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Module - 3 Optoelectronic Materials Device Physics Lecture - 25 Optical properties of materials

In the last lecture, we saw how light is absorbed by a material if we have a semiconducting material.

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This is a semiconductor. If we shine light on it with certain wavelength then, this light will be absorbed in the semiconductor throughout. This will create an electron hole pair. We also saw if we create electron hole pair by some other means in a semiconductor then, this electron hole pair may get annihilated and give light out. This is known as the emission from the semiconductor. This is due to annihilation of electron hole pair. But an optoelectronic device is more than just creation and absorption of light. We want to know how this light is going to be interacting with the rest of the material.

To explain this problem, let us think of our device. If you are just looking at the active region of the device only for the sake of simplicity, I do not want to draw the whole device. So, this is only the active region of an electronic device. If I am shining light from outside, this light will continue to go inside. But, some of it is going to also be

reflected. So, we do not only need to know what is happening here that is the absorption process.

We also want to know how much is going to be reflected back at the same time. Let us say, I am creating for an emitting device, light over here. This light is going to go in all the directions, some of what will be coming out. But, other may be lost in the device due to total internal reflection. That is why we need to understand the optical properties of materials because even though the device may be working well, it may not be giving any light outside. So, optical properties of materials are important for optoelectronic devices. That is a topic of today's discussion.

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So, today we are going to cover optical properties of material. What I mean by optical properties of materials is basically again whenever we say optics; we are normally concentrating on the visible light. But it does not mean that whatever we are going to do here is only good for the visible wavelength. This is equally good for infrared or UV region as long as if I look electromagnetic wave. Hence, you can always extend this discussion to other regions of the spectrum. When we talk about optical properties normally, what we are talking about is interaction of light with the matter the media or matter.

Now, what is light? Before we understand this interaction, let us understand what is light. Just like the material electronic structure when we talked about electron, we looked at as dual nature. In the same way, light also have dual nature. You can think of it as a wave as well as a particle. In today's discussion, we are going to be thinking of light as an electromagnetic wave. Hence, we must understand the theory of electromagnetic waves and basically Maxwell's equations.

So, our consideration here is going to consider light as electromagnetic wave interaction of the light with the materials. This electromagnetic wave with the material decides what is going to be the optical properties of the material. Now, when we talk about the optical properties of the material, normally we think in terms of transparency, opacity or reflectivity of the material. But these are basically phenomena which are based on intrinsic property of the material.

So, the optical parameters, the intrinsic optical parameters of a material are intrinsic parameters describing optical properties are; n, which is what we call refractive index. k, which what we call extinction coefficient. Remember, we have used this parameter k earlier for wave crystal movement of electron. That is why I have designed this particular k, which is extinction coefficient with slight tilt on the top, so that we distinguish between the two parameters.

Now, other properties which we normally confuse with the optical properties; other derivatives of this intrinsic properties are reflectance R, absorption and T transmission. Basically, a material has its optical properties defined by parameters n, n extinction coefficient. If I am looking at any light coming in, how much of it is reflected back is given by R, how much of it is transmitted is given by T. There is some amount which is getting absorbed in the material, which is given by A.

So, effectively if I am looking at these properties, R plus T plus A is always 1. These parameters R, T and A are actually dependent on the intrinsic property of the material, which is n and kappa. Now, how do we derive n and kappa? That is what we will do next. So, what is light? It is as i just explained light is nothing but an electronic EM wave.

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This solution can be obtained. It is a solution of the Maxwell's equation. In case of vacuum, Maxwell's equations are these, four set of equations that give the relationship between the electric field and the magnetic field in vacuum. The relationships are basically interrelationship of these two parameters. These four equations derive this interrelationship. In this parameter, epsilon naught is nothing but electrical permittivity of the vacuum. Mu naught is magnetic.

When we try to write these equations for a material, Maxwell's equations are going to be modified, when you are talking about for any matter or media. Now, matter or media is not vacant space. It has electrons. It has other phenomena going on, which are going to define its properties.

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Hence, those properties are going to change, modify the existing EM equations for matter and media. The additional parameters are given below. These are basically matter generally has some charge density per unit volume. It may also show some polarization behavior, which is basically the volume density polarization, is volume density of electric dipoles. M is magnetization, which is volume density of magnetic dipoles. We also have current density, which are current amperes per unit area. If we include these effects into the Maxwell's equation by including them in the Maxwell's equation, we are basically saying that polarization and magnetization is going to change the effective field inside the media. This is going to be used.

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Maxwell's equations in a medium will be: AXE = - HOSH - HOSH $\overline{\nabla x H} = \epsilon_0 \frac{\partial \overline{E}}{\partial t} + \frac{\partial P}{\partial t} + \overline{J}$ = - 1 7.P + Peo = -V.M Dielectric displacement D = E = 60E B = NH = Ho(H+M) Magnetic induction

This is going to change the Maxwell's equations into the following form; basically instead of H. We also have the magnetization included in here instead of simple electric field. We have polarization plus the current density included here. In case of the third Maxwell's equation, we also have the charge density included here. Now, these four equations can be further abbreviated. We use the abbreviation defining the properties of material, which is basically the dielectric displacement instead of electric field.

Dielectric displacement D is given by epsilon electric field. Epsilon is a dielectric constant of the material, which can be written as the electric field in the vacuum plus the polarization. We can also write as magnetic induction is given by the term H plus magnetization. By writing, using those abbreviations, we get further modified version of the Maxwell's equation which can be easily solved.

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The new set is fairly simple. The curl of the electric field is related to the magnetic induction. Curl of the magnetic field is related to the displacement vector plus a current density divergence of the displacement vector. It is basically defined by the density of the, charge density in the material. Divergence of the magnetic induction is going to be 0. Now, we are going to define these equations as 11, 12, 13 and 14. Now, these equations are basically defining all EM interaction with the material.

An additional relationship is also required, which relates the current density to the electric field. This is known as the conductivity of the material. In summary, what we have done is we are trying to define the interaction of light with matter. The three parameters that come out, which define this interaction is the electric permeability of the media, magnetic permeability of the media and the conductivity of the medium. Now, this is basically defining the properties of the material. We will see how that defines our optical properties.

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So, let us solve these equations for finding a solution. Let us look at the wave equation solution in an absorbing media. We will assume it to be isotropic for the present discussion. So, the properties in all directions are same in order to make this solution simple. We make following assumptions. Basically, density of charge is 0 as well as conductivity is 0. So, we are pretty much talking about a dielectric material here. There is no free charge in this. Material density is 0, free charge conductivity is 0.

We assume that the magnetic permittivity is mu naught, which is the same as magnetic which is the same as for vacuum. Hence, this is a non-magnetic medium. Now, this is not a bad assumption because at the optical frequency, most of the mediums are not magnetic; even the magnetic materials at a high frequency of a optical wave. The magnetic activity does not take place. Hence, normally this is true for most material. Those materials do not show magnetic properties at optical frequency.

So, normally true for optical frequencies. Now, from equation 11 to 12, 11 to 14, which were shown here from 11 to 14, we are going to try to solve for solution. We will take the curl of the first equation. This is going to be given by this expression. Further, write this, simplify this and write, take it the curl inside. Now, this can be by using equation 13, we can further simplify this part. This will become, this is obtained by using the relationship 13 and assuming epsilon independent of time. Now, we can try to simplify this expression. The double curl can be written.

Now, using the expression 14, we know that this is 0. That gives us an equation for wave, which is basically this equation. A solution for this equation will be our light in the media. So, a light in the media will be solution to this equation. If we take the terms for the vacuum, that would be the light, the equivalent wave equation for light in the vacuum. So, let us look at the solution and what are the characteristics of this solution.

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So, the wave equation is basically a wave equation. This wave has a velocity v, which is going to be given by 1 over square root of mu naught epsilon. So, this is a velocity of the light which is represented by the wave equation 15. So, light wave is basically a solution of equation 15. This is the velocity of light. Now, let us look for a possible solution for this equation. So, basically our light wave is a solution for equation 15. If we assume that the wave is moving in the positive direction, one possible solution is given by once again. We have another k vector here. I am representing this by this from k, which is wave vector for light wave.

So, in general, in this course, you would have seen that k is used many times. The first k you were introduced to was momentum for the electron. Then, crystal momentum; then, we used extinction coefficient, when I changed its shape because that is defining the property of the material. Now, we are using another k, which is basically defining the wave vector of the light. I have changed the symbol slightly so that you do not confuse between the crystal momentum and the wave vector of light.

So, this k is defining basically wave vector for light. In this, we have the solution for a wave, which is moving in positive r direction. Now, if I use equation 17 into 15, we will find a solution which will define our properties of the material in terms of light. By doing that, I will find this relationship; if I substitute 17 into 15, I will get k square.

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k square is now, dielectric constant of the material. It is defined by the relative dielectric constant also. These are the terminologies, which you must have seen elsewhere. So, dielectric constant of the material is also defined as epsilon r. It is basically epsilon over epsilon naught, where epsilon r is known as the relative dielectric constant. What we will find is that this epsilon r has also written as a complex number, given by epsilon prime plus i epsilon double prime.

Now, from the Maxwell's equations in vacuum, we will find that the light solution, the solutions for the light wave that we obtain will have a velocity c. This will be given by; this was seen earlier over here. I showed you that in the media, the velocity for light will be given by 1 over square root of magnetic permeability times the dielectric constant. If the media is not there then, basically the speed of light which is the vacuum speed of light that is a speed of light in vacuum is going to be given by the permeabilities of the vacuum for magnetic and electric field.

Now, applying for these new definitions to equation number 18, we are going to get k square is equal to omega square over c square epsilon prime plus i epsilon double prime.

We know that in this is in medium or in the material; we know that k square is equal to omega square over c square in vacuum. This is basically saying that our light as it goes from the vacuum to the medium, its speed is reduced by a factor square root of epsilon prime plus i epsilon double prime. This vector, this factor is known as n. So, normally we define that in a medium, factor N.

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This factor N is given by; we further know that this factor N is a complex number because it is a square root of a complex number. Some more parameters, material parameters are defined from here given by; this is all optical properties of the material. Remember, we talked about n, which is basically refractive index and kappa, which is the extinction coefficient. So, this has to be related to the relative dielectric property of the material by square root. Now, why is this n and i k? Let us see how N is represented by this, which gives us the optical properties of the material. You will do this derivation in the reverse direction in the sense; we will assume a light wave. We will show that the definition of the relative velocity gives you the optical property of the material.

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So, let us assume that light is, there is a material which has a refractive index n and absorption coefficient extinction coefficient k. Then, consider a plane wave, which is falling on this material in the z direction. Now, as this wave is propagating inside the medium then, what will happen to this wave? This wave is going to be modified because its k and omega vector are change. As we saw that k vector now is basically omega over c n plus i kappa. If we include this into our wave equation, we get e is going to be equal to the amplitude of the electric field.

Now, this equation wave equation is basically a damped wave equation. The magnitude of the electric field is reduced by this factor. This is damped damping factor for the electric field and speed is also changed by a factor n. So, the damped wave is propagating with a phase velocity of c by n. So, basically the c by n is a factor by which the velocity of the magnetic wave in the medium is reduced.

If you remember your high school science, you remember n is defined as c over v, which is the velocity in the vacuum divided by the velocity in the medium. So, from Maxwell's equation, we basically get optical properties of the material. They are defined, that is defined in the same way, that the velocity of light is reduced in the medium as oppose to in the vacuum. That is the refractive index of the material. Now, let us focus on this damping factor. If there was no absorption in the material then, the magnitude of the electric field would remain same in the material. So, if there is a electric field going in it has some magnitude e naught then, this magnitude is going to be dampened as it goes through the material. That is basically denoting the absorption of this electric field in the media. This absorption is being defined by this parameter kappa, which we called extension coefficient.

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So here, we have finally. To summarize so far what we have done is; we have shown that the optical properties of the material n and kappa are basically related to epsilon for the material and epsilon r for the material. It is given by epsilon prime plus epsilon double prime. So, both the n and k are related to the basic property of the medium, which is epsilon prime plus epsilon double prime.

Now, we would like to see how this n and k is related. n and k is going to be related to the actual observed properties of the light to get to the basic optical parameters of the parameter of the material. We basically measure reflectance, absorption and transmission. We do not directly measure n and k from the information from reflectance, absorption or transmission. We try to derive what are the basic optical properties of the material.

So, it is important to show the relationship between what we measure and what are the actual n and k. The difference basically lies in the fact that when we measure, we do not actually measure. We do not measure the magnitude of the electric field. We do not measure e. What we are measuring is the intensity of light. So, in any experiment, optical

experiment in which we are looking at how is light going reflected or transmitted or absorbed inside the material, we are actually measuring the intensity of light.

Now, how is the intensity of light related to the EM wave equation? Intensity of light is proportional to the e square. So, all the measurements that we do are actually done not on e, but on intensity. The detectors that we have the source, we have, we use the intensity in the terms of dual nature of light. This is basically number of particles per centimeter square per second number of photons that are emitted and this is what we are going to measure.

So, let us when we measure intensity, we are going to measure properties like R, T and A. I will first show the relationship between absorption and n and kappa. This is a term that we also used in the earlier lecture where I was talking about the absorption coefficient. If you remember, we talked about intensity of light. If i naught is a intensity of light falling on a material of this dimension x then, what I am going to measure is the intensity. Here, we will be at innovated by a factor alpha x. Alpha was defined as absorption coefficient.

This alpha was important to us because that is what defines how many electron and holes pairs are generated in the device. We use that alpha factor to calculate how many electron hole pairs will be e generated in a device. Now, what we want to do is we want to show how this absorption coefficient, which is measured on the intensity of light, is going to be related to the basic optical parameter of the material, which is n and kappa. Now, we are going to decide how n and k are going to be related to the properties that we measure in light experiments, which is basically absorption coefficient or the absorbance in the material.

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So, let us consider. In this derivation, we consider a slab. We consider a thin slab of material. In order to make the derivation simple, I am going to assume. So, this is my thin slab of the material, which has the dimension delta z. This has refractive index n and it is in a bulk of the material, which is also refractive index n. The reason I am assuming the bulk of the material and the thin slab to be both same refractive index because if the refractive index is different, you have some of the light being reflected back.

But if I assume it to be the same, which means I can easily ignore that there is no reflection, R is 0 here. Then, this will propagate. There will be some absorption here. Something will be transmitted. What I am interested in is trying to figure out how much, what will be this absorption in terms of n and kappa. So, from electromagnetic theory, we already know that, i is going to be propositional to magnitude of E square. From experiments, we know that the light intensity that we measure is related to absorption coefficient alpha.

It is important to realize that light as subject of interest has been there for a much much longer time than the Maxwell's equations. Hence, a lot of terminologies were developed before that the EM wave relationship was realize. That is the reason that we have to today find this correlation between the solution to the light as Maxwell's equation and the terminologies that exist in optics like absorption coefficient and reflectance etcetera. But it is interesting to note that both explain each other very well. Now, alpha is what we call absorption coefficient. So, since we can now try to see what this is going to be equal to, we know this i is related to E square. So, this is going to be 1 over E square, modulus of E square. I can take from my earlier equation, an expression for E in the media. So, modulus of E square is nothing but this from earlier equation, where we derived the E. This is the wave equation for light in media. If we include, if we do the complex conjugate multiplication here, we will get E naught square exponential.

Now, we can write what is alpha basically. This will say that del E square over del z is going to be equal. So, if I now look at what is alpha, alpha is basically this term divided by 1 over E square. Then, I am only left with 2. So, this is the relationship between absorption coefficient and extinction coefficient. Absorption coefficient is defined for the light intensity, which is used in the optics literature a lot. The extinction coefficient is defined to the permeability of the material property, which we have just shown is related to the permeability of the material for electric field and the magnetic field.

Hence, this shows the one to one relationship between optical parameters of the material as well as the dielectric parameters of the material. The relationship of a with n and kappa is simple. But, now you want to derive for reflectance and transmission.



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Let us first look at the derivation for reflectance. In the earlier discussion, we made the slab very thin inside the bulk material so that there was no discontinuity in the refractive index. Hence no reflectance, but if I have a discontinuity, I can almost assume that there

is going to be some reflectance except under certain special conditions. Hence, in order to derive the equation for reflectance, I must first do the condition or the assumptions used to deal with EM wave at the interfaces.

One important point to note about reflectance is just like in absorption, when the material property is basically deciding the absorption coefficient, reflectance is slightly different. Sometimes, it may not be the material property. Reflectance from a very sharp discontinuous material is a property of the material refractive index. I am assuming the refractive index of the air to be 1. n is equal to 1 and ambient is equal to 1. This is for the material. There will be some reflectance.

But it is not always the property of the material. This, you can think of a situation, where you have a very rough surface. This is known as a specular surface. This is known as a rough surface. Now, although this material might still be n, the reflectance is not a material property. It can be actually a surface property in some extent. So, we need to understand, the surface is to really understand reflectance. But we are interested in here to relate the optical properties.

As we observe with the material intrinsic material properties, we are going to consider this case, in which we have very sharp discontinuity. In this case now, the reflectance is going to be decided by refractive index of the material or optic or kappa of the material, not by the roughness of the surface. So, this is a case that we are going consider here. Now, what will be the boundary conditions when we take up such a case so, boundary conditions?

The first condition is going to be that the tangential component of the electric field and the magnetic field are going to be continuous. This is not very surprising. Why should these to be continuous? This is because intuitive way of deriving this condition is that you cannot have on a dielectric for which we have defined our wave equation that there is no current. There is no charge density. If these are not continuous, means that there is a current at the surface.

So, in the situation that there is no charge in the material, these two vectors have to be continuous across the boundary. Now, let us consider situation in which if when we said these things continues, what will happen? So, consider a very sharp discontinuity.

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Let us take the medium to have n 1 refractive index here, n 2 over here. Let us take a general case where the light is coming. We define the incidence angle from the normal theta. The incoming light wave has the wave vector k. We assume some wave vector k prime for the reflected light and at some angle theta prime. I am not defining this theta prime as equal to theta. You have already seen in your high school probably that the reflectance is at the same angle.

But we would like to derive that condition here, same thing about refracted light which is at the angle phi and wave vector k double prime. So, this is your reflected ray and this is your refracted ray. So, k a is for the incident reflected and refracted ray. We can further define that n parameter, which is basically n 2 over n 1. This may be useful in simplifying the expressions at a later stage. Now, if I write down the EM wave equation for incident reflected and refracted light, I am going to get, I can write it. Now, general expression the incident wave as having the magnitude E i, the reflected wave has having the magnitude some E prime.

I am also not assuming that the magnitude of the wave is going to remain same, given by k prime omega prime t. The transmitted wave is going to be E double prime. So, I have taken a very general case. I am assuming, I do not know anything about light. When the light wave comes, it has some wave vector, some magnitude and some frequency. As it gets reflected, it has a completely different magnitude, wave vector and a frequency as

well same thing for the refracted light.

Now, let us apply the boundary condition at this point to see what would be the some of the relationship between these parameters in all this. Let me specify r is taken relative to 0 and 0 point is the origin here. If I can write the electric field vector this way from help of the Maxwell's equation, we also know which means at the magnetic field vector of the light is going to be basically for the refracted magnetic field vector. It is going to be k prime and for the transmitted it is going to be k double prime.

If we look at this equation, we also see that the condition that is going to be satisfied here is going to be that that the two vectors, the wave vector and the magnitude are going to be perpendicular to each other. This is because for EM waves are transfer electric field and a magnetic field vector are at 90 degree to each other and that is at 90 degree to the wave vector.

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Hence, we can write the condition that the relationship between all 6 vectors is going to be such that k dot E is equal to going to be k prime dot E is going to be k double prime dot E double prime. These are with this relationship. Then, it basically says that Ei vector the tangential component the Er vector the tangential component of it and Et vector, E reflected, E transmitted vector the tangential component of it. Now, taking these tangential components at the boundary and using the boundary condition, we will get basically the Ei tangential component plus the Er tangential component should be equal

to the E transmitted tangential component.

So, what we are trying to say here is basically the E wave. This is let us assuming for the discussion that it is perpendicular to this. It is going in this direction. What we are saying is at this point the entire tangential component. If we add up for the incident and the reflected ray, that should be since it has to be continuous across the boundary, it should be equal to the 1 that is for the refracted ray. So, if we add up add up for the incident and the reflected one across the boundary that should be equal to the tangential component in the media n 2. That is this condition we have just written here.

Now, this equation must hold true for all values of r. As a simplification, if we take it for at r is equal to 0 then, we can forget about the k dot r terms. We will get basically E tangential for the incident term exponential i omega t. Now, this equation for this equation to hold true for all t's, it requires omega has to be equal to omega prime has to equal to omega double prime. Hence, although we did not assume in the beginning that the frequency is going to remain unchanged, it turns out that upon reflection from a sharp interface, the frequency of the reflected and refracted light is going to be same thing, we can do from this condition.

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For all rs, the equation is to be true for all r. It is also required that k dot r has to be equal to k prime dot r has to be equal to k double prime dot r. Now, this condition itself requires that all these vectors k, k prime and k double prime have to be coplanar. Now, from here, we get k r sign theta is going to be equal to k prime r sign theta 1 is going to be equal to k double prime r sign theta 2. No, sorry, sign phi. By definition we know that the k vector is nothing but n square omega square over c square.

We can also write that omega square over c square is equal to k square over n square. If we take that definition, we get the condition that across the interface; we will get relationship which is going to be true here. If we look at that from these two expressions, this basically means that k has to be k prime. Once again, we did not assume that before definition. But, it turns out that after solving it, this is going to be true only when k is equal to k prime.

Now, if we substitute that, this also gives us that theta is going to be equal to theta prime. We also get the equation that n 1 sin theta is going to be equal to n 2 sin phi. This is nothing. What is then what you have studied in high school? Snell's law that defines the reflection at a interface. So, what we have done in today's lecture to summarize.

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We have realized the importance of the optical properties in optoelectronic devices. We have derived the optical properties of the material from the EM wave, electromagnetic wave equations and its relationship with Maxwell's equations. Then finally, we showed a relationship between alpha and kappa are related E derived conditions of reflection using EM waves. So, this brings us to the end of this lecture.