

Electronic Properties of the Materials: Computational Approach

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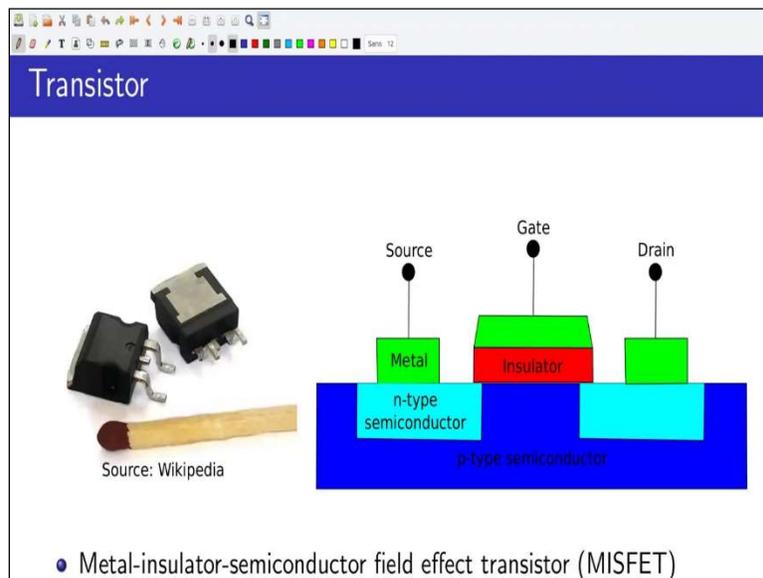
Indian Institute of Technology - Kanpur

Lecture: 1

Introduction

Hello friends I am Somnath Bhowmick from Department of Material Science and Engineering, IIT, Kanpur. Welcome to the first lecture of the course on Electronic Properties of the Materials. In this lecture I shall briefly explain the scope of the course.

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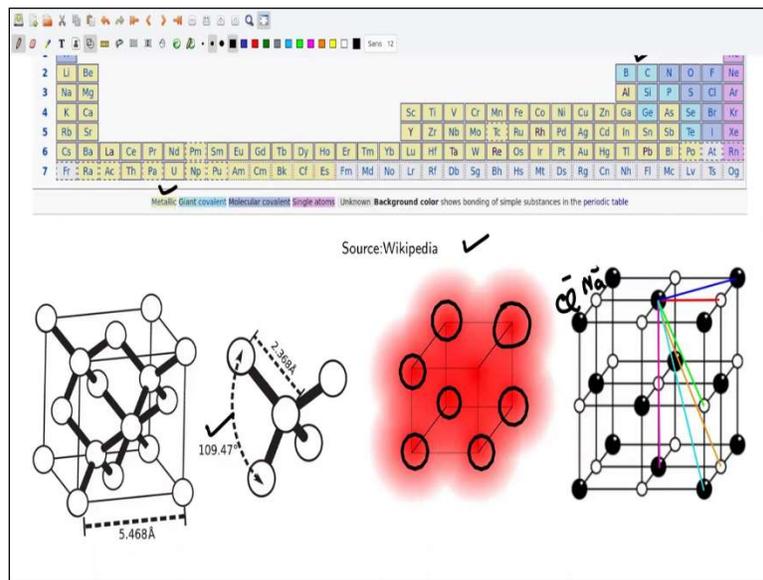
Let me start by showing a transistor which is one of the basic building blocks of modern electronics in particular I am going to talk about metal insulated semiconductor field effect transistor. In the left hand side actual devices are shown the matchstick is shown as a scale to give you some idea

about the size of the actual devices. In the right hand side main components of the device are shown schematically.

Current flows from drain to source via a region known as the channel region. And the current can be controlled by applying a gate voltage. No different class of materials used in the device. The channel region is made of semiconductor there are three metallic contacts in source drain and gate this is shown by the green colour. The gate electrode is separated from the body or channel region by an insulating layer right this is shown in the red colour.

Thus we need three different classes of materials to make the device metal, semiconductor and insulator.

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Let us explore the periodic table in search of metals semiconductors and insulators when individual atoms come together to form a solid their properties depend on the type of bonding holding the constituent atoms together. Looking at the periodic table most of the elements form a solid by a metallic bonding and some of them forms a solid via covalent bonding for example if you look at this region right the yellow region all of them they are forming a solid via metallic bonding.

And if you see this small region shown in blue they are forming a solid covalent bonding. Covalent bonding takes place via hybridization and overlap of atomic orbitals. For example in silicon sp³

orbitals form the covalent bonds with a bond angle of 109.47 degree. Metallic bonding takes place via valence electrons which becomes free from the core and forms a sea of free electrons. The ionic cores are submerged in the sea of the free electrons ionic cores are much heavier than the free electrons and remain fixed at certain points known as the lattice points.

For example if you look at this figure this dark region these you can consider as coarse and then outside the core electrons you have this diffuse region right and these are the valence electrons and you see that these ionic cores right they are at some points known as the lattice point and they are very heavy and they do not move. And the valence electrons may become almost free and they will move around in the solid and that is how the metallic bonds are formed.

Ionic bonds form among positively and negatively charged ions arranged in a lattice point. Obviously ions of opposite charge are held together by coulomb interaction for example if you take sodium chloride then this black points these are the chlorine atoms and the y points these are the sodium atoms and that is how they are arranged in a lattice and they are held together by Coulomb interaction.

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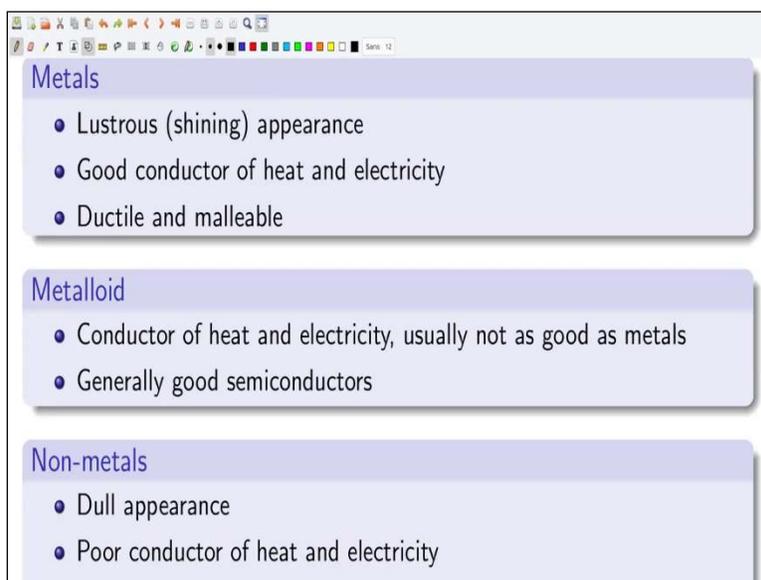
Group	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
Period 1	1 H																	2 He
Period 2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
Period 3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
Period 4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
Period 5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
Period 6	55 Cs	56 Ba	* 71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
Period 7	87 Fr	88 Ra	* 103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
			* 57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb		
			* 89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No		

In this slide I show the classification of elements in terms of their property the elements forming metallic bond are metals. There are further subclasses for example we have alkali metals we have alkaline earth metals we have transition metals and you see these gray boxes these are like

classified as other metals. Elements forming covalent bonds like boron, carbon, silicon, germanium etc these are known as metalloids.

You need two different elements to form ionic bond. When an element combines with oxygen nitrogen chlorine iodine etc to form compounds like oxides nitrides chlorides iodides etcetera such compounds are generally classified as non-metals. Generally these are formed by ionic bonding.

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Thus based on bonding we have broadly divided the materials in three different categories metals, non-metals and metalloids. Metals have shining appearance they are good conductor of heat and electricity and they are ductile that means they can be deformed without breaking them. On the other hand non-metals are dull in appearance and they are very poor conductors of heat and electricity and they are usually brittle that means they break easily.

Now metalloids their properties lie in between the properties of metals and non-metals. So, metalloids are conductor of heat and electricity but they are not usually as good as metals and these metalloids they are generally very good semiconductors.

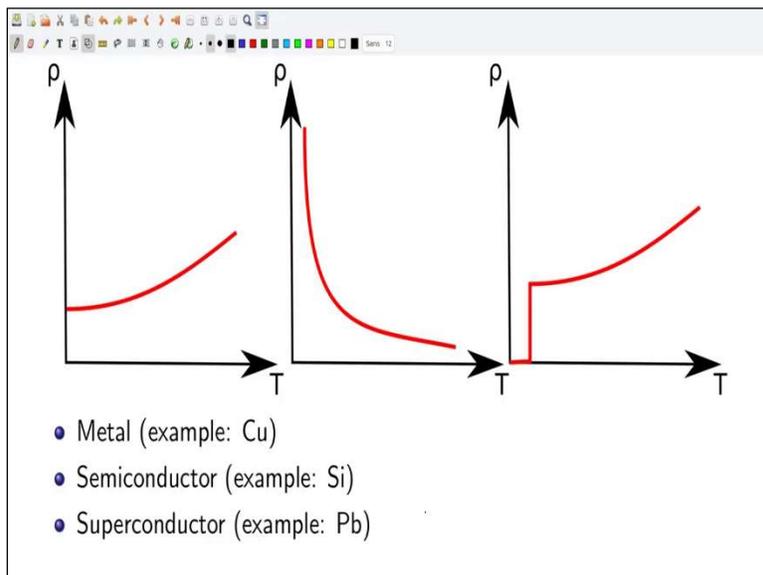
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Thus we know that the properties of metals non-metals and metalloids differ significantly because of bonding. Since this course is on electronic properties of materials I show you a comparison of electrical conductivity of different elements present in the periodic table. So, if you look at the metals mainly this reddish region then you see that the conductivity is very high that is of the order of 10 power 6.

Whereas if you look at the metalloid like silicon and germanium the value is only 10 that means there is a difference of 6 orders of magnitude. In this course we will try to understand why such a huge difference exists between metals and metalloids.

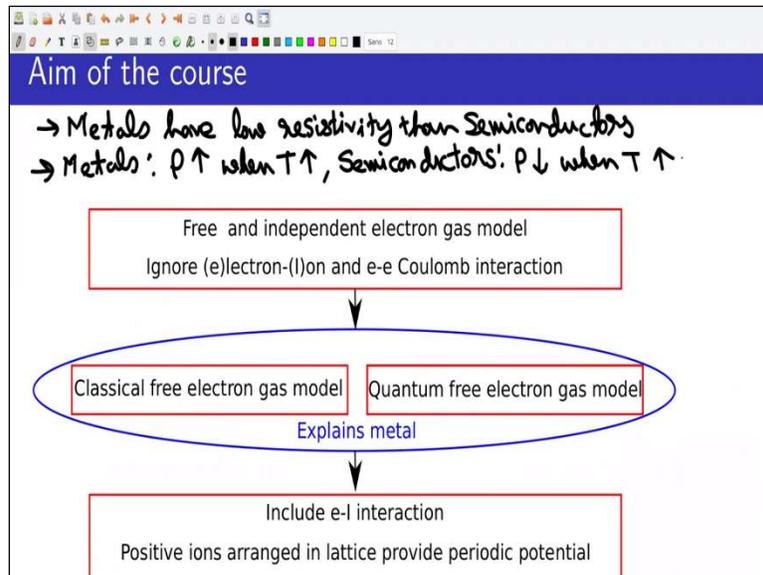
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Not only the order of magnitude of electrical conductivity in a metal and semiconductor differ but also the way its resistivity changes as a function of temperature that also differs completely. For example if you take copper and increase its temperature then its resistivity is going to increase. On the other hand if you take silicon and increase its temperature then in that case the resistivity decreases as a function of temperature then there is a third class of materials known as superconductors.

For example lead in such materials below certain temperature the resistivity suddenly drops to zero this is just for your information and we are not going to discuss about superconductivity in this course.

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Let me briefly explain the aim of the course. So, far we have seen that metals have low resistivity than compared to semiconductors and the difference is 6 orders of magnitude approximately moreover the resistivity increases in metal with increasing temperature whereas in semiconductors resistivity decreases when temperature is increased. So, we will try to understand why do, we observe such things.

In order to understand that we will start with free and independent electron gas model and such a model ignores the electron ion and electron-electron Coulomb interaction and such model can be explained at two different levels. First is classical free electron gas model and the second is

quantum free electron gas model. And we will see that the free electron gas model particularly the quantum free electron gas model can explain some of the properties of the metals very well.

And then we have to go beyond free electron gas model and we have to include electron ion interaction. Where the positive ions arranged in a lattice provides the periodic potential for the valence electrons and once we do that then we will see that we can get very good explanation for the properties of semiconductors and insulators.

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Fundamental concepts and technical skills

Fundamentals:

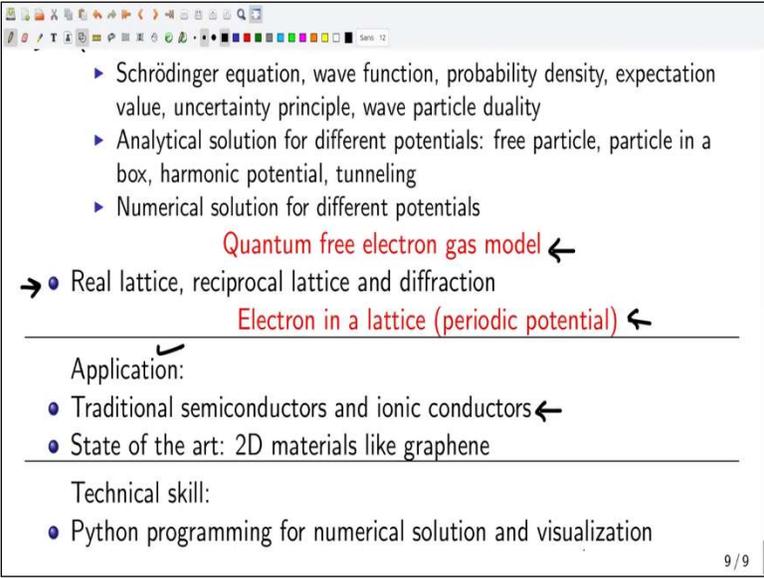
- Classical mechanics and electrodynamics
Classical free electron gas model
- Quantum mechanics
 - ▶ Schrödinger equation, wave function, probability density, expectation value, uncertainty principle, wave particle duality
 - ▶ Analytical solution for different potentials: free particle, particle in a box, harmonic potential, tunneling
 - ▶ Numerical solution for different potentialsQuantum free electron gas model
- Real lattice, reciprocal lattice and diffraction
Electron in a lattice (periodic potential)

Application:

Let me briefly mention the fundamental concepts and technical skills to be developed during the course. So, we will start with classical free electron gas model. For classical free electron gas model we need to know a little bit of classical mechanics and electrodynamics. Then we do quantum free electron gas model and for that we need to know the basics of quantum mechanics for example Schrodinger equation, wave function, probability density, expectation value, uncertainty principle, wave particle, duality etcetera.

Then we will learn the analytical solution for different potentials like free particle, particle in a box, harmonic potential, tunnelling etcetera. After that we will also learn how to solve Schrodinger equation numerically for different potentials. Then we do electron in a lattice or electron in a periodic potential for that we need to learn a little bit about the basics of real lattice, reciprocal lattice and diffraction.

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▶ Schrödinger equation, wave function, probability density, expectation value, uncertainty principle, wave particle duality

▶ Analytical solution for different potentials: free particle, particle in a box, harmonic potential, tunneling

▶ Numerical solution for different potentials

Quantum free electron gas model ←

→ • Real lattice, reciprocal lattice and diffraction

Electron in a lattice (periodic potential) ←

Application:

- Traditional semiconductors and ionic conductors ←
- State of the art: 2D materials like graphene

Technical skill:

- Python programming for numerical solution and visualization

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So, after we are done with the fundamental part we will learn a little bit about the application and in application part we will learn about traditional semiconductors and ionic conductors like silicon, sodium chloride etcetera. And then we will learn about state of the art for example 2D materials like graphene. Throughout the course python programming will be used for numerical solution and visualization.