

Physics of Functional Materials and Devices
Prof. Amreesh Chandra
Department of Physics
Indian Institute of Technology Kharagpur

Lecture – 50, Week 12
Summary

Greetings again. This is the final lecture of this course on Physics of Functional Materials and Devices. Over the last 49 lectures, we have covered a series of topics and sometimes you may get confused as to why we have covered these topics and is the topic which is being covered related to the topic which was covered next or if you consider a given topic is it related to what was discussed prior to that given topic. So, let me summarize the whole course in this lecture and you will find that each and every topic is related to what you were taught right from the first week onwards. So, in today's lecture let me discuss the salient features covered in the course. why and how these topics were chosen and they are related, why are the topics which were covered important in today's world.

We started with this slide discussion which was on the choice of the topic. we saw what was the reason because of which we chose the topic physics of functional materials and devices and not physics of materials. Why did we choose an additional term functional? Because in today's world what is happening? If you see people are always trying to have functionalities which are two or more in the same device. So, you need a device, but you need lot of functions to be performed by the given device.

And therefore, you must also try to find out the materials which can give you lot of functionalities that means, they can be used for different functions and same discussion holds good for devices. and that is why in today's world the course which becomes important is physics of functional materials and that is why we chose this topic. If you look into the way we started, we started with discussing solid materials and then we lot many materials, but they were solids. For example, we talked about transition metal oxide, we talked about transition metal sulfides, metal organic frameworks, conducting polymers, carbons and many more. What was the reason why we talked about these materials? The basic idea was that when you choose different elements to make a material let us say Mn or cobalt oxides or copper oxides.

What are you doing? You will find that these material elements they combine and they arrange in different orders. They can have different shapes. or sizes. Because of the particles having different shapes and sizes the crystal structure which is there having

different lattice you have different properties of these materials. Those properties will define the application of the material.

There were various ways which were discussed that will give you an idea how to change the properties of a material. Suppose you change the size of the material that means, you go from bulk to nanomaterials. So, we have discussed both properties of bulk materials and then when you go to nano size how the properties change. Functionalization of shape and morphology that means, you can have different types of particles and their shapes and obviously, their properties would be different. You saw in the previous lecture itself where we talked about SEM TEM, we had talked about capped carbon and we have talked about bowl like carbon.

You could see those particles and immediately tell that the properties of these two particles even though they are carbon would be different. We have talked about solid particles and then hollow particles. You could see that the area which was becoming available on solid particle and on hollow particles was entirely different and therefore, their response would be quite varied. Then you can have porous structures or dense structures, they will have their own properties. If you change the band gap of the material that means, you tune the conduction band and balance band formation in a material, then you can change the conductivity of the materials and therefore, their electrical properties can change. This is what we have discussed. So, we have talked about from bulk to nanomaterials and then from insulators to conductors or capacitors to battery applications of these materials. So, you can have different shapes and sizes of particles and obviously, the response characteristics of these materials both physical as well as chemical would be very different. This is what we discussed. Now, the point which you also saw that the crystal structure also plays very important role in deciding the properties of the material.

If you have let us, say you have rock salt type structure or a zinc blend structure or a perovskite or a spinel structure. The way the atoms are arranged they are quite different and because of this the response characteristics of these materials are also quite different. How will you make these materials? composites which are routinely used in large number of applications. How will you make these systems? Then we saw that you have to have quite a few synthesis protocols which can actually tune the properties and you can have the capabilities to make materials ranging from bulk size to nano sized. You had synthesis protocols which are classified under two broad headings.

What are those? Either you had the top down approach or the bottom up approach. So, from bottom up approach what were you doing? You were actually having the raw materials they were reacting and you were then reaching the final molecular formula and getting a solid solution or a single phase material. In the top down approach what were you doing? You were having the materials which were already formed and then you were reducing the size of the particles of these materials by crushing it in a top down approach

or cutting it as per the requirement in the shape which is desired for a given application and you are using techniques such as ball milling or lithography. So, knowing and understanding the synthesis protocols became essential. So, that you could get various types of materials and then use them for different applications.

When you go from large size particles so, you can go to 2D structures, 1D structures or 0D structures. So, then we had defined the quantum well structures, quantum wire structures, and quantum dot structures. To investigate the applications of these materials, we saw they can be used for energy applications, truck delivery or medicine, you can use them in electronic or sensor technologies. So, clearly till now everything is moving as per the logic.

So, you first decide the material which you want to make, find out using Hume Rothery rules or ab initio calculations whether those materials will actually form or not, use synthesis protocols to make those materials. Once you have those materials classify the nature of those materials, what type of materials those are and then find out the applications of those materials. So, once again it is absolutely essential to get the chemistry of materials right, if you want to do proper physics of materials or devices. You have various types of synthesis protocols which were discussed. Then if you see the formation of the lattice, what were we discussing? We saw that now you have a solid structure.

These structures can actually arrange themselves in crystalline or non-crystalline manner. So, short range ordering or long range ordering. So, crystalline long range ordering, non-crystalline short range ordering. the crystalline you can have single crystals or polycrystalline samples. Obviously, if just by looking at the lattice which is drawn with limited number of atoms, you can find out the properties of these two lattices would be different.

Following our discussions on solid materials then we went on to talk about the formation of alloys. Because this is one thing which is known to mankind for centuries and you find evidence of mankind knowing about alloy formation for generations after generations. what is the concept of parent or solvent and solute while you form an alloy was introduced. So, the metal which occurs in higher concentration is parent or solvent and the chemical element which is used alloy with this parent or solvent is the solute. So, by changing the concentration of solute you will get different composition of alloys and they will have their own properties.

It was also clearly explained that do not expect that every material which you make will be a perfect material. In fact, you will always have certain level of imperfections in the materials which are synthesized. And if you have imperfections then what are their nature, how will they impact the properties of these materials and how do you actually use these concept for your advantage. So, we talked about the requirement of moving away from the consideration of having perfect material to realizing the fact that you will have

imperfections. We talked about crystal imperfections, point defects, line defects, burger vectors and interfacial defects.

These particles which are formed can have different nature. They can be metallic, insulator or semiconductor. This was described using the nearly free electron model. So, we had the reduced zone scheme or you took the extended zone scheme to explain the origin of band gap. And you can also use the flat band diagram to understand that there is energy band gap in solids if you have periodic arrangements of atoms.

Periodic means you are getting certain arrangements which can be explained by crystallographic rules. Immediately we understood that by changing the crystal structure what will happen? you will get different extended zone scheme or the reduced zone scheme. That means, the nature of band gap will change when I go from one crystal structure to the other. That means, its electrical properties, the insulating properties or semiconducting properties may change when we go from one structure to the other. You can modify the molecular ionic covalent or metallic bonding structures and you will have the properties tuned when you go from one arrangement to the other.

If you transform from one arrangement to the other what are doing, we are actually undergoing a transformation. Then it became absolutely essential to understand the nature of transformation. What do we understand by transformation? Is the transformation of only one type or you can have various types of transformation? And when a system is undergoing transformation what are the consequences? is it always occurring at a constant rate or the rate of reactions can also change while the system transforms from one ordered state to the other or one state to the other. And if it actually transforms there must be certain factors which influence this transformation. So, all these things were also discussed.

Once you saw the transformation then there are classifications of phase transitions. We talk two of them either in terms of Rehnfest or Burger classification mechanism. So, the material is formed. If you have any system or a material, then you have migrations within a material from region of higher concentration to region of lower concentration till a homogeneous condition is obtained that is what is called as homogenization. And if that process is occurring what is that process called? That is called diffusion.

So, to actually understand what is the role of diffusion in solids, liquids or gases we spend significant amount of time. So, once the material is formed you know how to change certain properties and then we start investigating about a given material what all things can happen inside a material. So, we talked in terms of diffusion and if you have diffusion, then you can have different concepts. Then rather than mass transport, if we talk in terms of energy transport, then you can talk what is the heat capacity, the thermal expansion, the stresses and the conductivity of the material when there is temperature variation. Then came two important features of these materials which are to be used in applications.

We spent a lot of time on magnetism and its origin in the solid materials which we were discussing. We also discussed about the magnetism in alloys and what happens to magnetism when we go to small sizes of the particles which are forming the magnetic material. That gave us the route to understand the origin of magnetoresistance, giant magnetoresistance, colossal magnetoresistance, various types of giant magnetoresistance such as alternate layer, matrix model or hybrid systems. They have large change in the resistance when the magnetizing field is changed. Once you had the magnetic material which were solid, what will happen if you go to a condition where you take these magnetic particles and disperse them in a fluid, then you will start calling them as ferrofluids.

What are the typical properties of these fluids and how they are being used in our daily lives that was then discussed and we saw that they have large number of applications. Then came our discussion on applications. We started using the materials that were introduced in initial weeks, they were to be used for various applications to prove that they are actually functional materials. To prove that their functionalities they were used in sensors. For example, they can be used in electrochemical sensors or they were used in energy storage devices, large number of them.

And you would find examples like cerium oxide, iron oxide, cobalt oxide, chromium oxide, they have applications in all these fields. And now you will get an idea how to make just let us say copper oxide, how to modulate its shape and size, how to transform it from conducting to an insulator and then how to use this transformed material in various applications. So, right from beginning to the end everything is consistently following the logic. To understand all these materials in the last phase of the course, we also gave you brief introduction towards the characterization tools which are routinely used to investigate the properties of these materials before they can actually be used in devices. This will give you a feel that you have to have large number of characterization tools, understand the characteristics of a given material before even you can plan to make a device.

Once you make a device then again you will have to have the performance of the device is characterized thoroughly before it can go to the end user. Then we had also given you a very quick overview that there are additional topics which must be understood before a device is actually industrially viable, what would be its lifetime? What would be the cost? What would be the carbon footprint? And how will you dispose those devices once they have lived their life? So, these are additional questions which need to be answered before anything can go to the market. And we gave you an example of battery. You must have realized that the work on batteries are going on for more than 175 years. And even today there is massive research activities going on all around the globe to improve the battery performance.

So, this topic must have shown you that characterization of materials and devices are also very critical before you can use any material or device for end application. I hope you

enjoyed this 12 week course. If you have any queries you can write to us. in the forum or you can discuss them during the second live session which will be held before the examination. Thank you very much for attending the course on Physics of Functional Materials and Devices.

On behalf of my teaching assistants Ms. Puja De and Ms. Joyanti Halder, I wish you the very best of luck for all your endeavors.