

# A Synopsis on Science

## A Journey through 13.7 billion years of “Matter”

from The Big Bang to a Green Earth

### Lectures 4-6

# The Properties of Matter

Tokyo University Institute for Solid State Physics

Yasuhiro Iye

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# Lecture Plan

Lectures 4-6: Yasuhiro Iye “The Properties of Matter”

Lecture 4: Modern Society and Material Science

What does the discipline of Solid-State Physics do

**Lecture 5: From an Atom to a Solid Object**

**Diverse Matter, Varied Physicality**

Lecture 6: Manipulating Atoms, Manipulating Quanta

**High-Tech and Nano-Science**

# Today's Talk

- From an Atom to a Solid Object
  - Diamonds are hard, Gold is soft
- Electron States in Solid Objects-Metals and Insulators
  - Copper Wire and Plastic
- Magnetism
  - Why does Iron become a magnet?
- Super-conductors
  - Super!

# From an Atom to a Solid Object

## Inter-atomic Forces and Crystal Structures



# The Forces that Bind Atoms Together

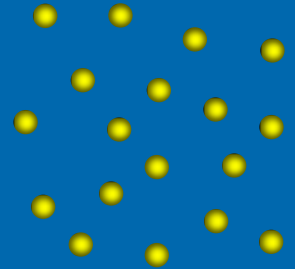
Groups of atoms are scattered at high temperatures (Gas)  
Below a certain temperature, they become Liquid, then Solid

The state of cohesion (Solid, Liquid) depends on the forces of attraction at work between the atoms

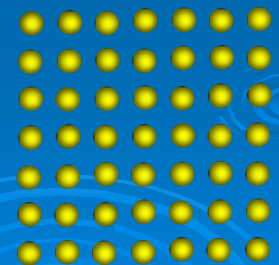
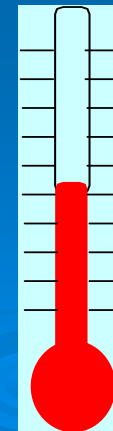
Crystal structure and mechanical properties reflect the type of inter-atomic forces at work

Diamonds are hard  
Gold is soft

Disordered State



Phase Transition



Ordered State

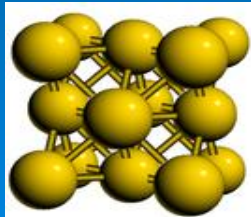
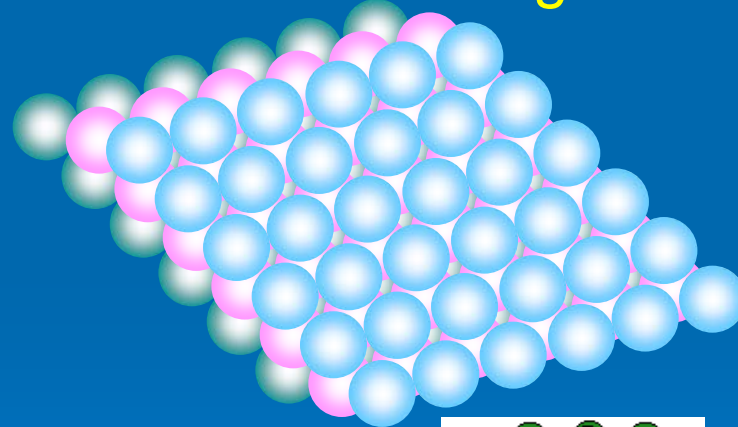
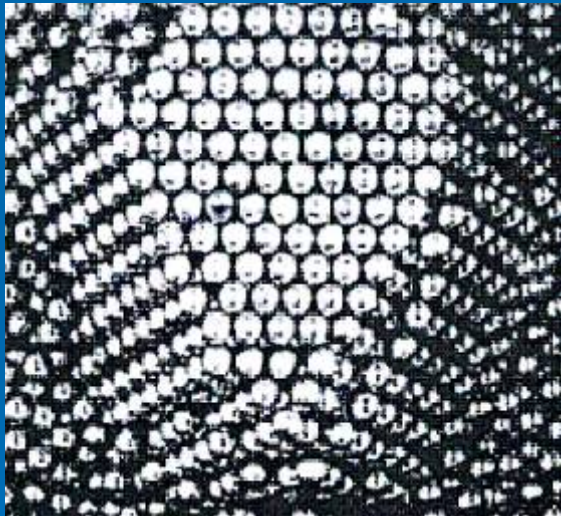
# Crystal Structure

What arrangement do atoms take at the lowest amount of energy?

What if you fill a box with Pachinko balls (solid spheres)?

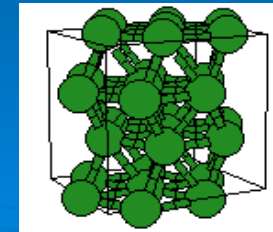
A Packing Problem

Close-Packing Structure  
Packing Ratio of 74%



Face Centered Cubic lattice

fcc



Hexagonal Close-Packing

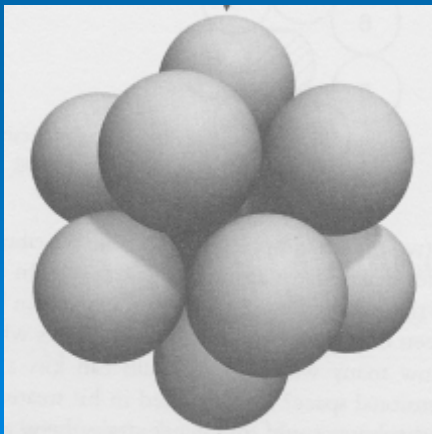
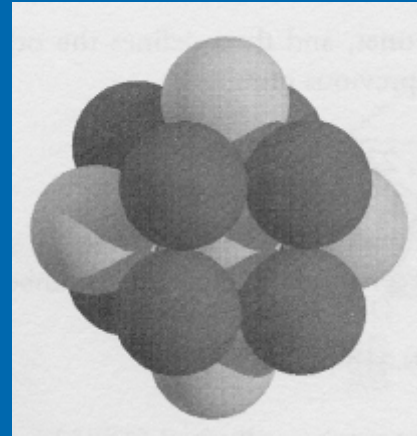
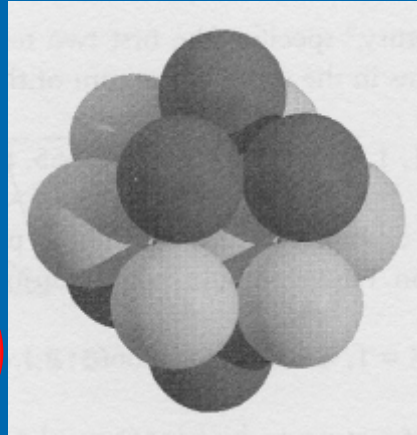
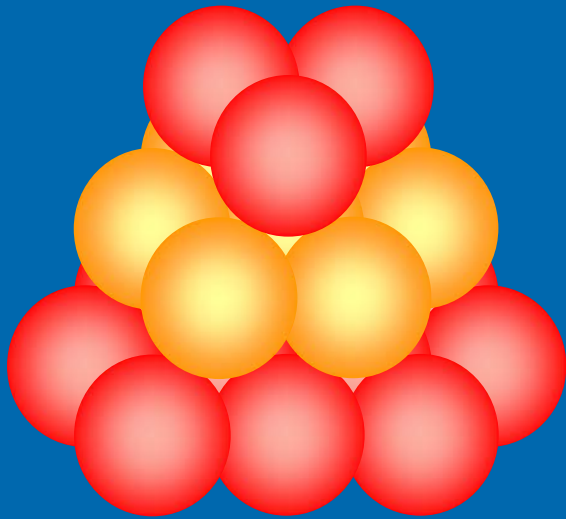
hcp

# [Digression] Kepler's Conjecture

Packing spheres without spaces in-between :  
3-D Packing



Johannes Kepler  
(1571-1630)



Icosahedral arrangement

The greatest number of same-sized  
spheres that can be packed around  
a single sphere is 12...

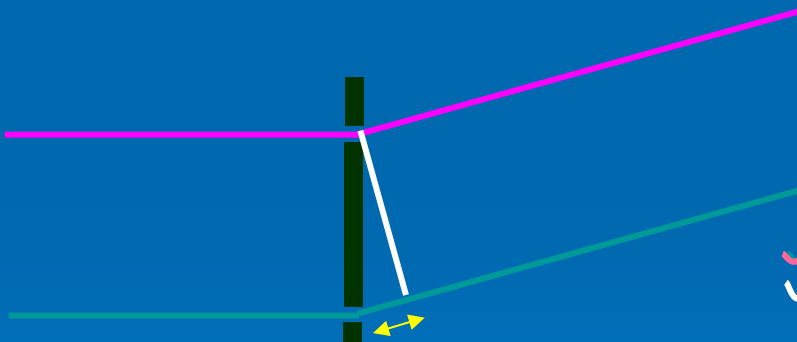
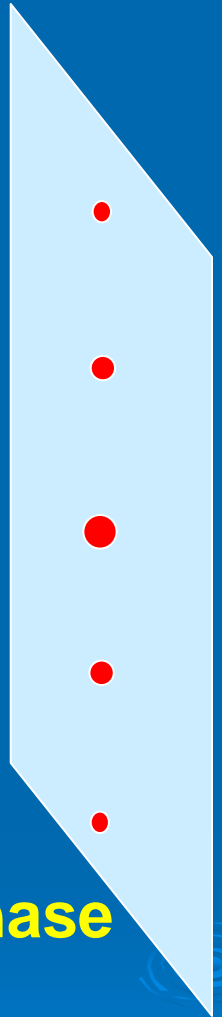
Kepler's Conjecture

A mathematical rigorous proof of  
this was finally established in 1997

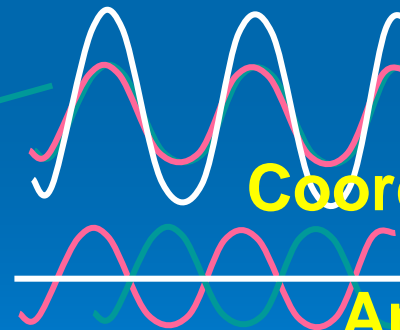
How do you investigate a crystal structure?

# Diffraction of Light

## Diffraction



Optical Path Difference



Coordinate Phase

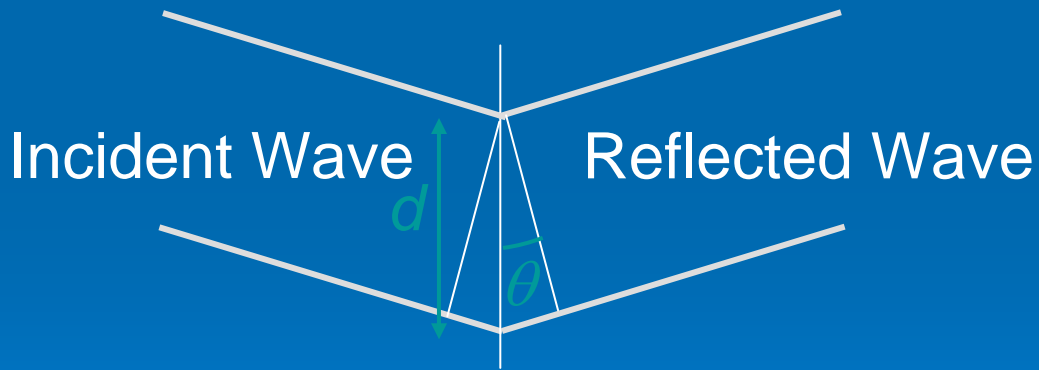
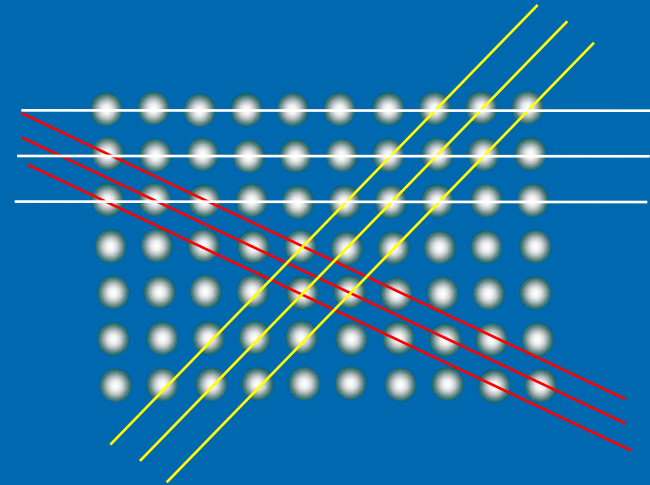
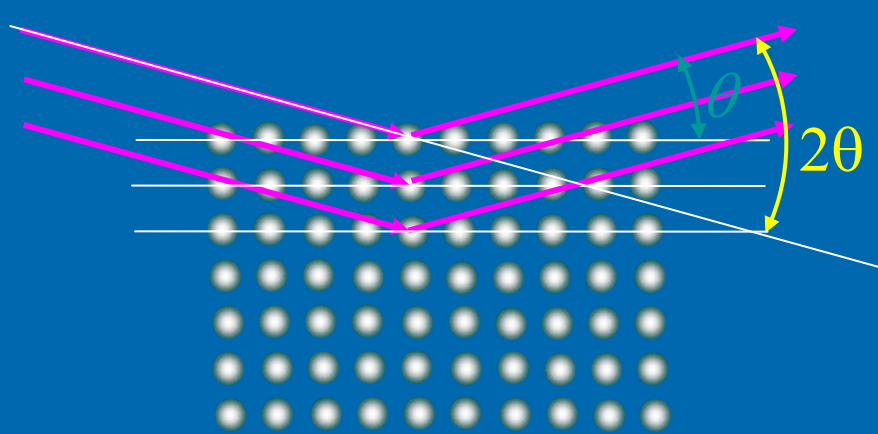
Anti-Phase

$$d \sin \theta = n\lambda$$

Inter-atomic Spacing  $\sim 0.3\text{nm}$   $\Leftrightarrow$   $\sim$  Wavelength of X-Rays

Diffraction of an Electron Beam or Neutron Beam can also be used

# Crystal Structure Analysis



$$2d \sin \theta = n\lambda$$

Bragg's Condition



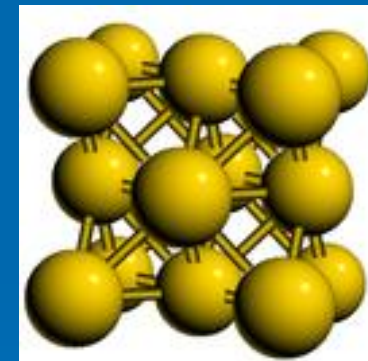
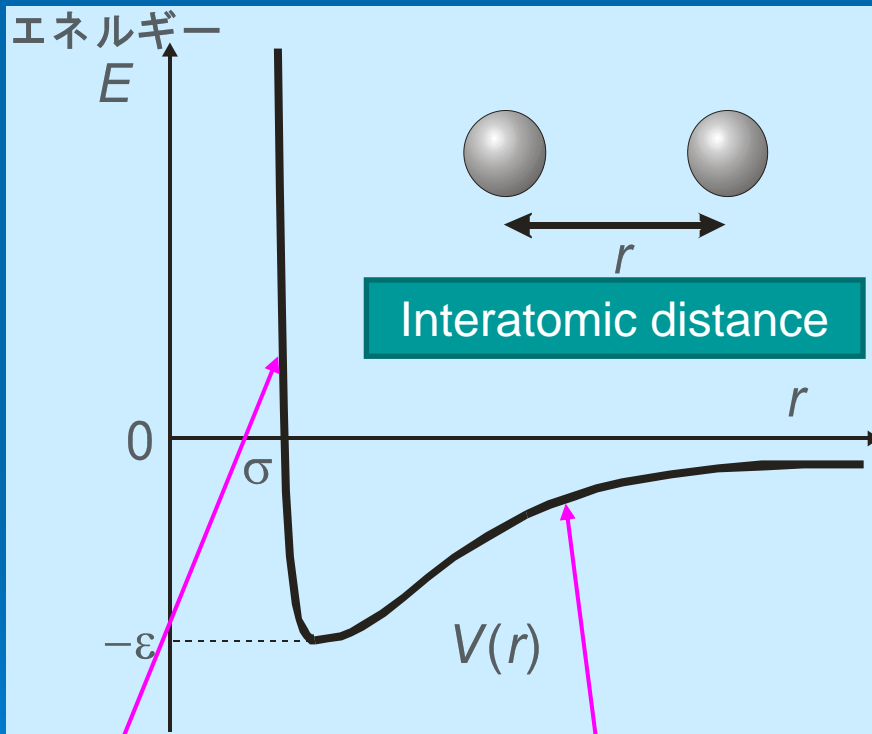
4-Axial X-ray Crystal Diffractometer

# Nobel Gas Crystals

Inter-atomic Force Potential

Ne, Ar, Kr, Xe

Close - Packing Structure  
Face centered cubic lattice (fcc)



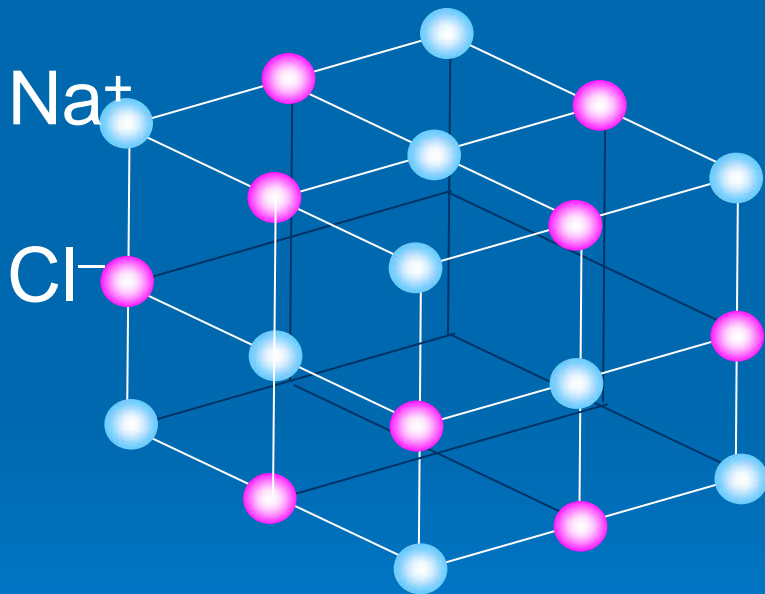
He is?  
Quantum Liquid

Rigid Body  
Central Repulsion Force

Van der Waals Attractive Forces

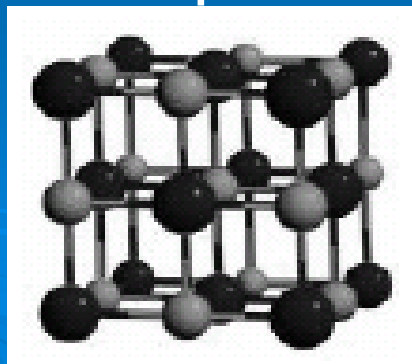
# Ionic Bonding

Coulomb Forces acting between positive and negative ions

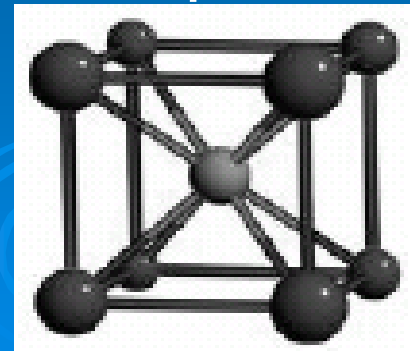


H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr

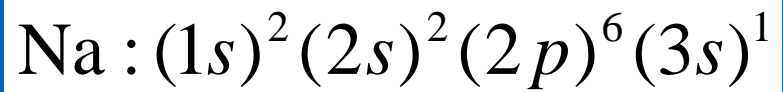
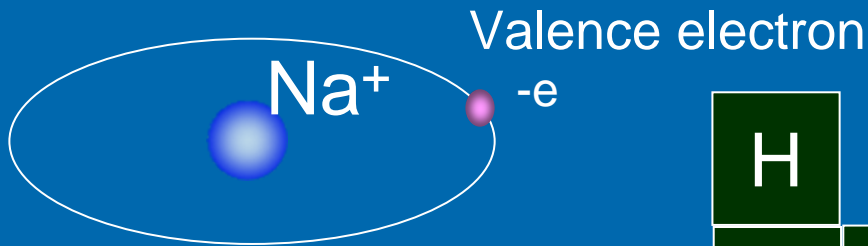
NaCl pattern



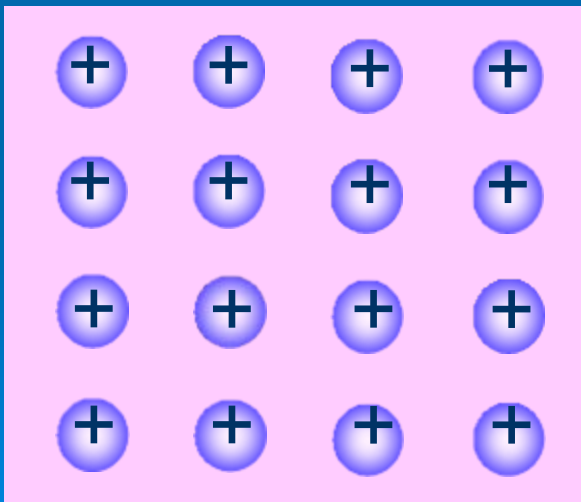
CsCl pattern



# Ionic Bonding



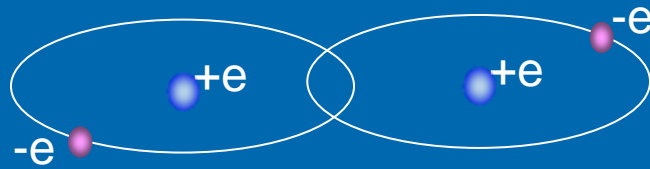
H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr



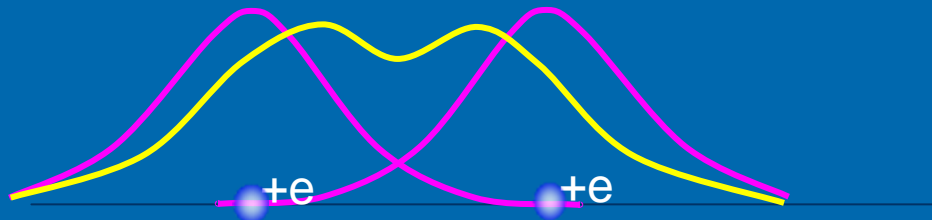
Positive-charged ions are embedded in a sea of negative electrical charge caused by the circulating electrons.

# Covalent Bonding

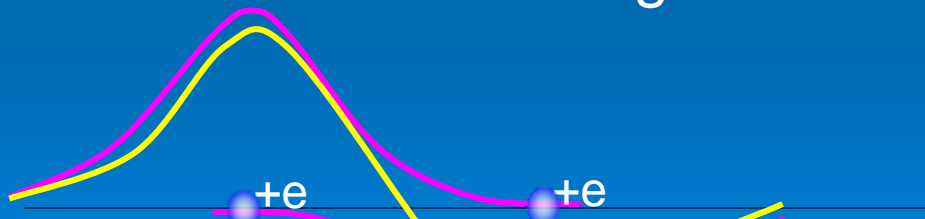
Hydrogen Molecule :H<sub>2</sub>



Molecular Orbit

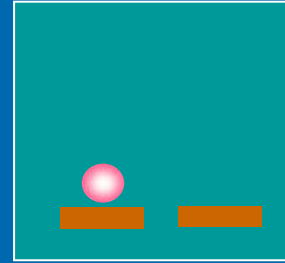
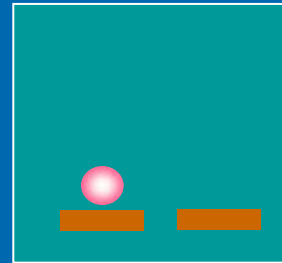


Bonding Orbital

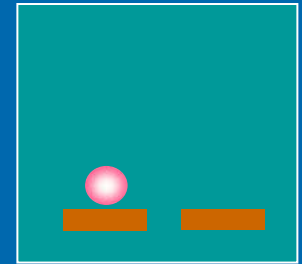
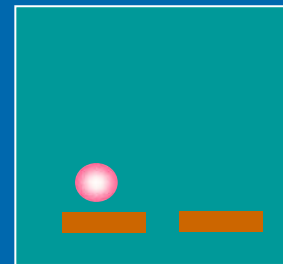


Anti-bonding Orbital

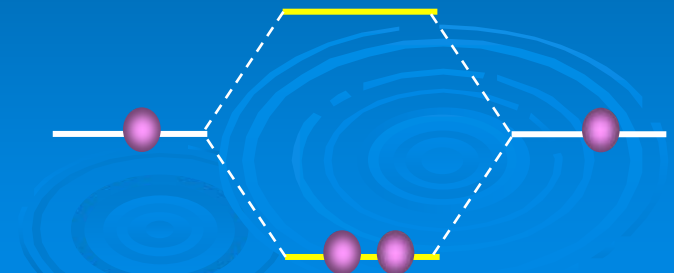
2 twin-bed rooms,  
1 child each room



Visit next door

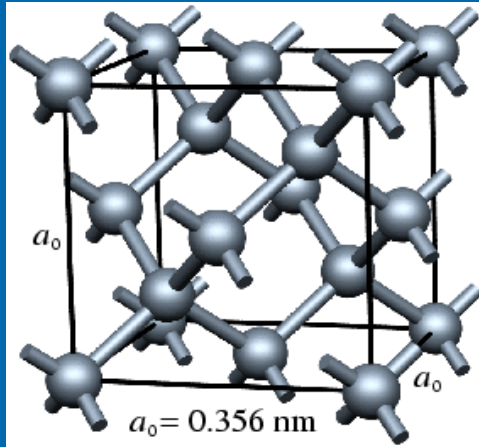


By broadening the area of activity, the energy is reduced



# Covalent Bonding

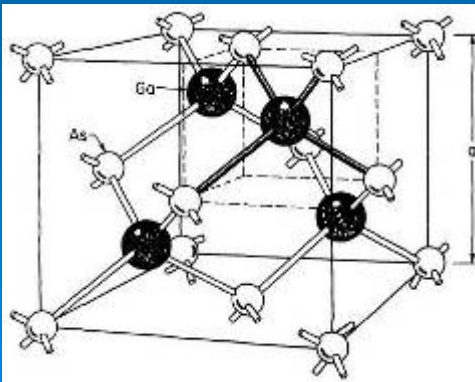
C, Si, Ge



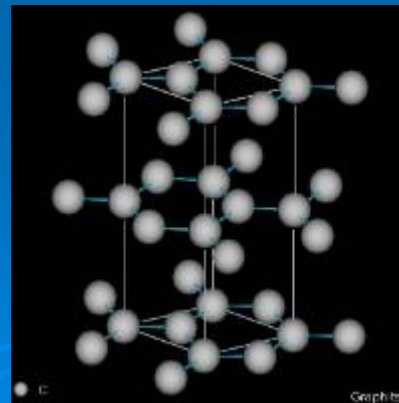
Diamond Structure

H							He
Li	Be	B	C	N	O	F	Ne
Na	Mg	Al	Si	P	S	Cl	Ar
K	Ca	Ga	Ge	As	Se	Br	Kr

GaAs, InP



Sphalerite Structure

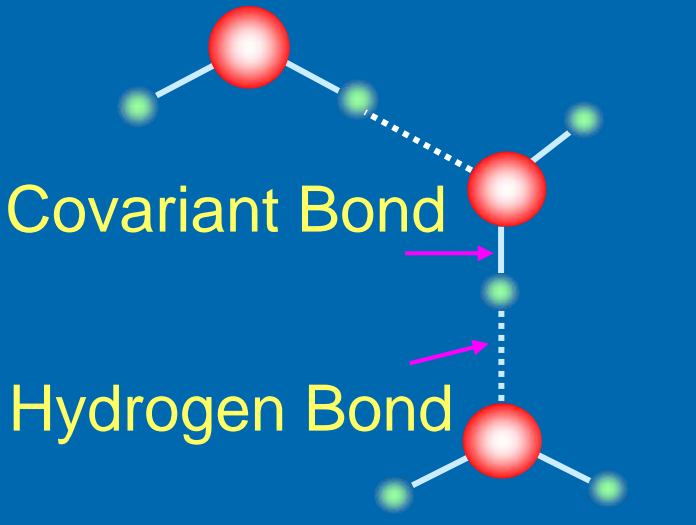


Black lead

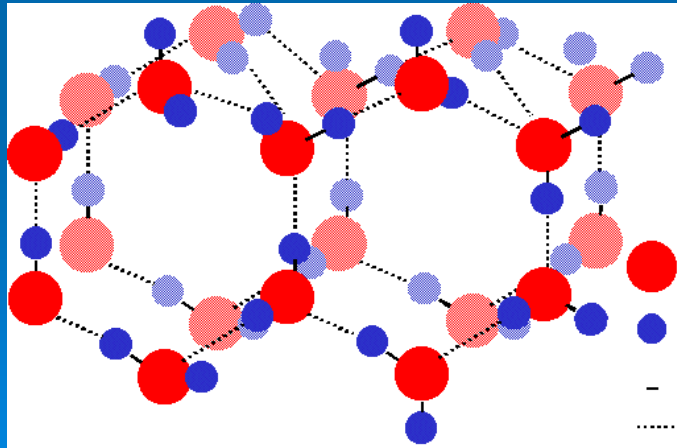
Layered Crystal  
Within the layers there is strong **covalent bonding**,  
between the layers there is weak **Van der Waals Bonding**  
=> easy to cleave

# Hydrogen Bonding

## Water Molecule



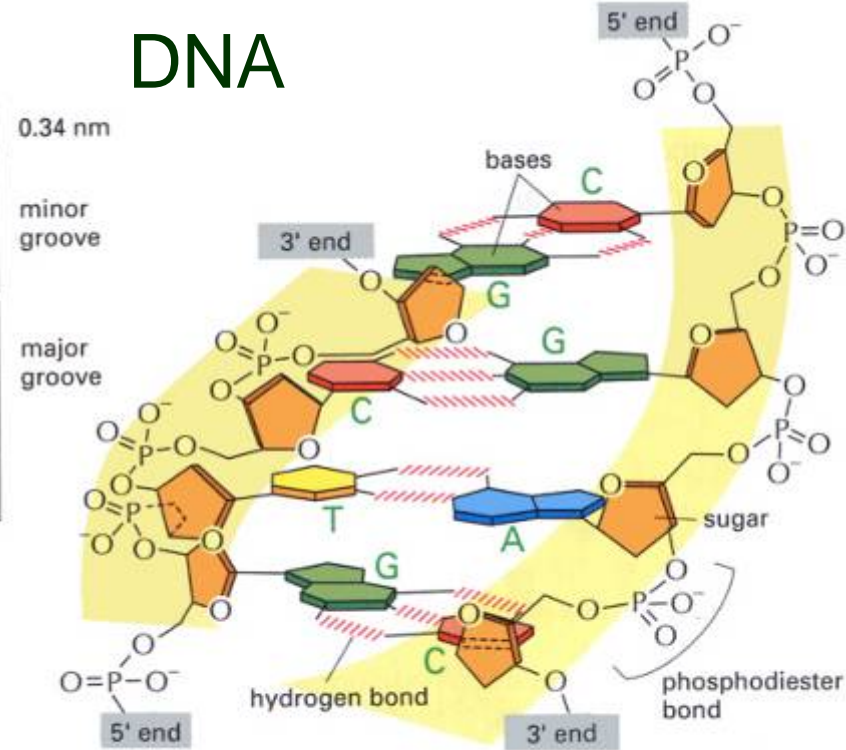
Hydrogen Bonding plays an important role in bio-molecules



Ice Crystal



(A)



(B)

# Electron State within Solids (Band Structure)

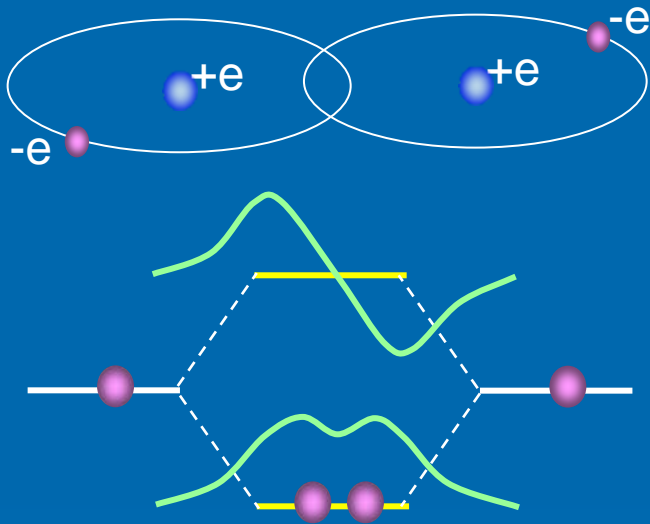


# Electron State within Solids

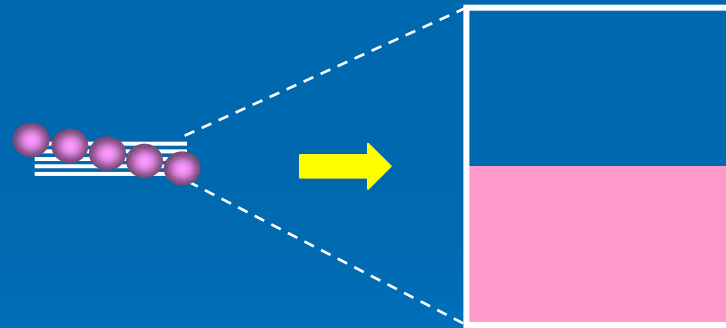
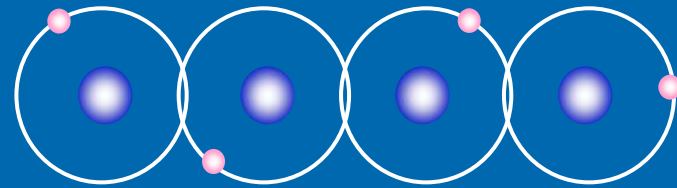
- Quantum mechanics deals with electrons' movement within the potential that makes atoms periodically line up
- There are two schools of thought
  - Atoms line up  $\Rightarrow$  **tight-binding model**
  - Depart from free space and bring in periodic potentials  $\Rightarrow$  **nearly free electron model**

# Lining Up Atoms

Hydrogen molecule :H<sub>2</sub>

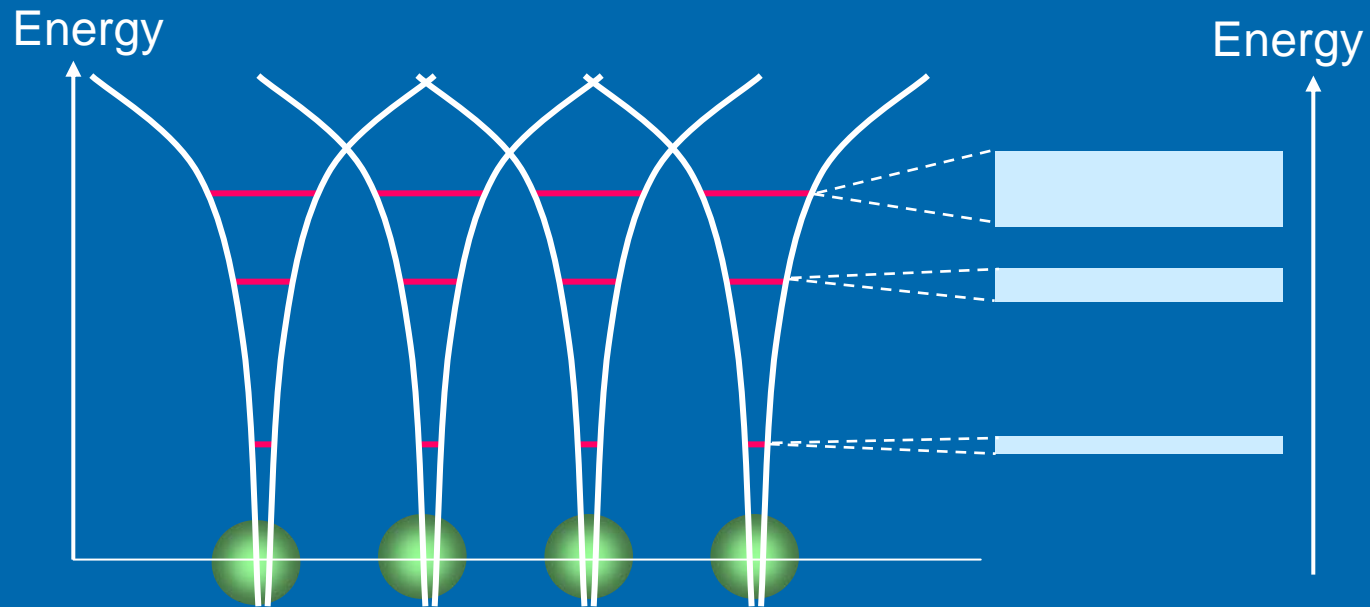


Hydrogen molecules periodically line up



The oscillation of electrons depends on the overlap of electron clouds of adjacent molecules, and electrons move around the entire crystal structure

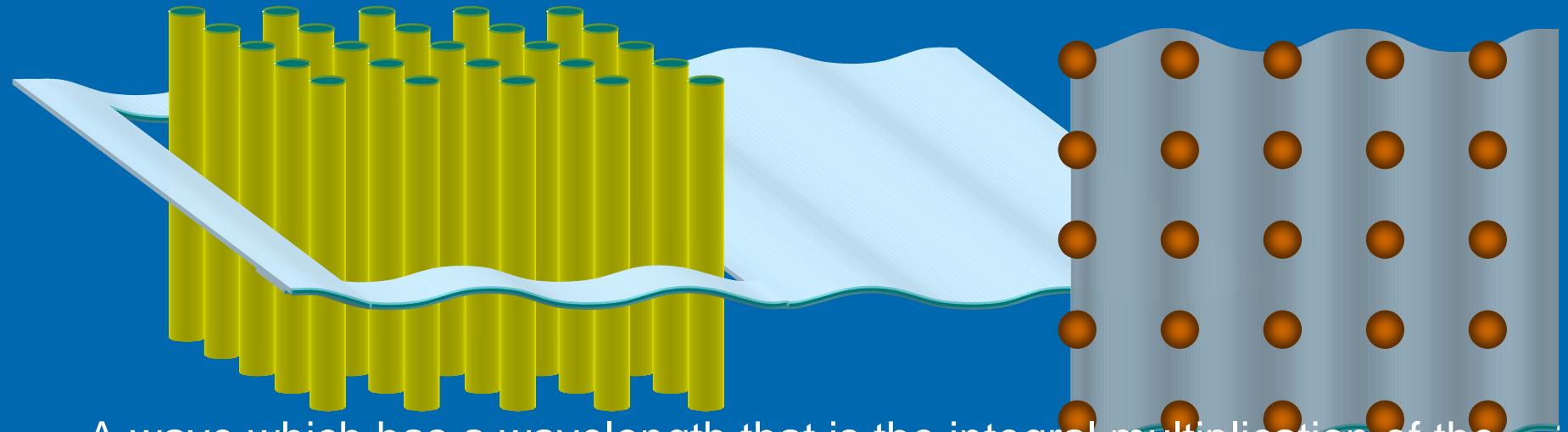
# Broadening of Energy Width due to Oscillation



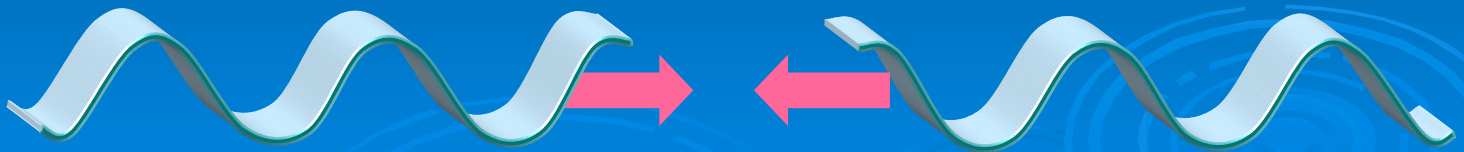
Depending on the oscillation of electrons,  
each electron energy level of a molecule  
expands and forms a band

# Wave Dispersion due to Periodic Structure

Waves breaking onto lines of stakes standing in a pond

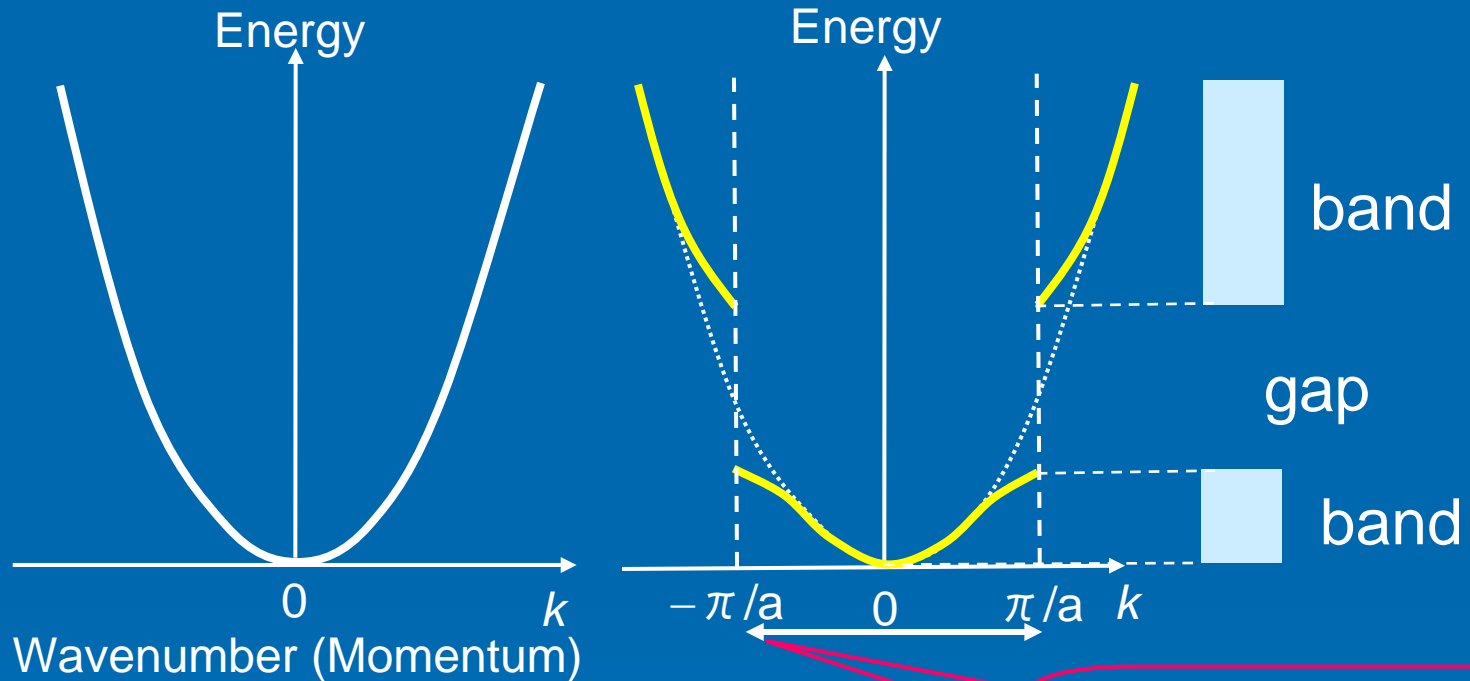


A wave which has a wavelength that is the integral multiplication of the arrangement period of the scattering body is strongly reflected (Bragg Reflection), and a standing wave is made by the interference between the incidence wave and reflected wave. => **at a specific wavelength a travelling wave is unable to be formed.**



$$e^{i(kx-\omega t)} + e^{i(-kx-\omega t)} = 2e^{-i\omega t} \cos(kx)$$

# Formation of Bands and Gaps due to Bragg Reflection

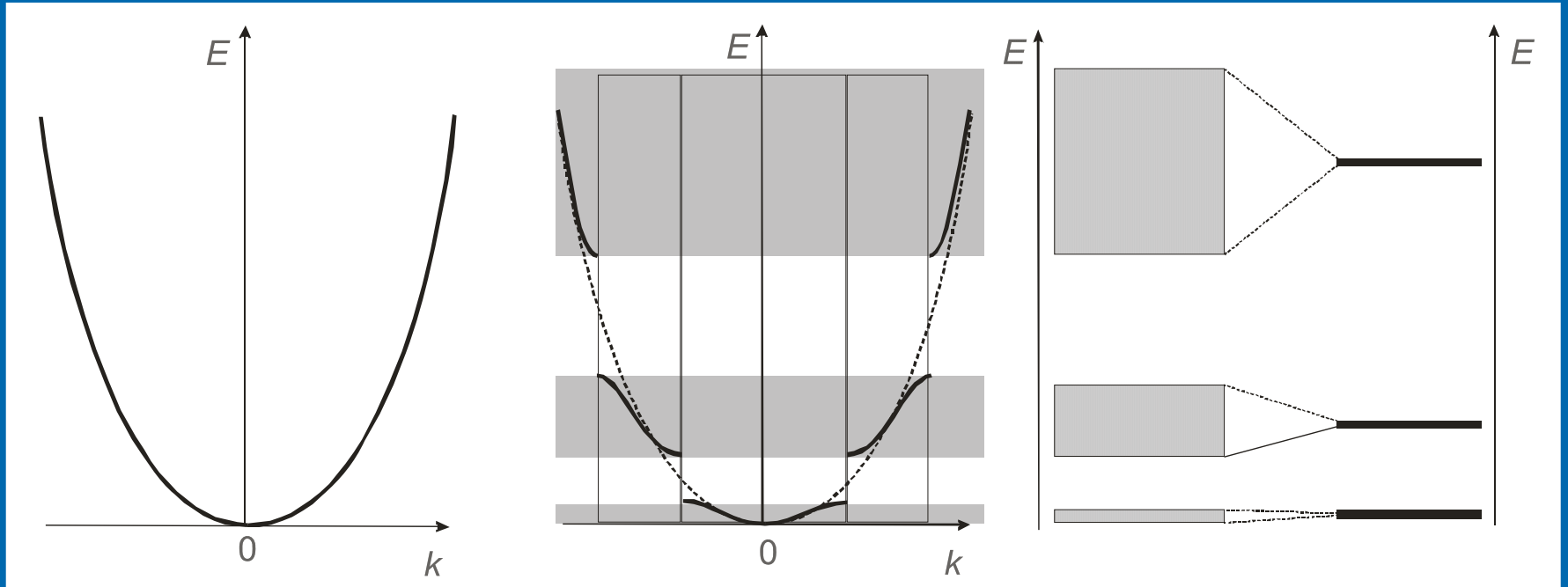


Energy range taken (**Band**)  
and not taken (**Gap**) by an electron

Wavenumber  
corresponded period

Role of periodic potential  $\Rightarrow$  Change the relationship (Dispersion Relationship) of an electron's energy and momentum (**Bloch Electron**)

# Electron Band Structure



Free Electron  $\longrightarrow$  Electron within a Crystal (Bloch Electron)  $\longleftarrow$  Isolated Atom

Nearly-Free Electron Model  
Roaming Electron

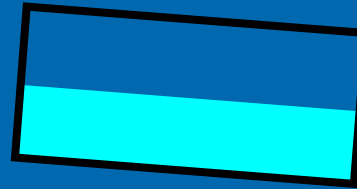
Tight-Binding Model  
Localized Electron

# Metals, Insulators, Semiconductors



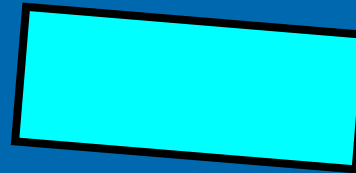
# Metals and Insulators

Half-packed Band



Electrical current  
can flow

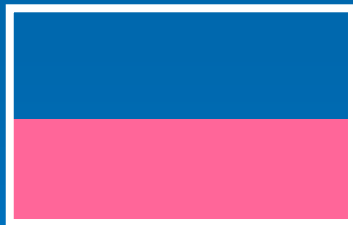
Fully-packed Band



Electrical current  
can't flow

Apply an Electrical Field

Energy ↑



Metal



Insulator



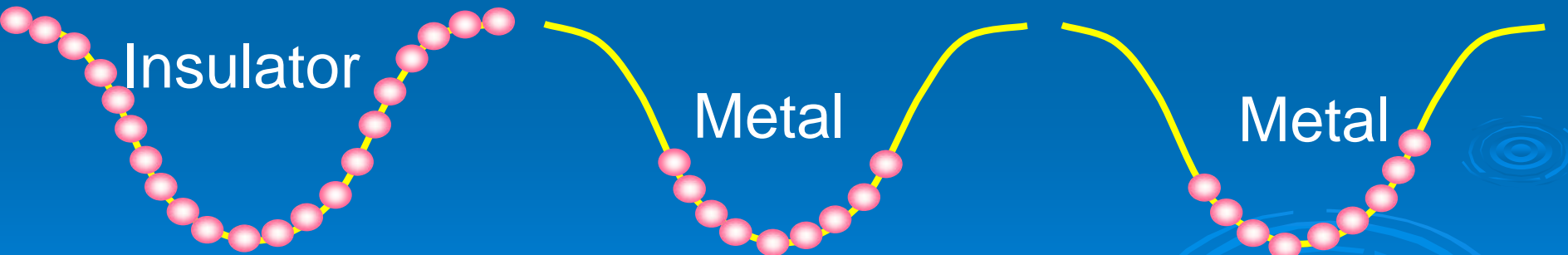
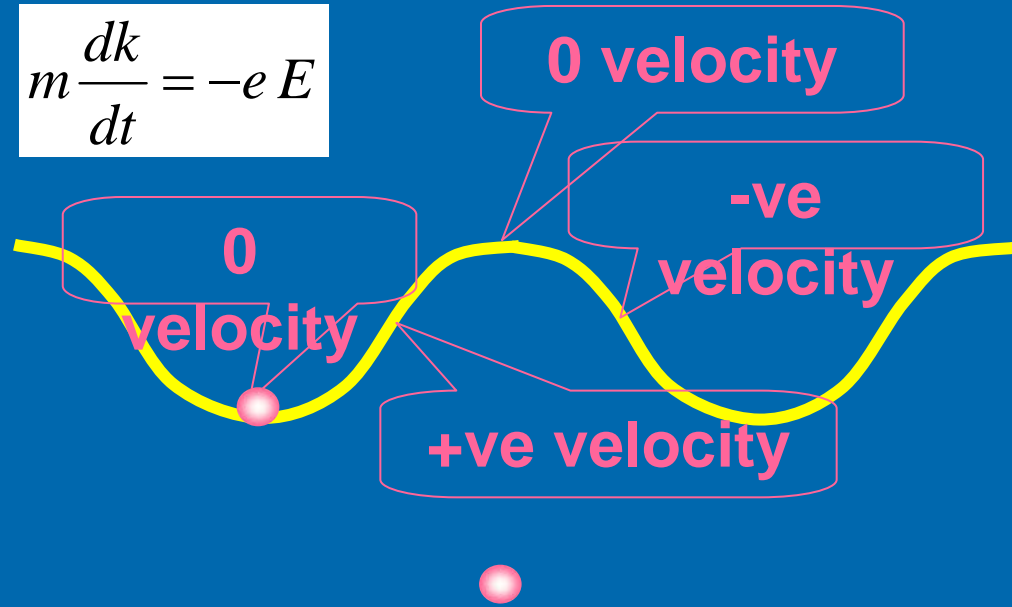
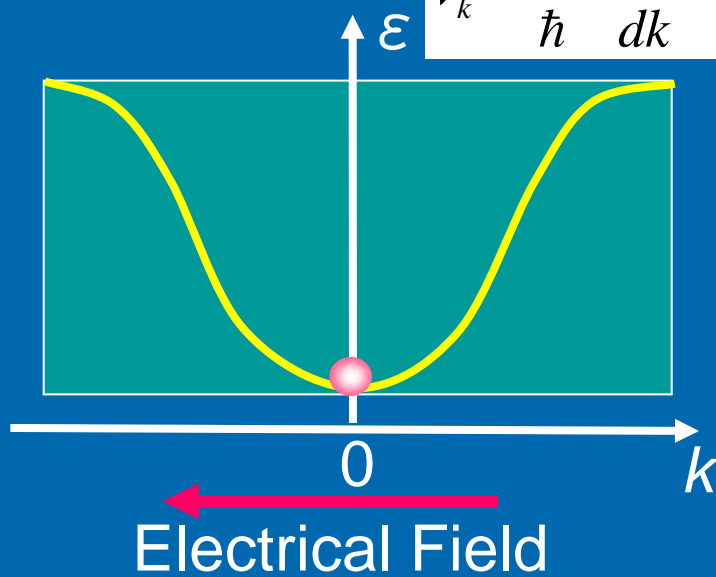
(Band Insulator)

# Movement of Bloch Electrons

Momentum Space

$$v_k = \frac{1}{\hbar} \frac{d\varepsilon(k)}{dk}$$

$$m \frac{dk}{dt} = -e E$$

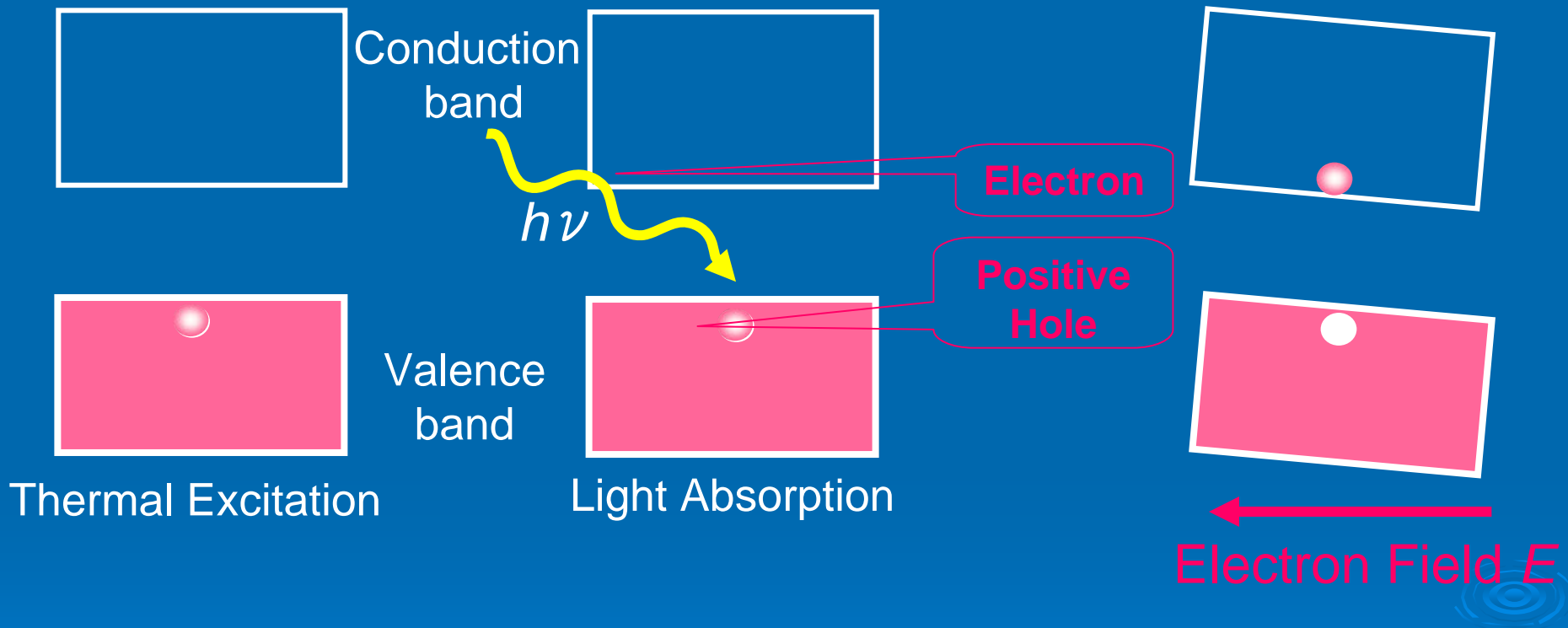


Even if you apply and electric field, the packing of electrons doesn't change

If there's absolutely no dispersion, do electrons just go and come back?

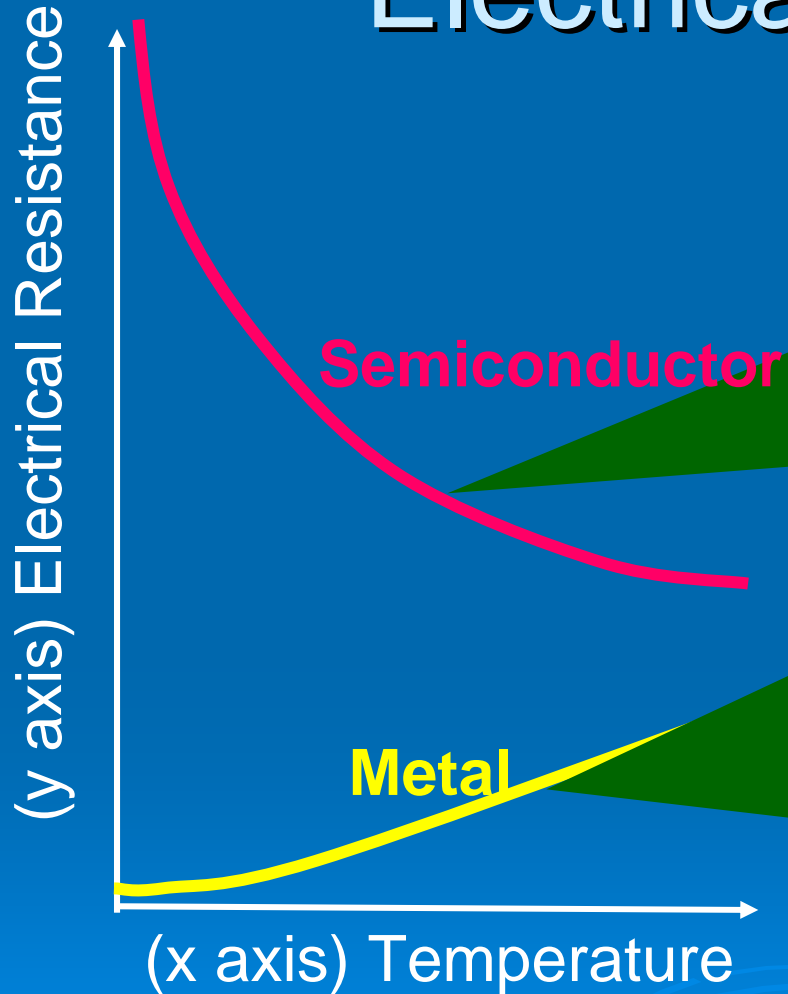
In real substances, the dispersion of electrons is usually slightly spaced-out to allow scattering.

# The Electrons and '(Positive) Holes' of Semiconductors



In semiconductors, the few carriers that are formed (Conduction Band Electron, Valence Band Hole) carry electrical conduction due to thermal excitation or light absorption

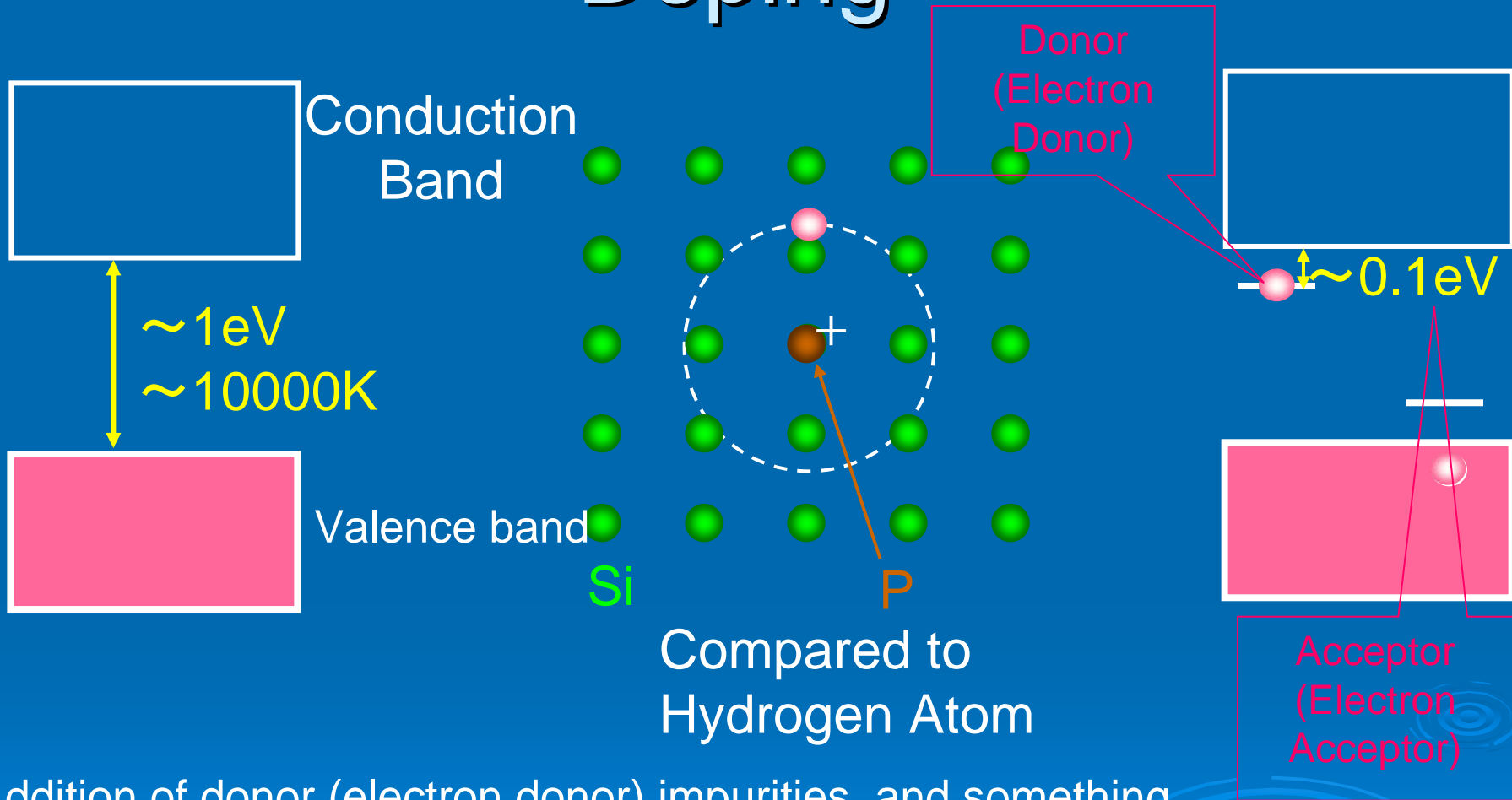
# Temperature Change of Electrical Resistance



In semiconductors (insulators), resistance decreases as thermal excitation increases due to rising temperature, to allow the multiple formation of (carrier) electrons and holes

In metals, the number of electrons doesn't change according to temperature. At high temperatures, lattice vibration works through the dispersion of electrons. Electron dispersion at extremely low temperatures is decided by impurities and defects etc.

# Doping

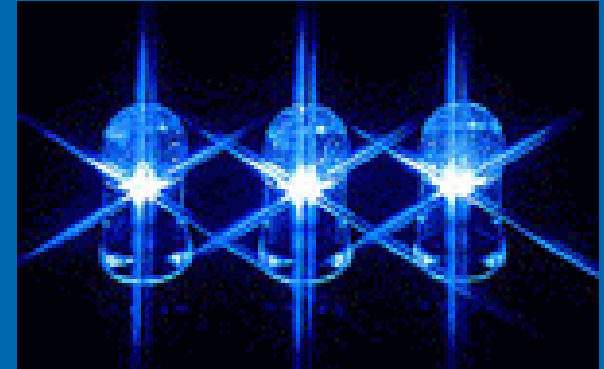
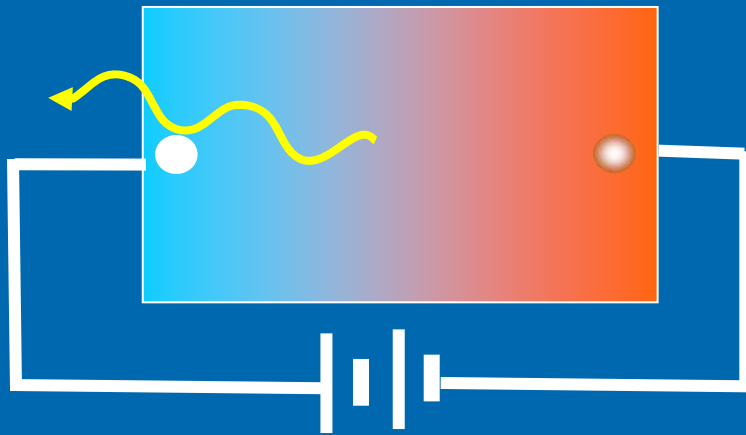


Addition of donor (electron donor) impurities, and something that supplies an electron to a conduction band is called an n-type semiconductor

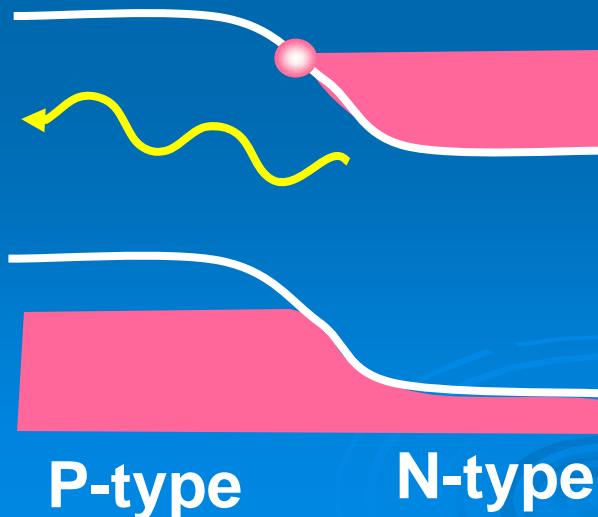
Addition of acceptor (electron acceptor) impurities, and something that makes a positive hole in a valence band is called a p-type semiconductor

# Light-Emitting Diode

p-n union



Light-Emitting Diode

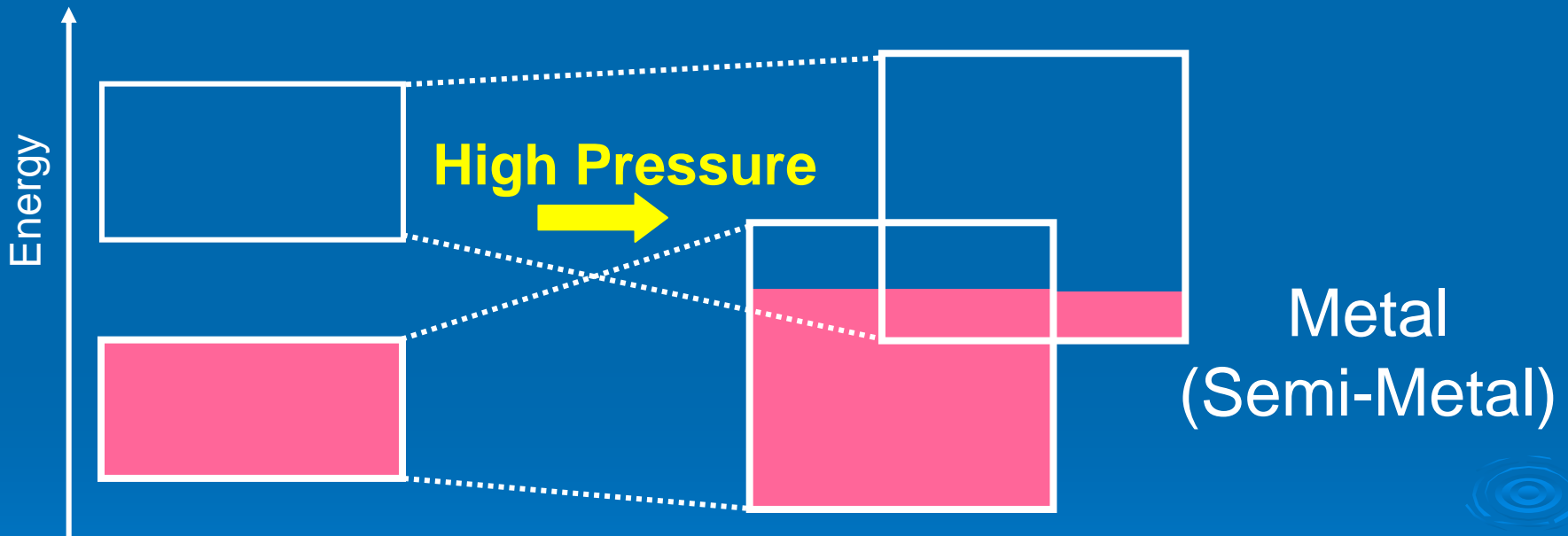
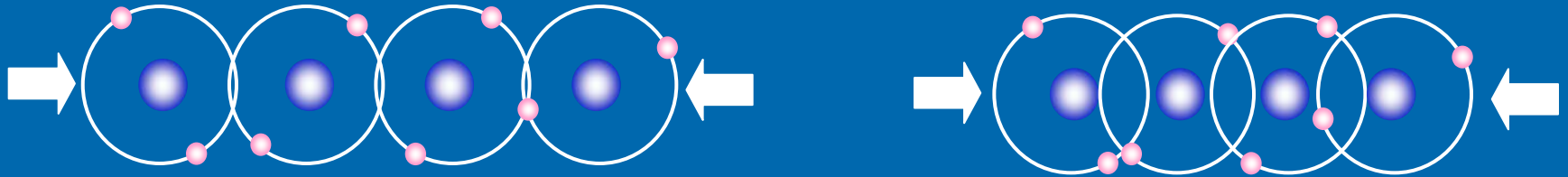


The color of the emanating light is determined by the band-gap of the semiconductor

1eV~3eV

Infra-red ~ Blue

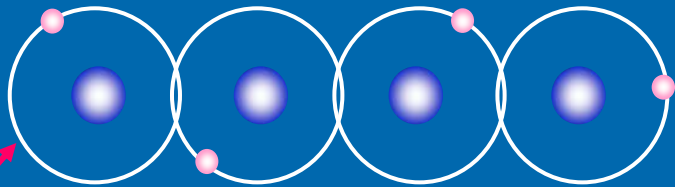
# (Simple) Metal-Insulator Transition



Insulator  
(Band Insulator)

Width of the Band broadens as the lattice is squeezed under high pressures, and the Valence Band and Conduction Band subsequently overlaps (Closing the Energy Gap).

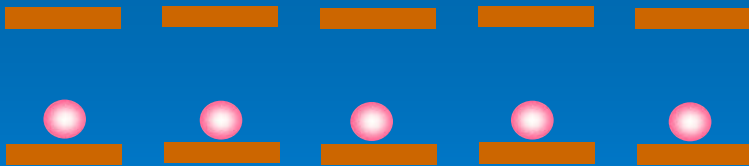
# Mott Insulator



In a situation where there are two electrons in the same orbital, the energy becomes higher by  $U$  (the inter-electron Coulomb energy)

When the number of beds and number of children is the same

⇒ no room for movement

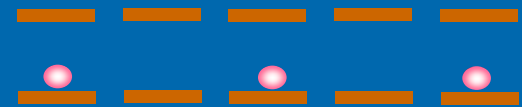


To move they must climb onto the neighboring bed

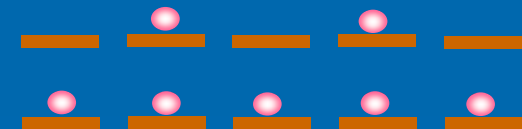
## Children Playing in Bunk-Beds

Children who come later have to get into the upper bed

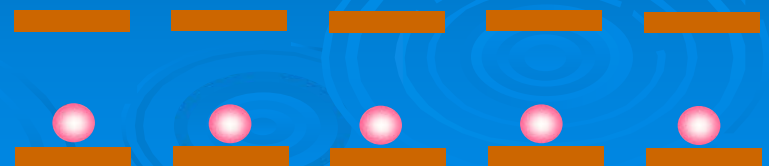
When there are more beds than children



When there are more children than beds



## Mott Insulator



# Strongly Correlated Electron System

- Like a Mott Insulator, a system where the strong coulomb interaction between electrons controls electron behavior is called a '**Strongly Correlated Electron System**'.
- Many remarkable phenomenon such as **High Temperature Superconductors** and the **Supergiant Magnetoresistance Effect** etc act as a stage for Strongly Correlated Electron Systems
- The behavior of Strongly Correlated Electron Systems is an **essentially difficult multifaceted problem**, and presently many researchers are concentrating their efforts into the elucidation of this quintessential physics.

# Magnetism



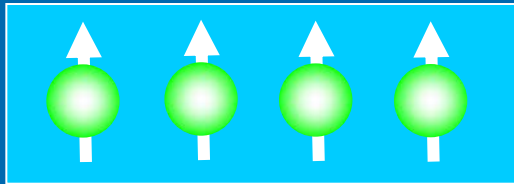
# Ferromagnetism

For a certain substance to be magnetic (ferromagnetic)

- 1) atoms (or molecules) must have magnetic moments (micro magnet)



- 2) these magnetic moments must align in the same direction

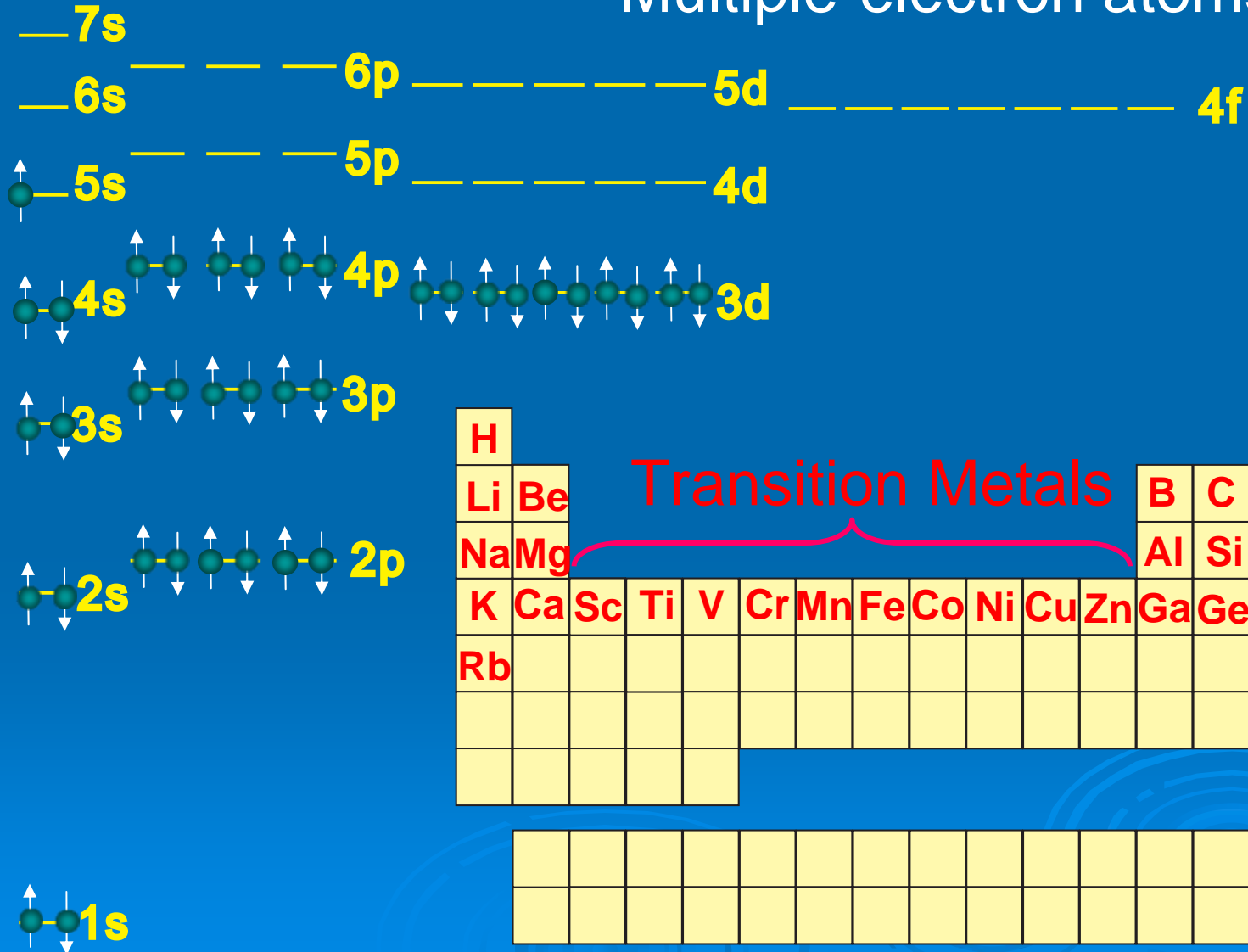


- 3) the macro specimen must have overall magnetization



# The Filling of Electron Energy Levels

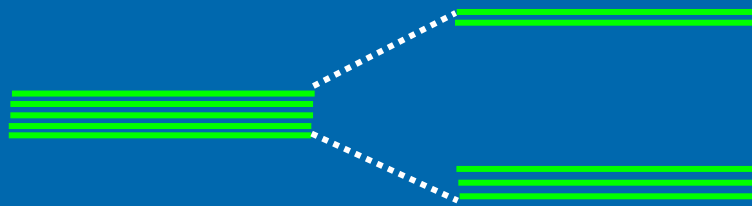
Multiple-electron atoms



# Electron Moment of Atoms (Ions, Molecules)

## d-Orbit of atom

5 positions each  
of  $\uparrow$  Spin,  $\downarrow$  Spin

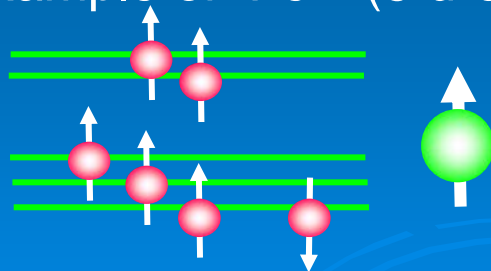


The 5 Energy Levels  
divide up depending  
on the environment  
(Crystal Field ) that  
atom is placed in

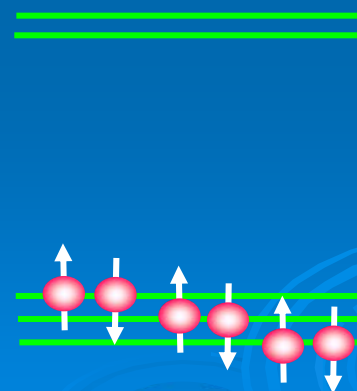
How do electrons fill here?

In avoiding as much as possible the repulsion coulombs between electrons, each orbital is occupied by single electrons of parallel spin before double occupation occurs.  
(Hund's Rule)

$\text{Fe}^{2+}$  The example of  $\text{Fe}^{2+}$  (6 d-electrons)



When division is small



When division is large

# Arranging the Magnetic Moments of Atoms

What is the force that arranges the magnetic moments of atoms?



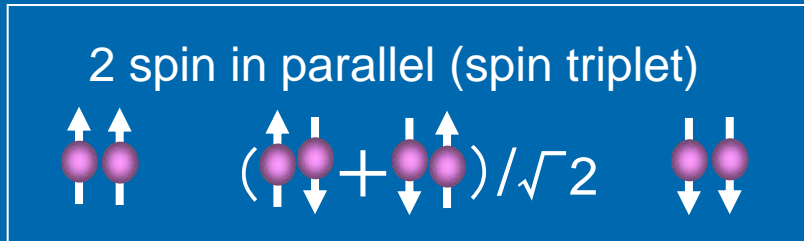
~~The magnetic dipole interaction of classical electrodynamics?~~

Interaction is too weak  
(Energy < 1K)

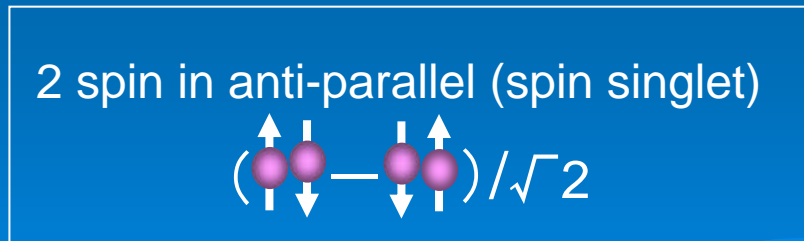


Quantum Mechanical Effect  
**Exchange Interaction**

(Difference in Coulomb interaction according to direction of spin)



↑↓ Difference in Coulomb Interaction Energy (Exchange Interaction)



$$\text{Energy} = -J \mathbf{s}_1 \cdot \mathbf{s}_2$$

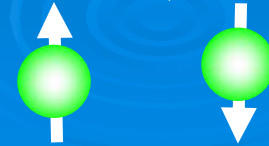
Ferromagnetic

$$J > 0$$

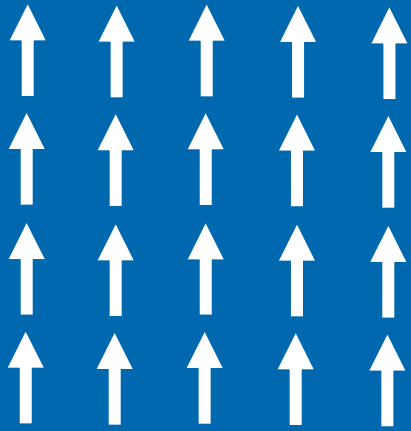


Antiferromagnetic

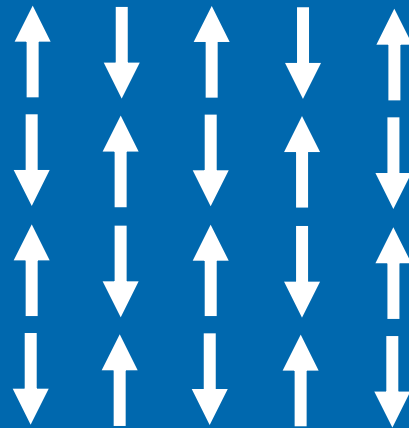
$$J < 0$$



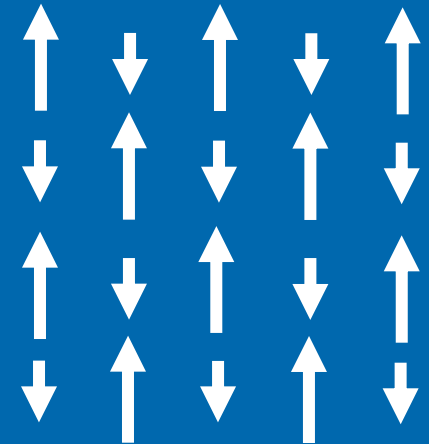
# About Magnetic Bodies



Ferromagnetism  
(Macro-magnetization)

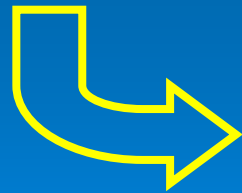


Antiferromagnetism  
(No macro-magnetization)

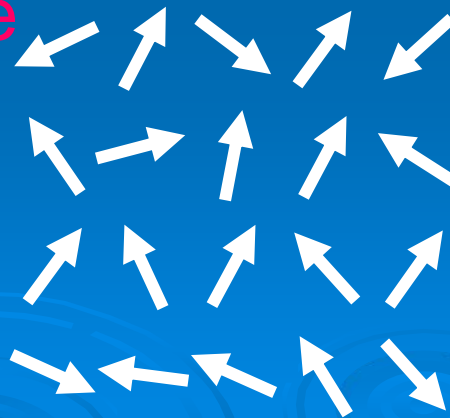


Ferrimagnetism  
(Macro-magnetization)

Ordered State



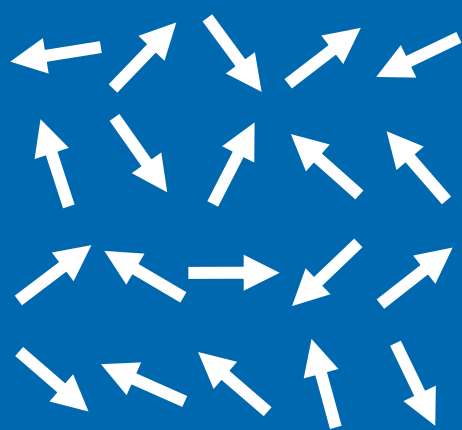
High Temp



Chaotic State

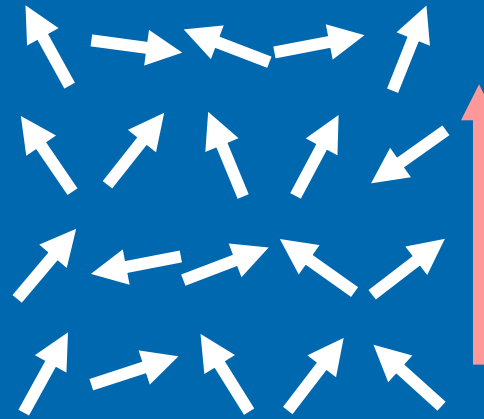
Paramagnetism (No macro-magnetization)

# Magnetic Order (Cooperative Phenomenon and Phase Transition)



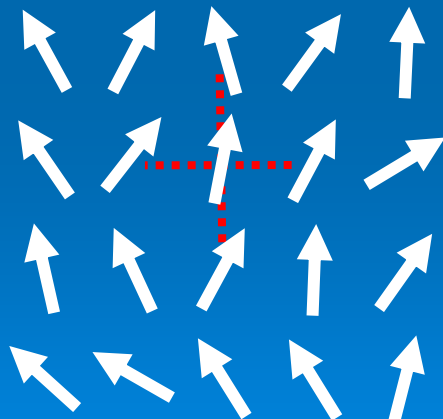
Chaotic State of High Temp

Apply  
Magnetic  
Field



Magnetic  
Field

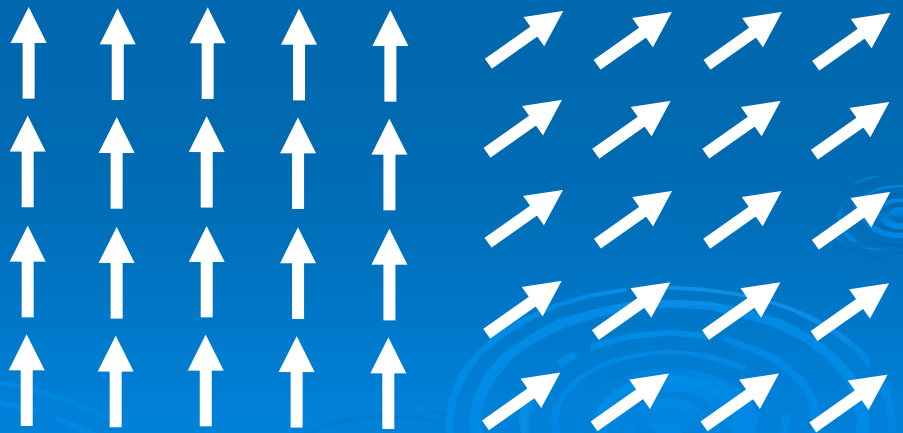
Low Temp



Tries to become parallel  
With the spin of their  
neighbor

Phase  
Transition

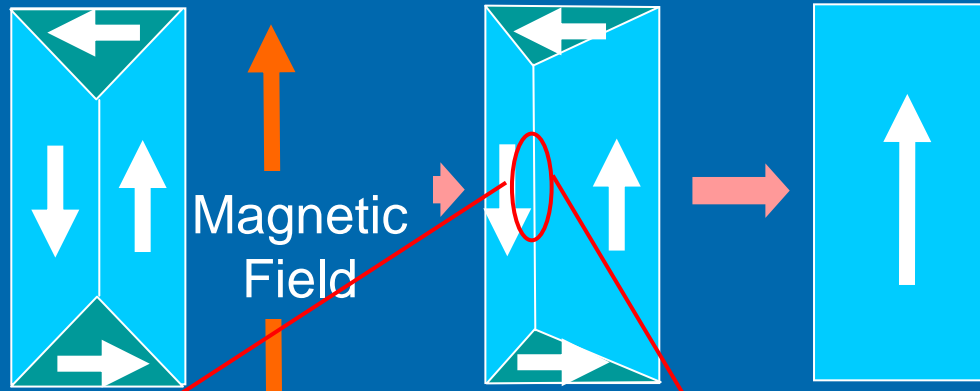
In terms of magnetic domain, the power arranging spin by changing-interaction is several hundreds tesla



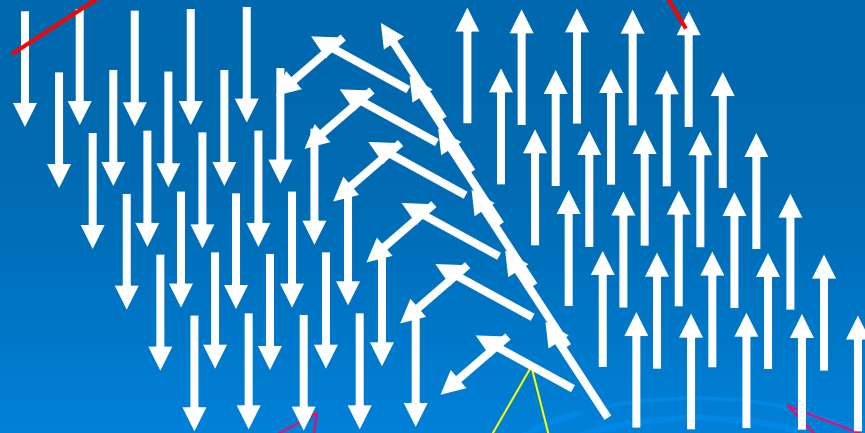
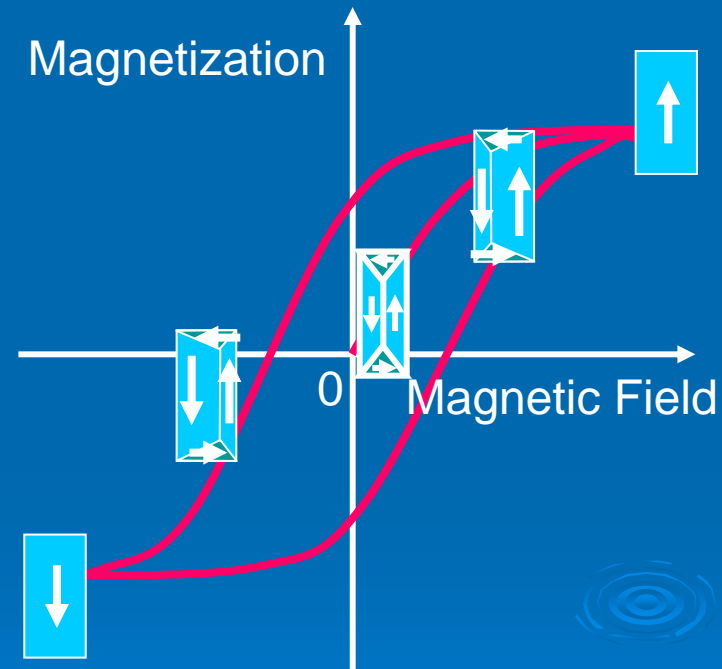
Ordered State of Ferromagnetism

# Magnetic Domains and Magnetic Domain Walls

Magnetization Process of Ferromagnetic Bodies



Magnetization Curve



Magnetic Domain

Magnetic Wall

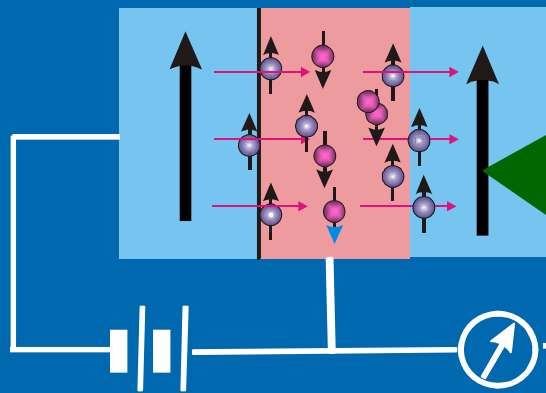
Magnetic Domain

# Spintronics

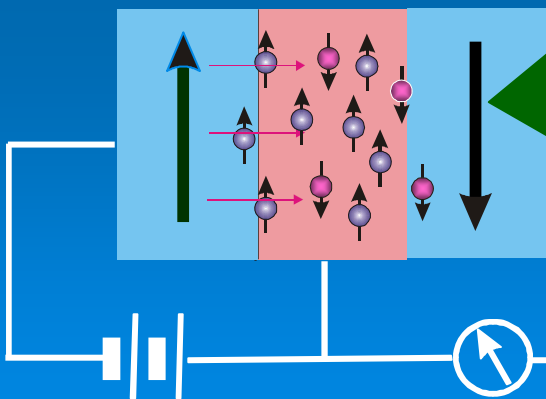
Electronics: uses the degree of freedom of electron's charge

Spintronics: uses the degree of freedom of electron's charge and spin

## Spin Valve Device

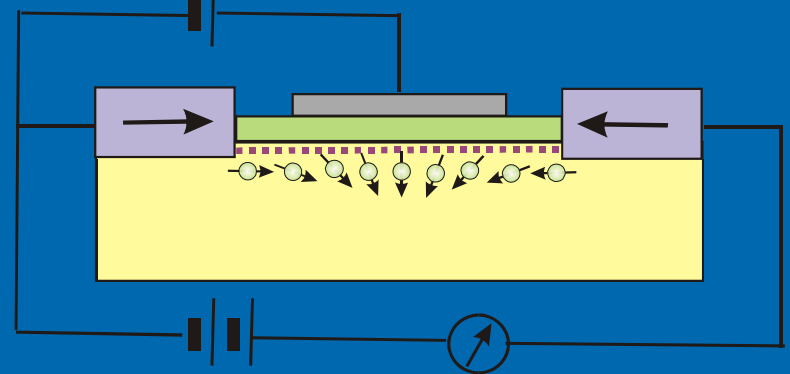


When magnetized is in the same direction, electrical current flows easily

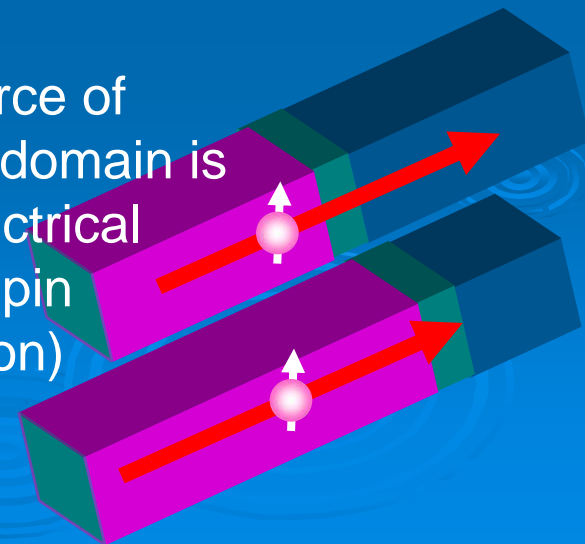


When magnetized is in the opposite direction, flow of electrical current is more difficult

## Spin Transistor



Driving force of magnetic domain is due to electrical current (Spin Polarization)



# Super Conduction



# The Super-conductivity of Elements

The Super-conductivity of Elements																		
H																		He
Li	Be												B	C	N	O	F	Ne
Na	Mg												Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pr	Au	Hg	Tl	Pb	Bi	Po	At	Rn	
Fr	Ra	Ac	Ru	Ha														

Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

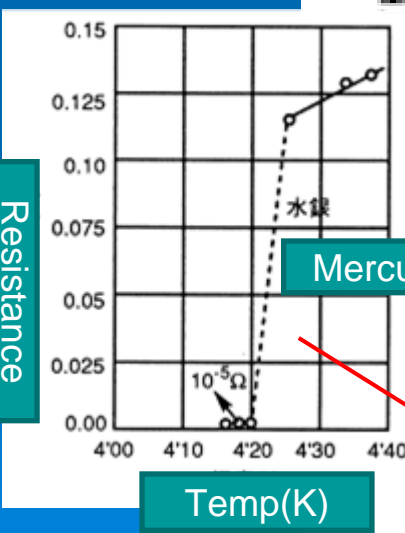
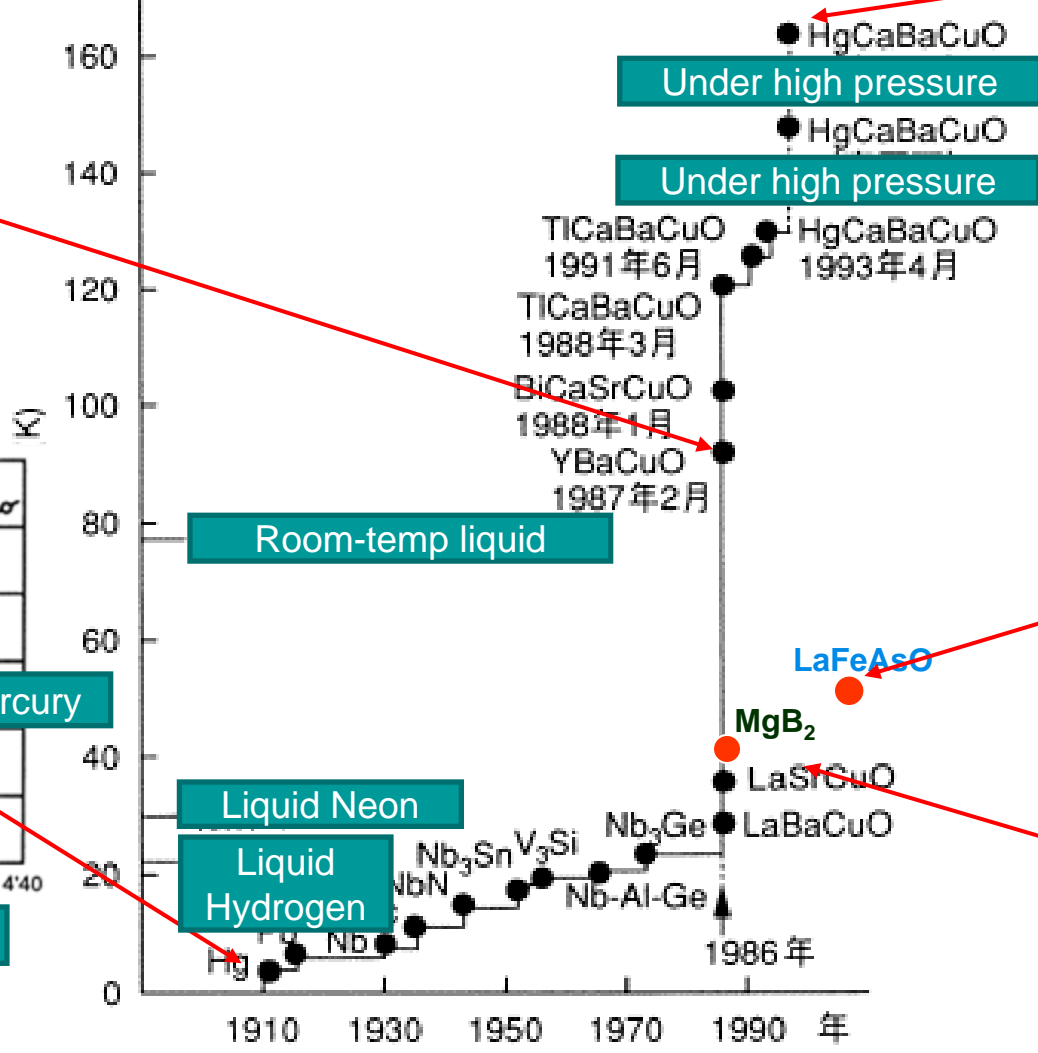
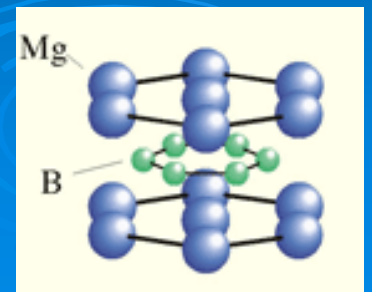
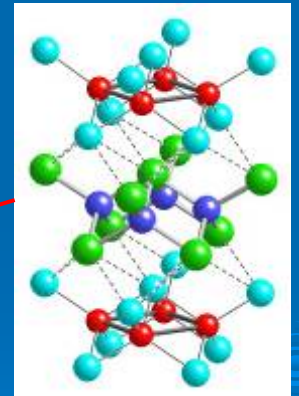
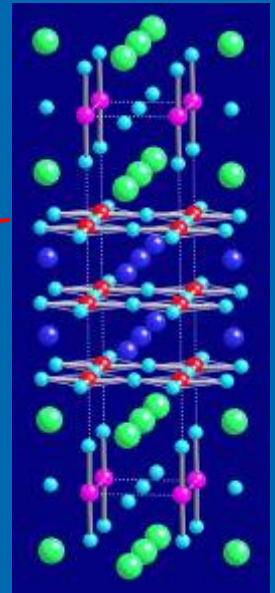
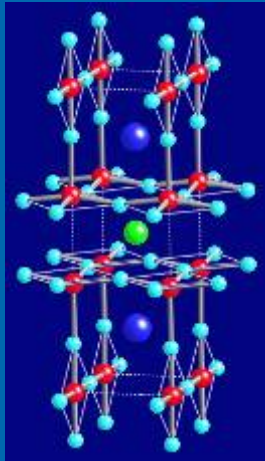
**Al** Substance which is super-conductive when in its normal crystalline form

**Si** Substance which is super-conductive only under special conditions such as under high pressure or in an amorphous state

**Cu** Substance in which a super-conductive phase hasn't been found

# Vicissitude of Superconduction Transition Temperature

Is room-temp super-conduction possible?



Resistance

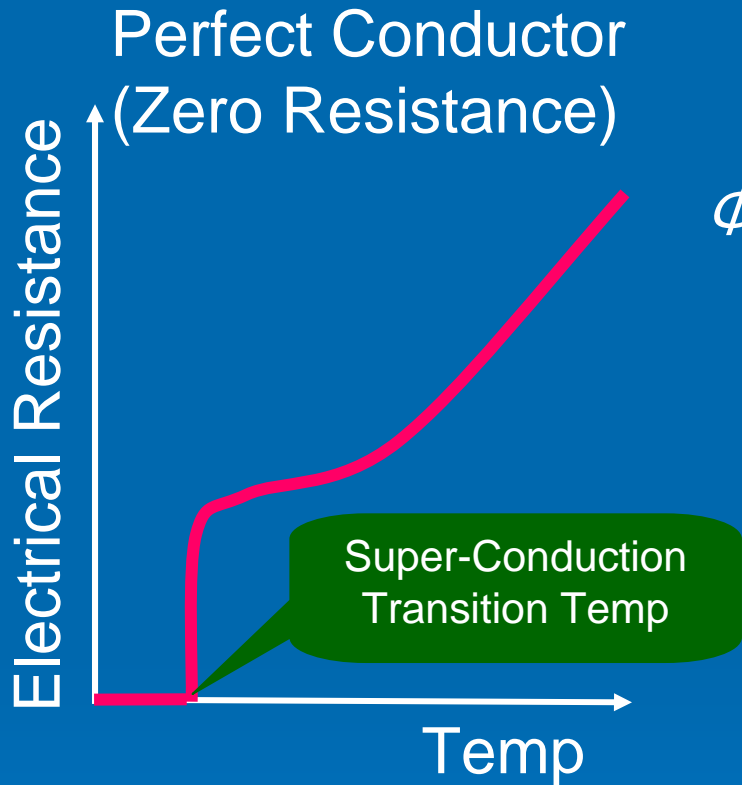
Temp(K)

Room-temp liquid

Liquid Neon

Liquid Hydrogen

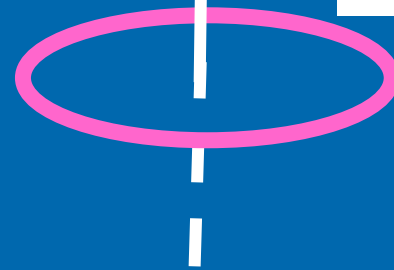
# Basic Properties of Super-Conduction



Quantization of Magnetic Flux

$$\phi = n \phi_0$$

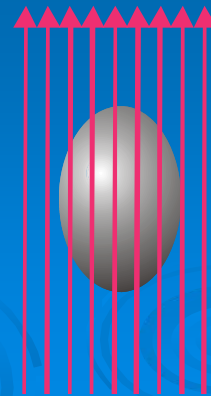
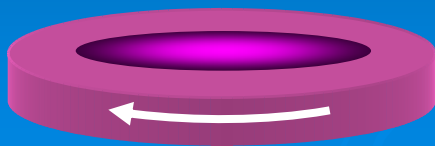
$$\phi_0 = \frac{h}{2e} = 2.07 \times 10^{-15} \text{ Wb}$$



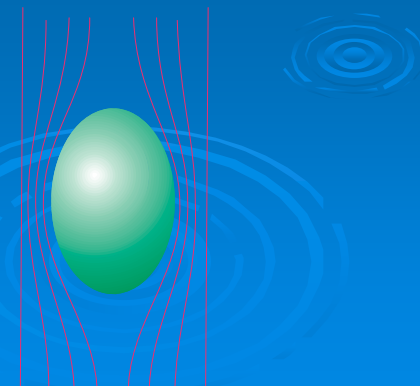
Same as quantization of rotation (swirl) in superfluidity

Meissner Effect (Perfect Diamagnetism)

Permanent Electrical Current



Normal Conductive State



Super-Conductive State

# Super-Conduction $\neq$ Perfect Conduction

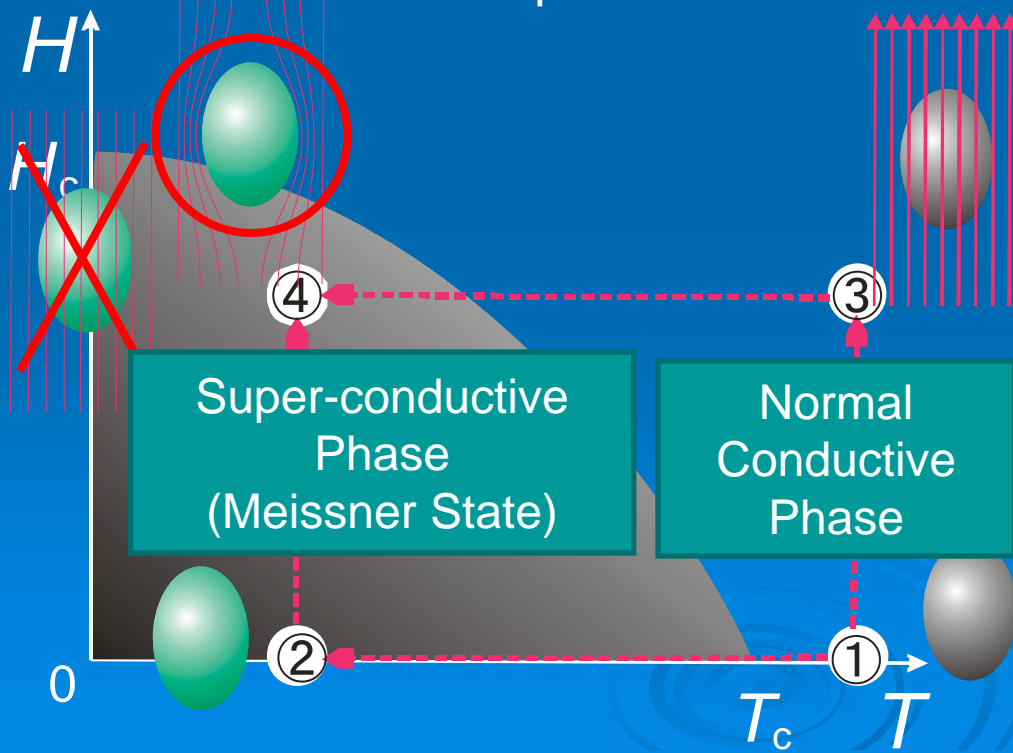
If you apply a magnetic field to a conductor, a shield current will flow (Lenz's Law), but it will soon decay due to resistance



In a perfect conductor, shield current continues to flow without any decay



However, in that case, the situation is dependent on how the magnetic field is applied



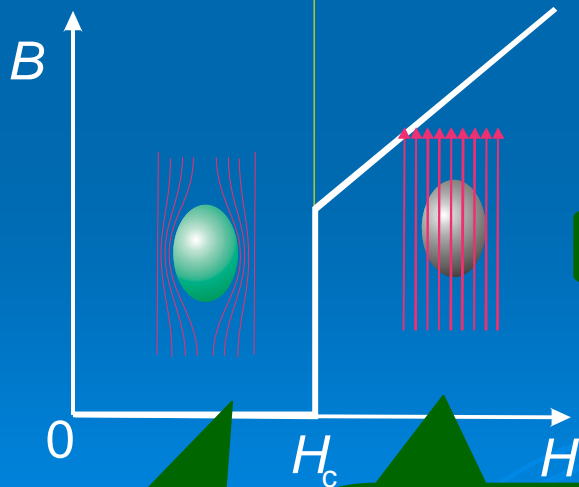
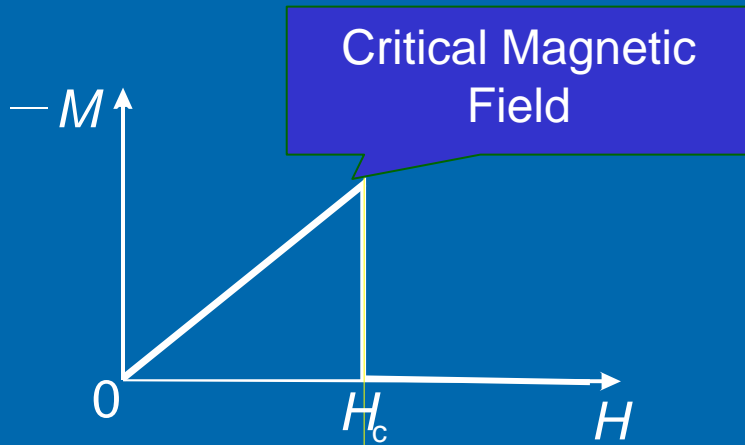
## Meissner Effect (Perfect Diamagnetism)

With a super-conductor, magnetic fields are completely eliminated

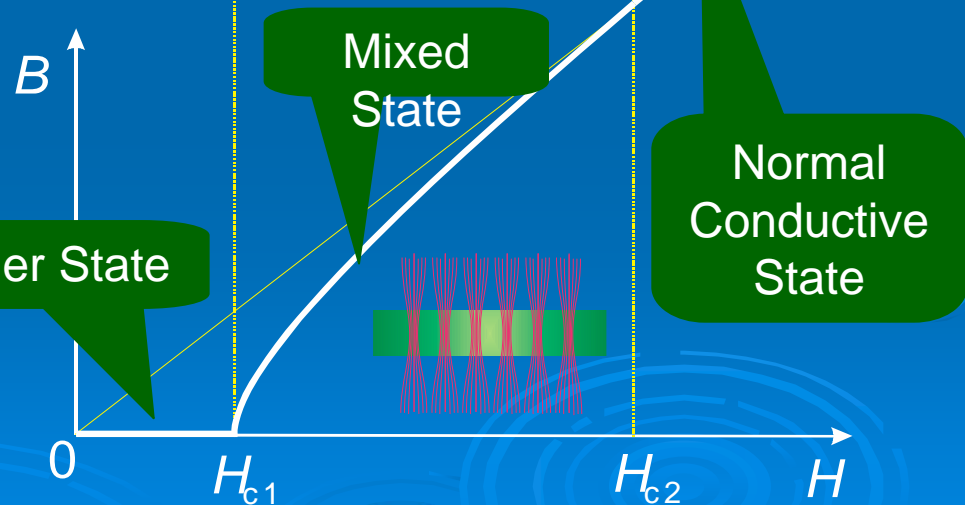
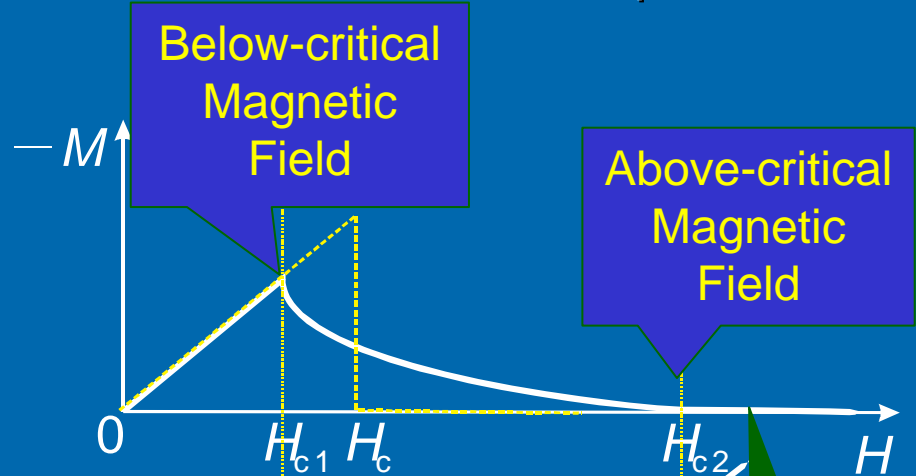
Super-conduction shield current is an electrical current that is flowing in a heat-balanced state

# First and Second Generation Super-Conductors

## First Generation Super Conductor



## Second Generation Super Conductor



Meissner State

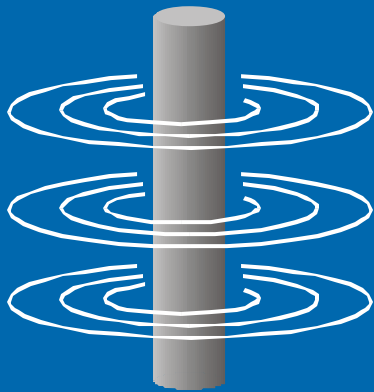
Normal  
Conductive State

Super-conductive substances that are use as practical materials are 2nd Gen Superconductors

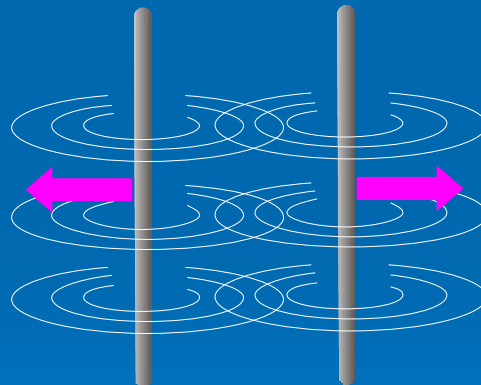
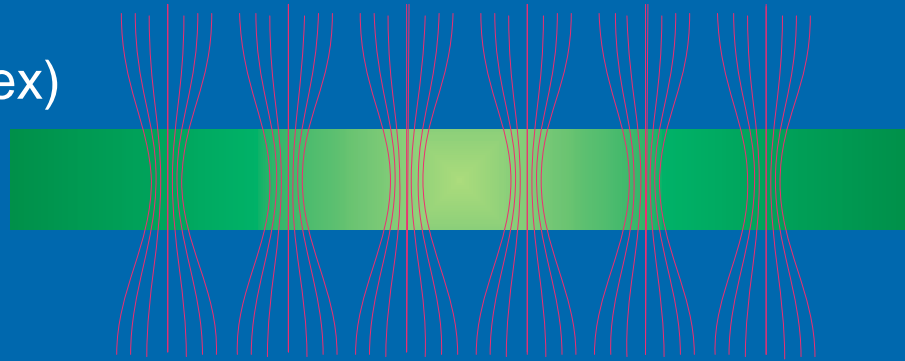
# Quantum Magnetic Flux (Vortex)

Mixed State of 2nd Gen Superconductors

Quantum Magnetic Flux (Vortex)



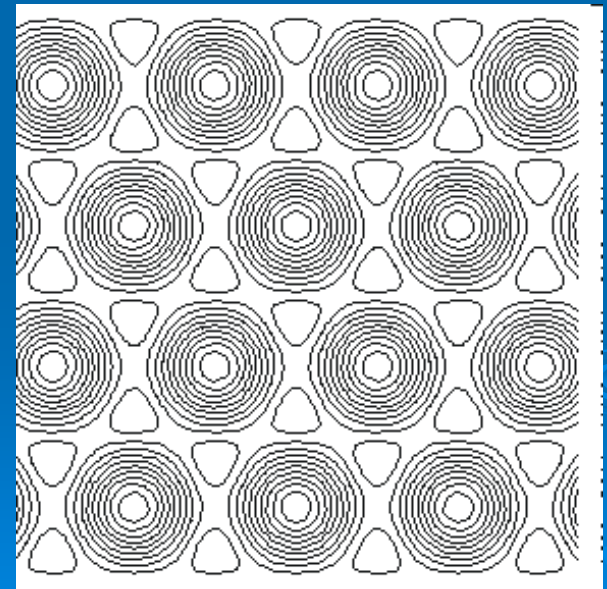
$$\phi_0 = \frac{h}{2e} = 2.07 \times 10^{-15} \text{ Wb}$$



Repulsive Force at work between Vortices

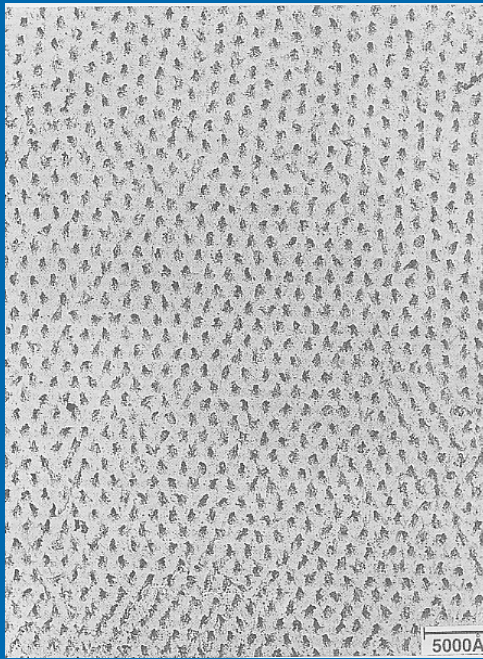


Triangular Lattice



Magnetic Flux Lattice  
(Abrikosov Lattice)

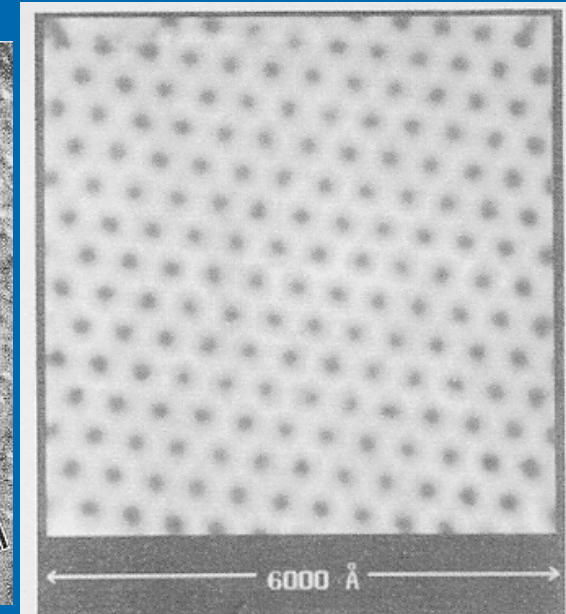
# Observation of Magnetic Flux Lattice



Bitter Method  
(Essmann & Traueble, 1968)

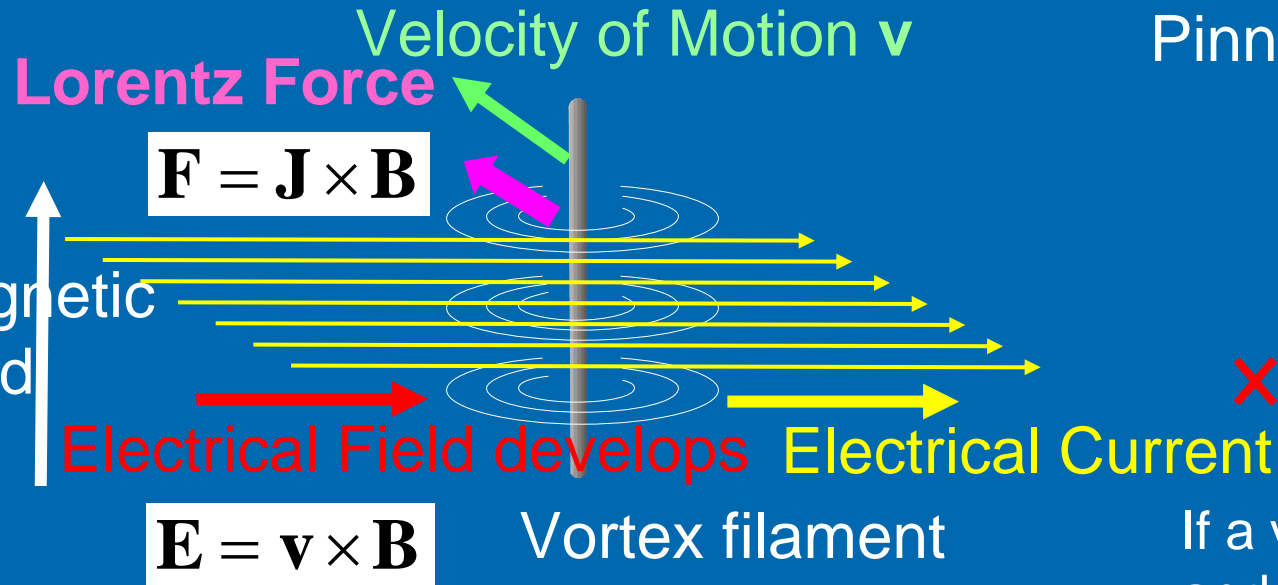


Lorentz Microscope  
(Tonomura Akira, 1992)

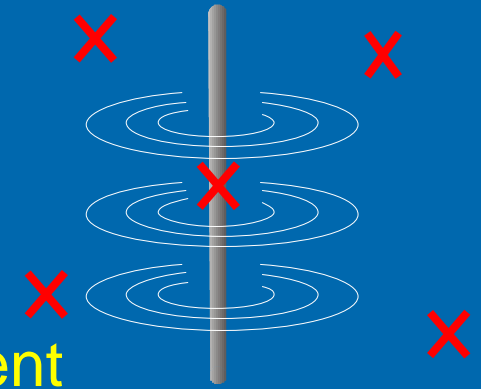


Scanning Tunneling Microscope  
(Hess, 1989)

# Lorentz Force and Pinning of Vortices



## Pinning of Vortices



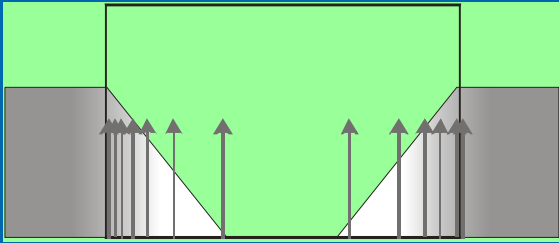
If a vortex is pinned and can't move, energy dissipation doesn't eventuate

Electrical field develops when a vortex moves. The creation of an electrical field in the direction of electrical current flow is the development of non-zero electrical resistance (energy dissipation)

**Lorentz Force vs Pinning**  
Current density that starts to move a vortex  
 $\Rightarrow$  **Critical Current Density**

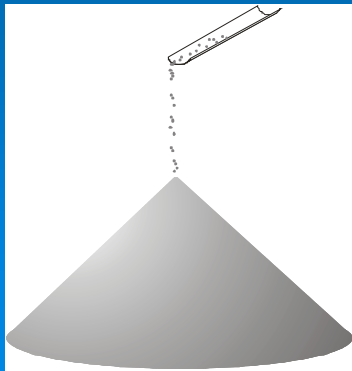
# “Hard” Superconductor

Strong Superconductor  
Pinning Vortices

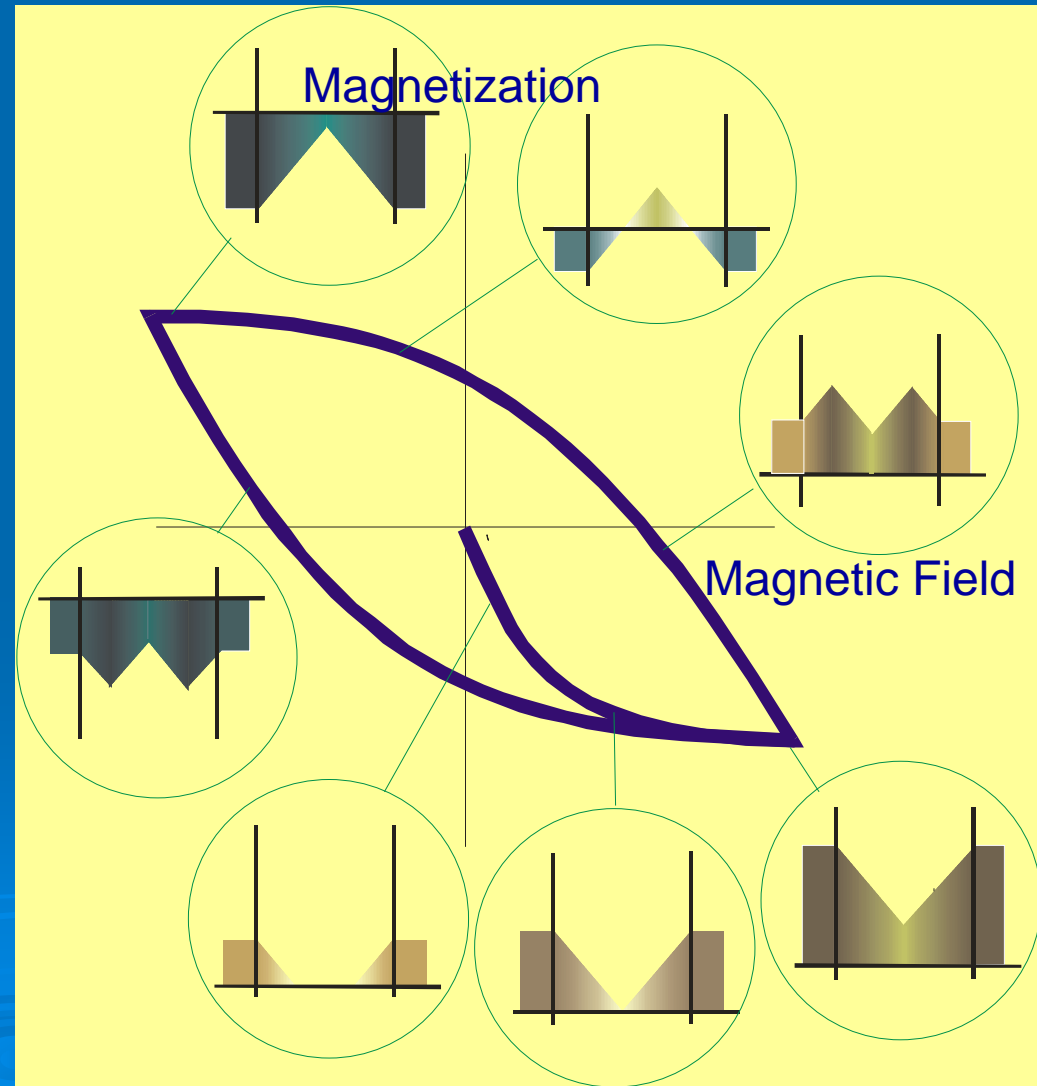


Shield current will flow  
until critical current is reached  
=>This decides the gradient of  
the magnetic flux density

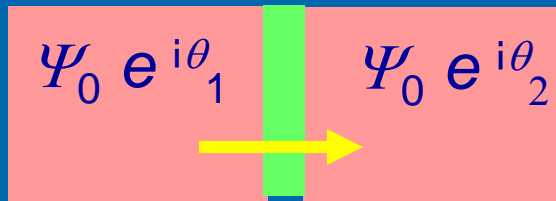
The shape of a sand hill  
(Critical state of self-organization)



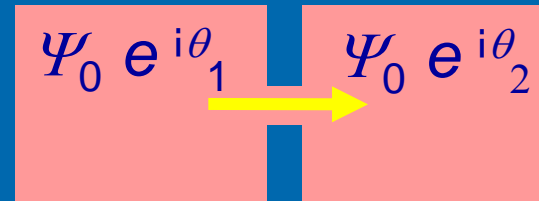
Magnetization Curve



# Josephson Junction



Tunnel Junction



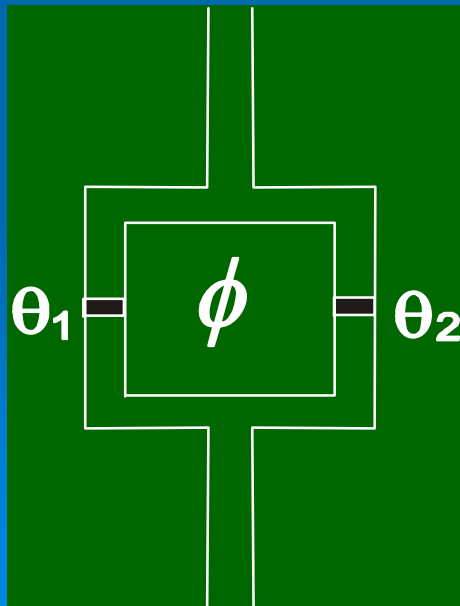
Weak Junction

Josephson Current

Depends on phase contrast of the junction

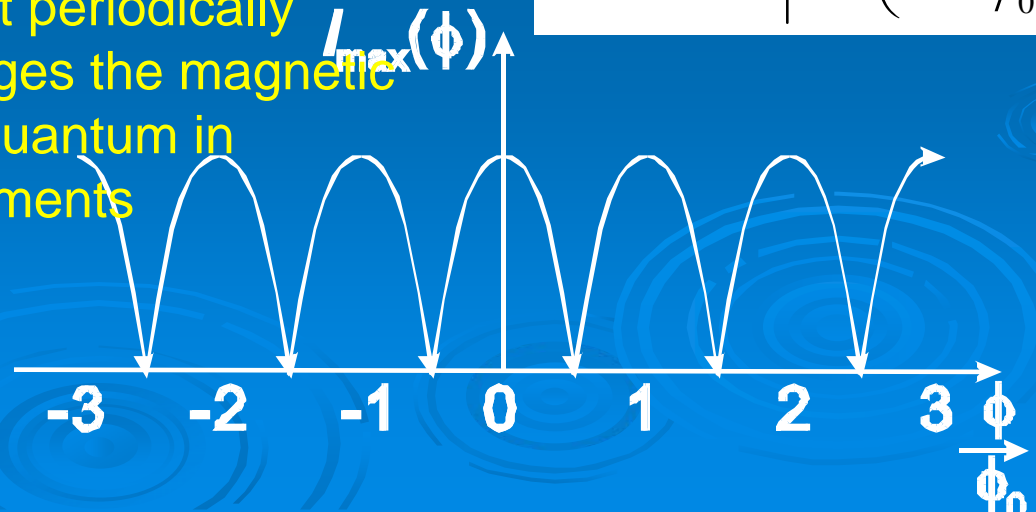
$$J = J_c \sin(\theta_1 - \theta_2)$$

## Superconducting Quantum Interference Device (SQUID)



A superconducting current that flows in a circuit periodically changes the magnetic flux quantum in increments

$$I_{\max} = 2I_c \left| \cos \left( 2\pi \frac{\phi}{\phi_0} \right) \right|$$

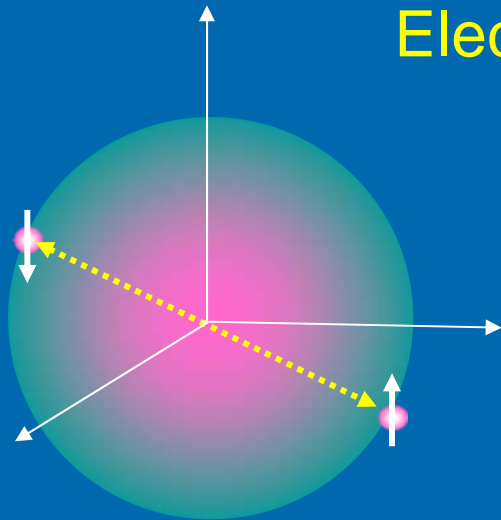


# Mechanisms of Super-conduction

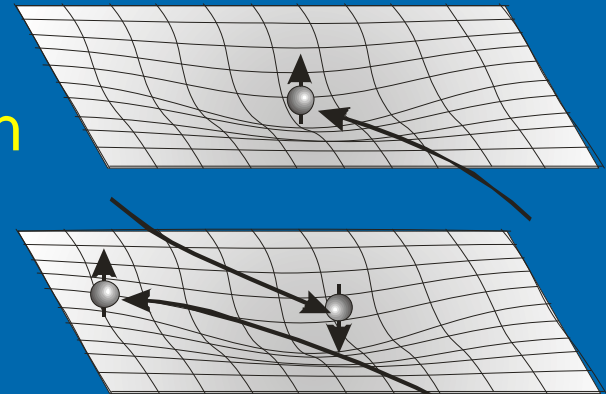
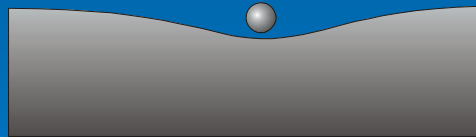
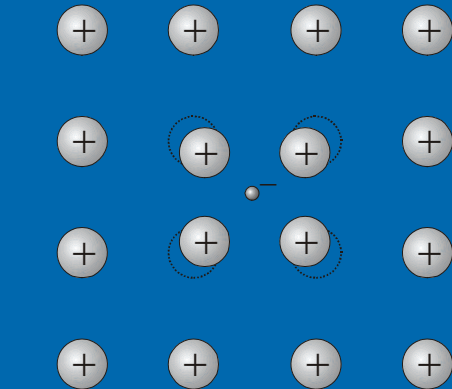
## Cooper Pair Configuration

Origin of Attraction?

Electron lattice Interaction



When attractive force acts on two electrons on the Fermi plane, a bound state (Cooper Pair) takes shape.



When the inter-electron attractive force that mediates electron particle interaction over-powers the inter-electron Coulomb repulsive force, pure attraction is able to function.

Super-conduction Transition Temp.

$$T_c = 1.14\Theta_D \exp\left(-\frac{1}{N(0)V}\right)$$

# Bardeen, Cooper, and Schrieffer (BCS) Mechanism

Inter-electron attractive forces  
overcome the inter-electron  
Coulomb repulsive forces



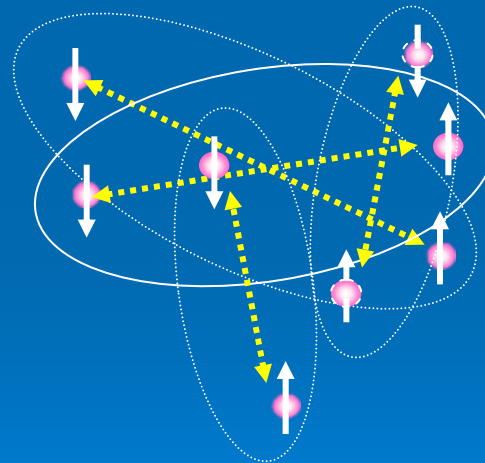
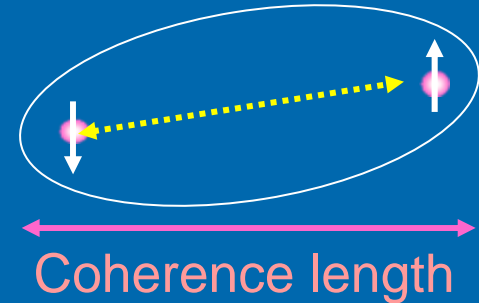
Formation of Cooper Pair



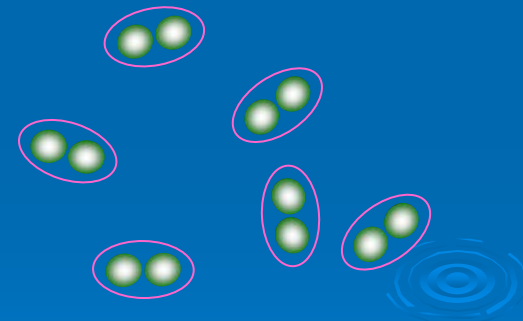
Bose-Einstein  
Condensation of  
Cooper Pair

=> Super-Conductive  
State

Size of Cooper Pair



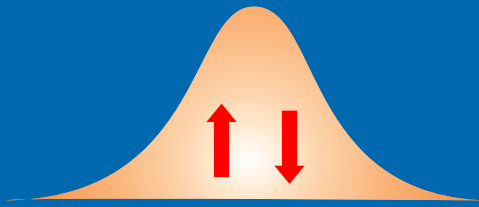
Cooper Pairs overlap  
each other



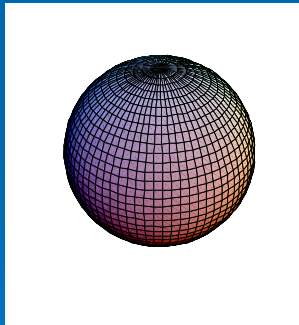
In the case of normal  
molecules, the size of  
the molecule is smaller  
than the distance  
between the particles.

# Anisotropic Super Conduction

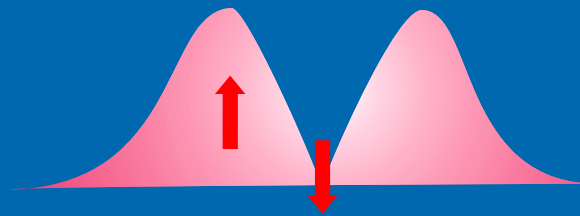
## Symmetry of Cooper Pairs



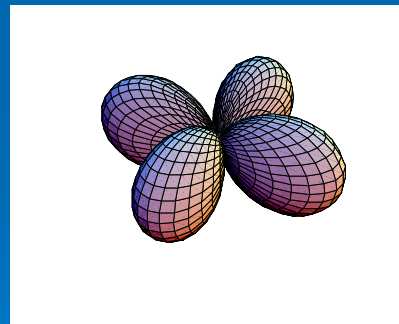
s wave ( $l=0$ )  
Spin Singlet



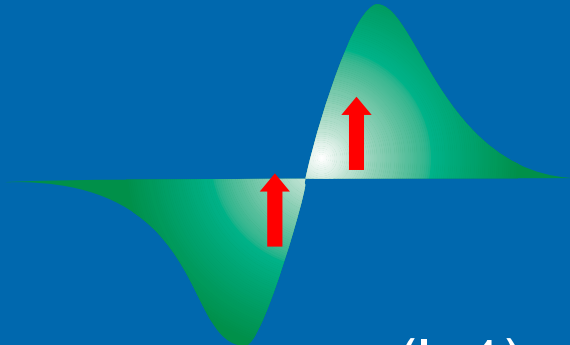
Super-Conduction of  
Most substances



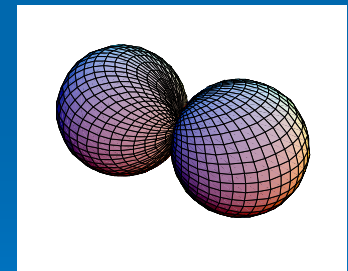
d wave ( $l=2$ )  
Spin Singlet



Copper-oxide High-temp  
Super-Conducting  
substance etc



p wave ( $l=1$ )  
Spin Triplet

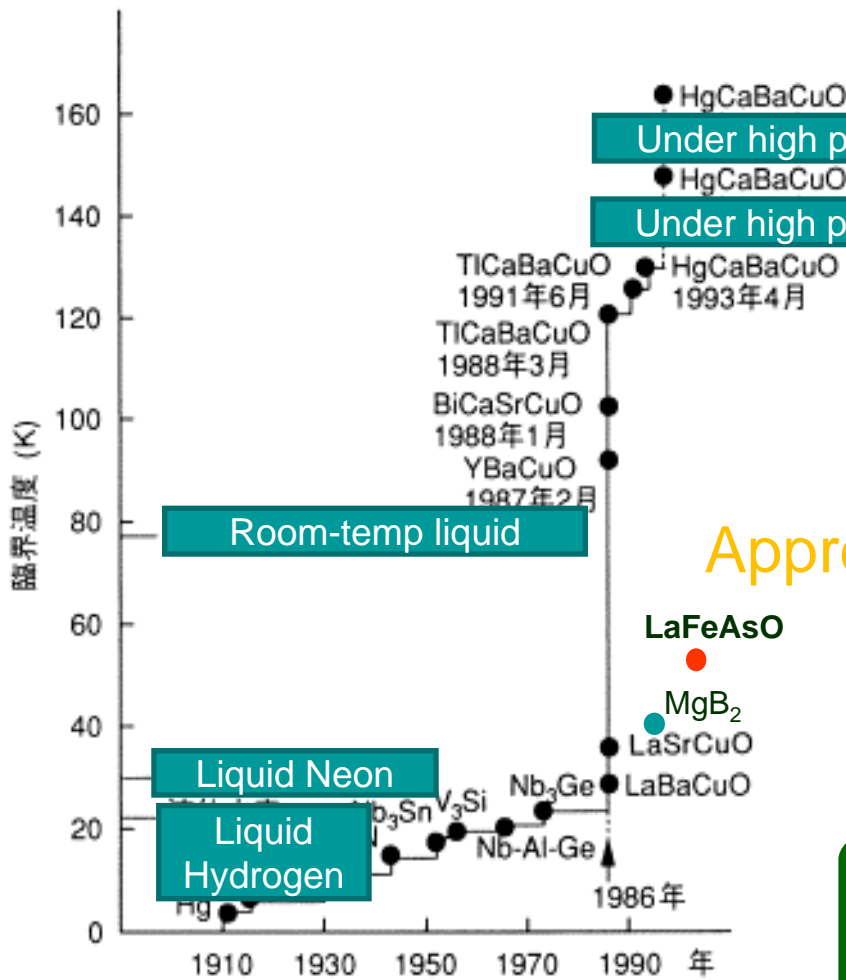


Ruthenium-oxide  $UPt_3$   
Super-conductivity of  
 $^3He$

# Exotic super-conduction

- Copper Oxide superconductors ( $\text{YBa}_2\text{Cu}_3\text{O}_7$ ,  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ )
- $\text{Sr}_2\text{RuO}_4$
- Heavy Fermion ( $\text{UPt}_3$ ,  $\text{CeCu}_2\text{Si}_2$ )
- Organic Superconductors ( $(\text{TMTSF})_2\text{PF}_6$ ,  $(\text{BEDT-TTF})_2\text{Cu}(\text{NCS})_4$ )
- $\text{MgB}_2$
- Alkali-Doped Fullerene  $\text{K}_3\text{C}_{60}$
- Boron-Doped Diamond
- $\text{LaOFeAs}$

# What is Room Temp. Super-conduction?



Super-conduction transition temp.

$$T_c = 1.14\Theta_D \exp\left(-\frac{1}{N(0)V}\right)$$

Characteristic energy scale of lattice vibration

Strength of electron lattice interaction

Approx ~30K is the limit?

$$T_c \approx T^* \exp\left(-\frac{1}{\lambda}\right)$$

Characteristic energy scale of prime excitation that intermediates inter-electron attraction

Strength of interaction

Room Temp. Super-conduction : there's no reason it isn't possible

# Summary

- Cohesive forces and crystal structure of atoms
- Electron state within solids (Band Structure)
  - Band
- Electrical Conduction
  - Metal, Insulator, Semi-conductor
  - Metal/Insulator Conversion, Mott Insulator, Strongly Correlated Electron System
- Magnetism
  - Magnetic Moment of Atoms => Exchange Interaction => Magnetic Domain
  - Spintronics
- Super-conduction
  - Fundamental nature of super-conduction (Zero Resistance, Meissner Effect)
  - BCS Mechanism
  - The search for superconducting substances => Room Temp. Super-conduction?