is the D(E) is not proportional to $\sqrt{E-E_c}$ in the conduction band, but constant between the quantized energy level as shown in the figure below. This sometimes is called the "2D quantization".



In the 2dimensional gas, the DOS of the *i*th subband (per unit area, unit energy) is

$$D_i(E) = \begin{cases} \dfrac{m^*}{\pi \hbar^2} g_v & \text{for} \quad E \geq E_i \\ 0 & \end{cases}$$

where g_v is the band degeneracy.

The total DOS is

$$D(E) = \sum_{i=0}^{\infty} D_i(E)$$

Now areal electron density in the *i*th subband is

$$N_i = \int D_i(E) f(E) dE = \int_{E_i}^{\infty} \frac{m^*}{\pi \hbar^2} \frac{1}{1 + e^{(E_F - E_i)/k_B T}}$$
$$= \frac{m^* k_B T}{\pi \hbar^2} \ln[1 + e^{(E_F - E_i)/k_B T}]$$

and total Q_n is

$$Q_n = -q \sum_{i=1}^{\infty} N_i$$

Now E_i can be only known from the Schrodinger equation as,

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2}+V_p(x)\right]\Psi_i(x)=E_i\ \Psi_i \qquad (1)$$

and $V_p(x)$ is the total potential energy as the result of the Poissons equation with

with $$\rho = q(p-n+N_D) \qquad (2)$$

where $$n(x)=\sum_{i=0}^{\infty}N_i|\Psi_i(x)|^2 \qquad (3)$$

(1) and (2) constitute the loop to be solved numerically.
Net effect of the quantization is the reduction of the density states thereby reducing Q_n for a given Ψ_s (surface potential) V_T is higher than the classical theory.

D. Breakdown of E(k) relation for bulk

- The E(k) diagram based on the assumption that the lattice is infinite (large N) with the periodic boundary condition may be invalid if the size of N is small.
  The situation may be met in the 'silicon nanowire MOSFET' with very very small diameter(less than 10nm).
-See the discussion in the paper(available in the PDF format)

ref>: On the Validity of the Parabolic Effective-Mass Approximation for the Current-Voltage Calculation of Silicon Nanowire Transistors
Jing Wang, Anisur Rahman, Avik Ghosh, Gerhard Klimeck and Mark Lundstrom

E. Energy band due to the strain in the silicon

— Band structure is modified due to the deformation of the regular crystal structure in silicon.

Typical example of the local deformation is the energy band structure caused by the 'lattice vibrations(optical phonon and acoustic phonon)'. They are considered as the perturbation to the electon transport.

ref>

- Efforts to use the strain to modify the energy band shape have been made for a long time to enhance the mobility of carriers.

  There have been two approaches: Using the epi layer such as Si1-x Gex as the relaxed layer to give the strained Silicon grown on top of the relaxed layer.

  ref> J. Welser et. al., 'NMOS and PMOS Transistors Fabricated in Strained Silicon/Relaxed Silicon-Germanium Structures' IEDM, 2002

- Another efforts is to use the silicon nitride film to give the stress from the side wall for NMOS and Silicon Germanium implantation

to the source/drain regions for PMOS.

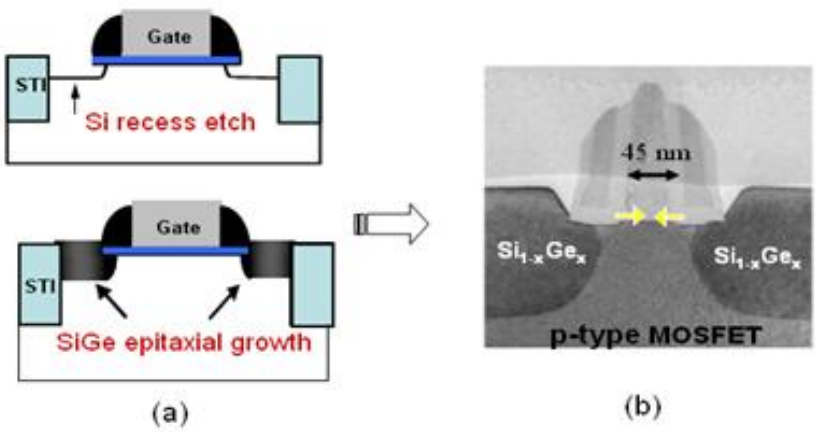


Fig. SiGe epi layer is formed to give a unaxial stress to PMOSFET

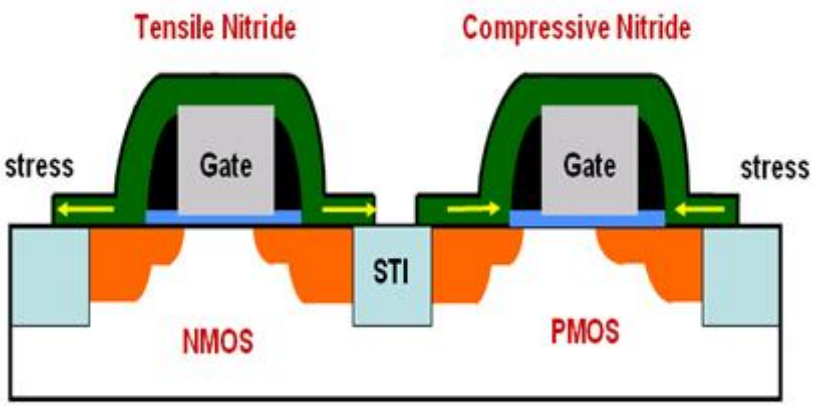


Fig. Silicon Nitride capping layer is introduced to give a uniaxial tensile stress to NMOSFET.

<some references but may not be the typical.

[1] S.-E. Thompson *et al., IEEE Trans.Electron Devices* ***51,*** 1790 (2004).

[2] M. Horstmann, A. Wei, and T. Kammler, in Proc. Intl. Electron Device Meeting (2005), pp. 233-236.

[3] C.-H. Jan, P. Bai, and J. Choi, in Proc. Intl. Electron Device Meeting (2005), pp. 60-63.

[4] K. Uchida, T. Krishnamohan, K. Saraswat, and Y.Nishis, in Proc. Intl. Electron Device Meeting (2005), pp. 135-138.

[5]For modeling of the mobility enhancement for NMOSFET, for example,

E. Ungersboeck,, et.al, Electron Inversion Layer Mobility Enhancement by Uniaxial Stress on (001) and (110) Oriented MOSFETs, SISPAD, 06

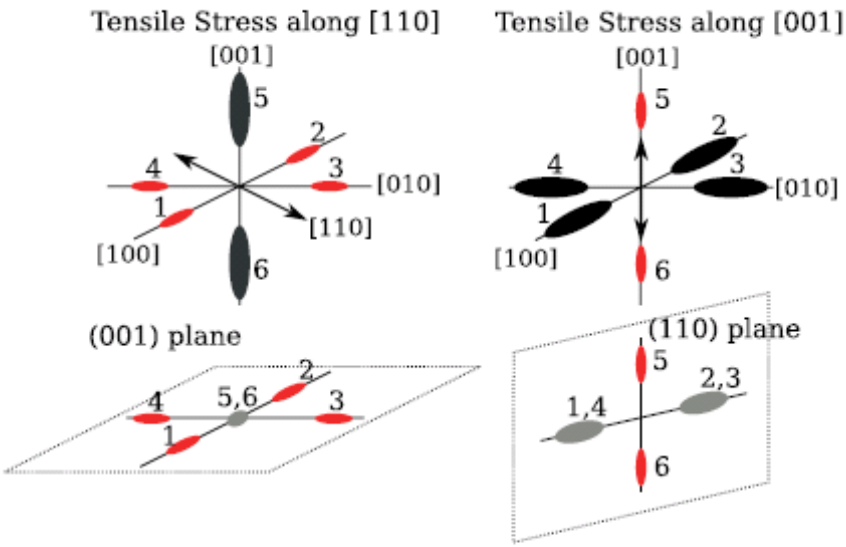


Figure 1: Constant energy surfaces of the Si conduction band under uniaxial tensile stress along [110] / [001] with projection on the (001) / (110) plane.

from ref. 5 above

- effects of strain on the performance of PMOS and NMOSFET

Y. Luo, 'Enhancement of CMOS Performance by Process-Induced Stress'

IEEE, TED, VOL. 18, NO. 1, FEBRUARY 2005 63

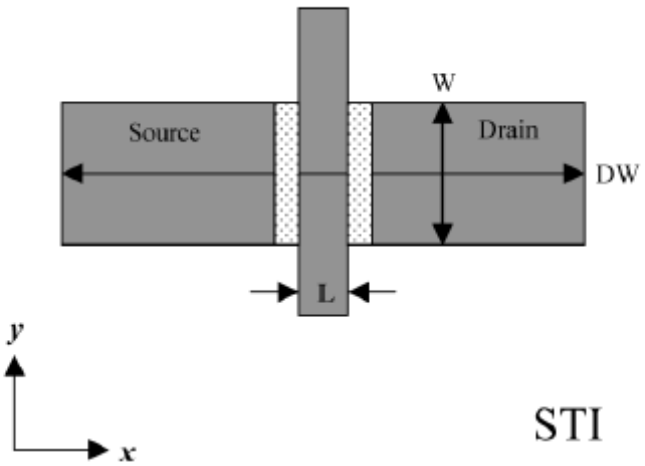


Fig. 1. Schematic of MOSFET for study, showing the three main parameters: channel length L, channel width W, and diffusion width DW. Stress components x, y are along L (DW) and W, respectively.

TABLE I

IMPACT OF STRESS COMPONENTS ON MOSFET PERFORMANCE

	axis	*NMOS*	*PMOS*
Tensile stress	*x*	⇧	⬇
	y	⇧	⇧
Compressive stress	*x*	⬇	⇧
	y	⬇	⬇

⇧ - enhancement; ⬇ - degradation