**Semiconductor Device Modelling and Simulation**
**Prof. Vivek Dixit**
**Department of Electronics and Electrical Communication Engineering**
**Indian Institute of Technology, Kharagpur**

**Lecture - 38**
**Semiclassical Transport (Continued)**

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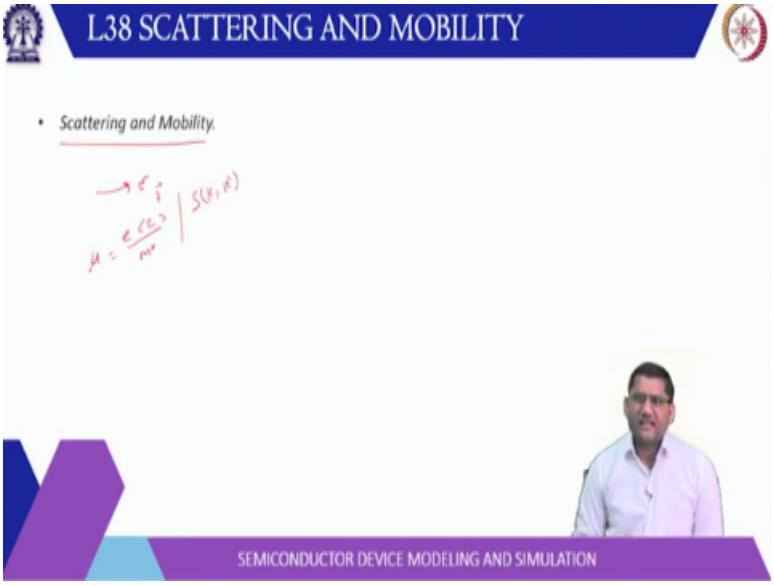


Hello, welcome to lecture number 38. Today we will discuss about the scattering, further discussion about the scattering and mobility. So, in previous class we have learned that due to scattering the distribution function actually changes. And if the electric field is in let us say Z direction, then distribution function also changes in Z direction so only k z component changes. And from that we can drive the expression for current energy density.

And we found out that we can define one parameter called mobility which is basically e then tau average divided by m. So, now we will discuss further about the mobility and there we assumed that S is the scattering between k to k prime. So, how do we calculate this scattering and how do we calculate these mobilities? So, that we will discuss in today's lecture.

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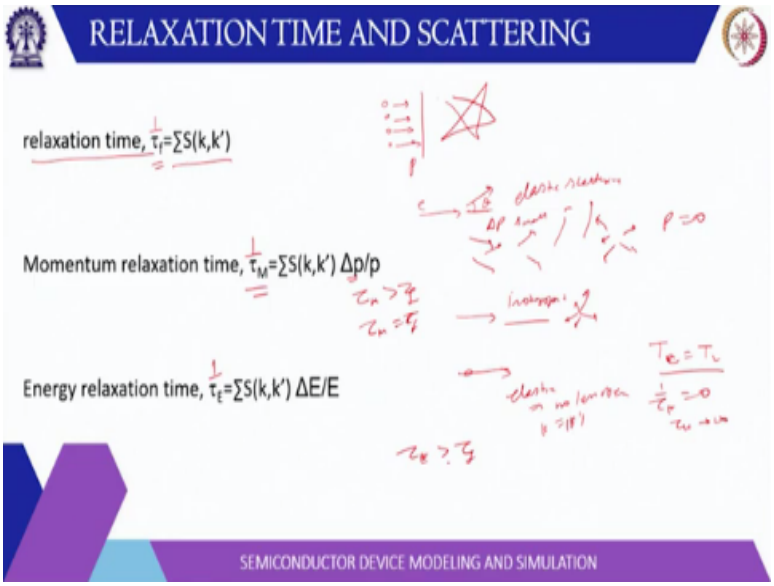


Now before we go further let us revisit this relaxation time. So, here tau f is the relaxation time which we defined that is sum over sum of S k, k prime. So, it is a sum of all the scattering rates from k to k prime. So, continue so the summation of this S will give you the summation all of the scattering rate and that will be 1 over tau. So, this relaxation time will give you the scattering rate. So, 1 over tau will be sum of all S k so it should be 1 over tau.

So, this relaxation rate can be understood like this. If you have some electrons and they are entering a piece of semiconductor with some initial momentum p then in this region they undergo some random reflection and so on. What will happen? They will lose their momentum; they will lose their energy but the timing may be different. So, this tau f is basically the mean time between collisions.

Then momentum relaxation time is again one over tau will be summation of all the scattering rate and for each scattering rate what is the change in momentum divided by p. So, if there is a process or if there is a scattering there is no change in momentum or very small change in momentum. So, for example that say this is coming here, this carrier is coming here and it is deflected by a small angle so that there is no change in energy.

So, you can consider some kind of elastic scattering. So, this is a change by small angle so in such scenario the delta p is very small. So, that means it will take lot of collisions to randomize

the momentum. So, the momentum relaxation time is the time taken to randomize the momentum. So, this momentum will take more time to randomize. So, that the momentum net momentum is zero so that time is tau M. So, that is called momentum relaxation time.

Now this tau M is more than this tau f because there are processes which have a small deflection. If there are some isotropic processes so isotropic is basically with equal probability of deflection in all the directions. So, for such scenario tau M will be same as tau f for isotropic scattering then there is a energy relaxation time. So, this is basically a time so the 1 over tau should be sigma S times delta E by E.

This is a time at which these electrons they lose their energy and T E becomes a T c carrier becomes latest temperature. Now if there are process which are elastic so in elastic scattering there is no loss of energy so k = k prime. So, for such processes the delta E will be 0 so for them tau E will be 1 over tau E will be 0 that means tau E will be infinite for elastic processes. For inelastic processes there will be some tau E so that means this tau E will be actually more than the tau f and tau M.

So, these are the different times that you may encounter in literature regarding the semiconductor. So, there is relaxation time, there is a moment of relaxation time, this energy relaxation time. So, in summary relaxation time is basically average time between two collisions, momentum relaxation time is the time taken by these carriers to randomize the momentum and energy relaxation time is a time taken by the carriers to get to the temperature of lattice. So, your carrier temperature become lattice temperature that time is energy relaxation time.

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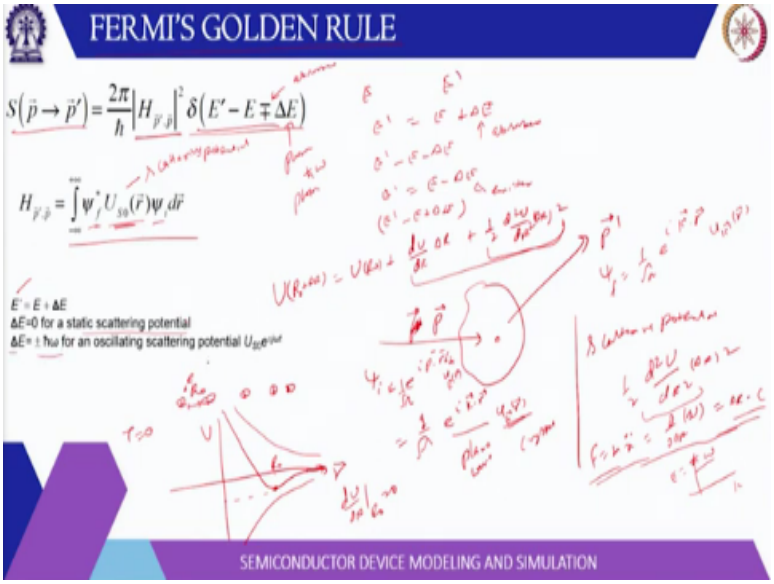


Now how do we calculate this scattering rate S? For that we have this formula Fermi's Golden rule. Now it states that scattering rate or a scattering probability from p to p prime where p is a momentum is 2 pi by H bar then this is H p, p prime square times delta E - E + - delta E. So, that means where E is the initial energy and E prime is the final energy. So, in the process some of the energy may be lost or some of the energy may be taken.

So, there should be some conservation of energy so that means E prime finally should be equal to initial energy plus some delta energy. So, that means if this is plus sign this energy is absorbed. So, the difference E prime - E - delta E so, this minus sign refers to the absorbed energy. And similarly, if E prime = E - delta E that means energy is imitate. So, that means E prime - E + delta E. So, this delta term basically tells you the in our about the energy conservation.

So, if there is a delta here it means some third particle will be there it could be phonon. So, phonon energy is H bar omega it could be a photon or any other particle. Now this H p, p prime is basically can be understood like this let us say this is your some scattering centre and initial particle is coming with certain momentum p and this is basically scattered with some momentum. This is let us say p this is scattered to p prime.

So, now this static scattering we cannot model using Newton's laws or we cannot model it classically. We have to consider the wave nature of the particle. So, in crystal these carriers they

can be expressed as a block waves. So, let us write the expression for the block wave. So, this is psi initial which is E to the power i p dot r by H bar times u as a function of position for vector k or it can also be written as then of course some normalization vector 1 over the volume.

Which can also written as 1 over volume times E to the power i dot k dot r times u k r. Now if you remember this solution for periodic wave inside the periodic potential so the travelling wave is modified by the periodic potential of the crystal. So, E to the power I dot k dot r is a plane wave equation for a plane wave and that is modifier the periodic potential with same periodicity as the crystal.

So, this is psi i there is the scattered particle f psi f will be again one over this normalized to volume times u 2 to power i dot k prime dot r times u k prime function of r. And then this H is defined as psi f star times psi i times u, u is the scattering potential. So, this is the scattering potential of the scattering centre. So, it could be four on impurity ionized impurity defect so on and this is the potential. So, this potential how does it arise? So, we can consider let us say phonon.

So, phonon is basically kind of vibration of these lattice atoms. So, at T = 0 they are fixed at their position and if you go back to some chemistry those things there are two types of potentials. One is due to the attraction others is due to the repulsion between the carrier. So, these carriers are attracted and these nucleus are repelled. So, this energy will be something like this. It will lower energy attraction force and then there is a energy something like this due to the repulsion which increases energy.

And the overall energy is basically something like this. This is the overall energy versus position r. Now there is a point of minimum energy that we call r 0. So, these are typical the distance between these two atoms, there is a minimum energy. Now this energy can be expressed as this potential u this will change if you change this position r. So, what is happening? At high temperature this lattice atoms are vibrating.

So, this u potential as a function of r, so let us say there is some change. This is r 0 + delta r small change is there. We can write it as u of r 0 + d by dr of u times delta r + half d 2 u by dr square times delta r square and so on. Now if this r is small so then this change in potential can be written as in terms of this higher order terms. Now you notice this is the minima so the del u by del r at r 0 is zero. So, the potential that is changing will be due to this term.

So, the scattering potential potentially half d 2 u by dr square times delta r square so that will be the scattering potential. Now in terms of discovering potential we can write the force on these atoms. So, force is equal to L times the position double derivative will be equal to the force and force is derivative of this energy. So, that will be d by d delta r of u or delta u you can say and that will be delta r times this term which we can write as a constant.

So, this will be basically this equation will give you the phonon characteristic. This elastic wave will have certain energy and by solving this equation you can get their phonon characteristic. So, you can get E k diagram very similar to we got for the carriers. And if you have E k diagram so E is here h bar omega so this energy of this phonons. This phonon interacts with these carriers to scatter them.

So, now is the final energy E prime which is equal to E + delta E. Now this delta E is zero for static scattering potential and delta E is + - x bar omega or scattering due to phonons because phonon will not have energy x bar omega. So, this will have plus sign if we are absorbing a phonon and it will have minus sign if we are releasing a phonon.

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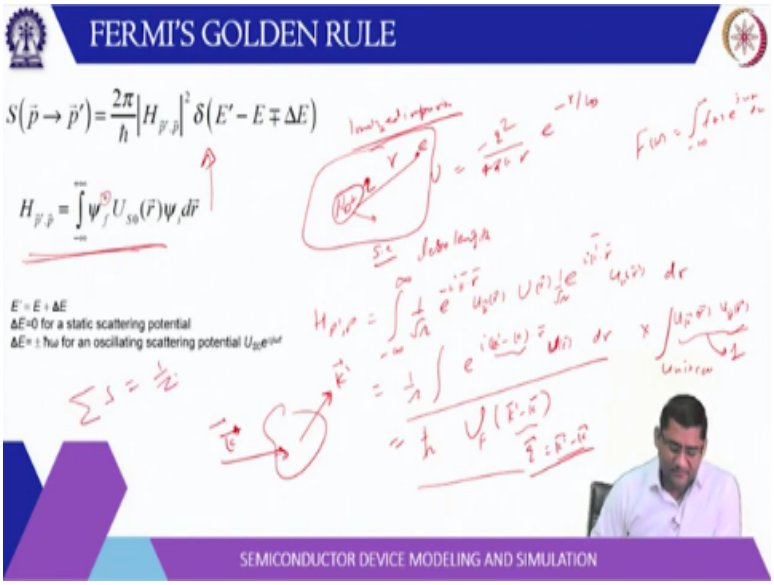


Then let us say we consider one scenario where let us say some let us say we consider ionized impurity. Ionized impurity will have a steady potential so let us say there is a some donor atom here N D plus, this charge is there. So, this charge will give let us say this is a charge some charge is q here. So, this will give out some potential that will be interacting with the moving carrier.

So, the corresponding energy will be U will be - q times q so that will be - q square divided by four pi epsilon r, r is a distance. So, this is the distance between the electron and this site. Now what will happen this because this is inside a semiconductor so this will get screened and we have discussed the device length well it is divided. So, it will get screened by the device length and then we can say it is e to the power - r by L D.

So, because the; field is getting actually reduced due to this screening. In metal the screening is such that the field does not extend. But in case of semiconductor the field extend to certain length then it gradually dies down and that is due to the device length because this carrier respond but they donate a much carrier like metals so field does exist. Now due to this scattering if we integrate it to get this H factor so let us integrate this H here.

So, H p prime p is integral - integral to infinity. Now psi we have already discussed is the block wave. So, this is one over volume times e to the power i tap k dot r times u k r times scatting

field. So, that we can write it as let us say some u as a function of position times 1 over volume at a k prime dot r u k prime r then we integrate it over dr for this position. So, this will be one over this then e to the power iota.

Now this is the first one is the star so there is a complex conjugate so this will come – i iota k r. So, you will have E to the power i tap k prime - k dot r then U potential dr and we can take this thing outside u k r, u k r k prime r. Now this is basically the product of this periodic potentials so this we can say it is one. So, your H p prime p can be written as because this is integral over the unit cell because this is a periodicity of the unit cell.

So, we can say this is 1 over sigma. Now if you look at this expression carefully it is basically the expression of Fourier transform. So, this is let us say we call it u f, u f is a Fourier transform of U and the vector here will be the frequency because if you recall that four a transform f omega = f x e to the power J omega X t x - infinity. So, this is basically F of k prime - k and that we call it vector q, q is k prime - k which is basically related to the momentum.

So, the difference of the momentum of the incident vector and the scattered vector so this from k prime to k. And since the momentum has to be conserved so some particle will be involved. So, let us say there is a phonon or some particle is there so that will take care of this momentum concerned energy also. So, this k prime - k will be the wave vector of that phonon. So, this is basically the some example is given to calculate this H prime.

Then once you have this S prime then we can get from this the S scattering rate. Now this S scattering rate is from for one particular set of combination k to k prime. Now when we sum it over for all the k primes so that sigma S that will give you scattering overall scattering rate. So, here we will consider some cases where the scattering rate is given for some situations.

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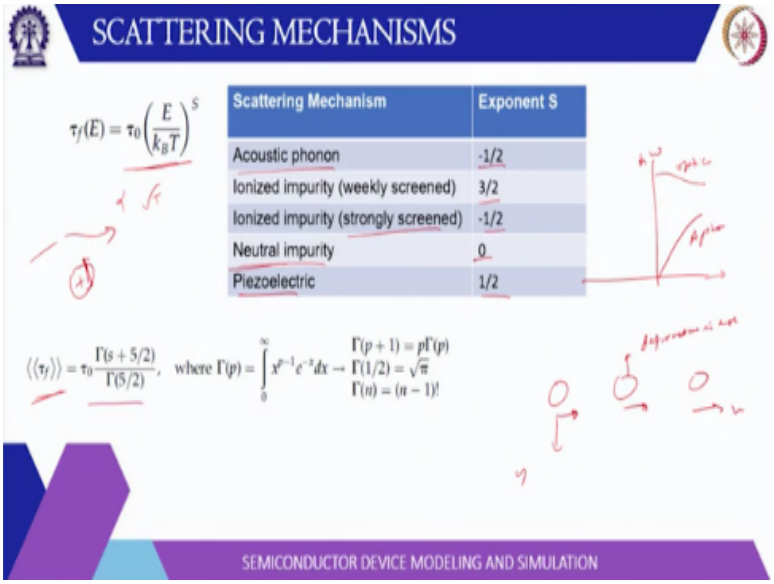


Now for acoustic phonon, there are two types of phonon, one is acoustic phonon one is the optical phonon. So, in acoustic phonon what happens? These atoms they oscillate in the same phase so the distance is not altered. Optical phonon are basically where they oscillate in opposite phase so there is one is going down other is going up. So, let us say this is x axis this is y axis so this will be optical phonon.

So, in this case the deformation is high in case of optical phonon deformation is high. So, generally they have high energy and then if you have this E k diagram so for this will be acoustic phonon and then this will be optical phonon, this energy H bar omega. So, for the acoustic phonon this scattering mechanism the tau is proportional to energy by k T power S where S is minus up. So, that means tau is proportional to square root of T.

Then in case of iodized impurity this is T to the power - 3 by 2 and if it is strongly screened that means there are lot of carriers then this power is minus up. And in case of neutral impurity, it does not have a charge so the mechanism is physical basically. In case of charge impurity that the scattering can be at a distance also because this electric field extend there. But in case of neutral impurity there is no electric field so the cross section of that scattering will be less here.

This is basically or not dependent on temperature. Then piezoelectric is scattering again it has exponent 1 by 2 and if you substitute this expression for tau in the previously derived equation

that we derived for we solved for the distribution function then we will get this some gamma functions there and these scattering rates are actually calculated using this average tau.

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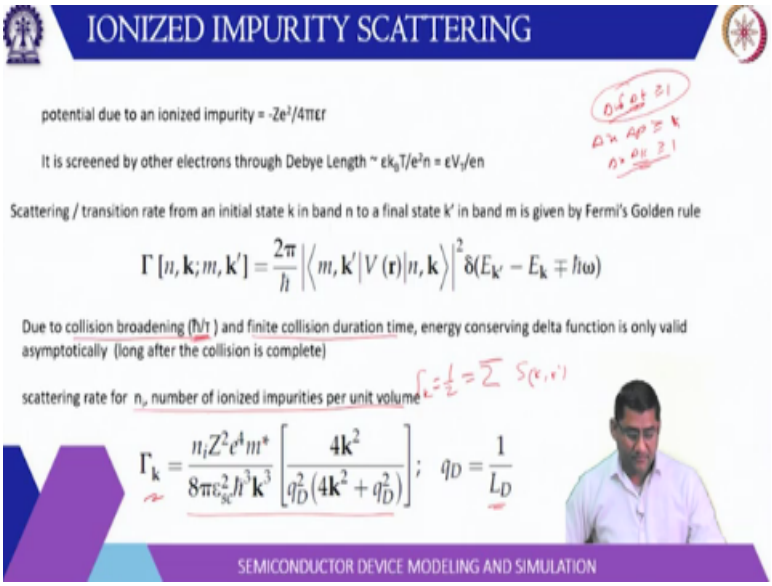


Now in case of ionized impurity scattering the potential due to ionized impurity let us say Z e is the charge on the ionized impurity. So, the potential is Z e square by 4 epsilon r and if it is the screen by some length so this is the device length epsilon k T by E square n. So, this was e to the power - r by L D which is Debye length and then corresponding scattering rate can be obtained from the Fermi's Golden rule.

And then of course if we sum it over that means we integrate it over that sigma S k, k prime then we will get the scattering rate 1 over tau which is given by gamma for k. So, this is the expression from the textbook. Now here two things are to be considered one is there is a collision broadening. So, collision broadening is it takes some finite amount of time for the collision to take place and that we call finite collision duration.

And this when it extends over a time so this due to this time and we can recall this rule that uncertainty principle that delta x and delta p they are related means delta x and delta p, position and momentum cannot be simultaneously determined with absolute accuracy. So, this is usually more than equal to some constant some h bar something or you can say delta x and delta k is greater than equal to one.

So, that means if the scattering is taking place so this delta k will take place over certain time or delta omega times delta t will be greater than equal to one, delta f h r omega delta omega delta t will be so these two are the Heisenberg uncertainty principle. So, if there is a change in there is a scattering event. So, if it is over zero time then the energy cannot be determined to the greater accuracy and because there is some finite energy change there has to be some duration of the collision.

So, this is usually given by the collision broadening is given by h bar by tau. So, tau and omega are inversely proposal. So, if there is a collision duration tau then energy will have this h bar by tau variation. Now when we calculate the scattering rate for ionized impurity let us say n i is the number of ionized impurity per volume we get this expression where L D is basically Debye length and others have their respective meaning.

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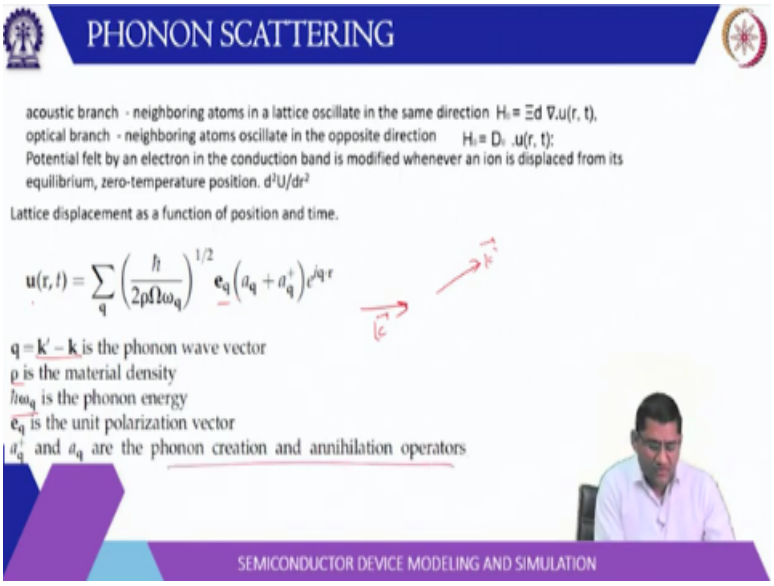


Now in case of phonon scattering as we already discussed there are two possibilities. One is acoustic phonon, there is optical phonon. So, in case of optical phonon the h factor that is a energy is basically the potential is given by the some deflection potential times the position because these atoms are oscillating in the same phase. But in case of a acoustic branch the unit cell is actually changing. So, this is basically related to the del U the gradient of this position vector.

This position vector is basically the position of this lattice atoms. So, there is a deflection potential d, d times del U. So, that will give you the H for the acoustic branch and this we have already discussed that the potential felt by electron in the conduction band due to this iron displacement from the equilibrium that is del U by del r square because d U by dr is 0 at that point. So, this energy has to be d 2 U by dr square.

Now the lattice displacement as a function of position and time can be solved for the phonon. So, k prime - k is a phonon wave vector so where k is the wave vector of the incident particle, k prime is the wave vector of the scattered particle. And here roh is the material density and h bar omega is the phonon energy so where omega of q is the wave vector. So, omega q is the corresponding frequency for the wave vector q and e is the unit vector.

These are the phonon creation Annihilation operators. So, from this U we can calculate the H and the scattering rates.

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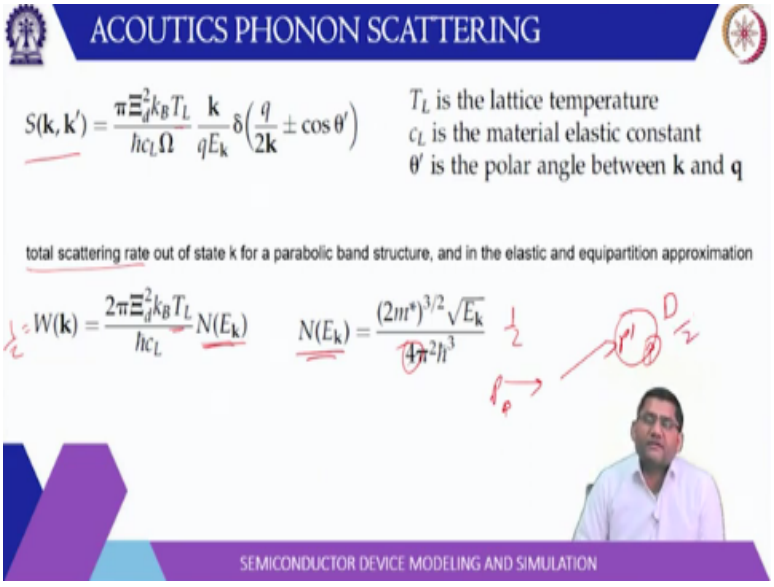


So, scattering rate the important point that we should pay attention here is that this is proportional to the lattice temperature. The scattering rate divided by 1 by E k so E k is energy and then total scattering rate will be 1 over tau. So, if you see here this is proportional to T times

the density of states. You can see one more thing here because we are scattering these phonons from a P to P prime.

So, for it to be scattered to P prime the density of a state here plays are all so it is proportional to the density of a state. So, this n E k is the density of a state for this k vector so that is 2m 3 by 2 power 4 pi square x square q times E k and there is a factor of 2 is there half. Because this P will scatter let us say this electron has spin up so this P prime will also have a spin up. So, if you consider the density of a state with a spin up then it will be D by 2 actually.

So, that is why this extra one by two factor is there because normally E k is 1 by 2 pi square h bar q.

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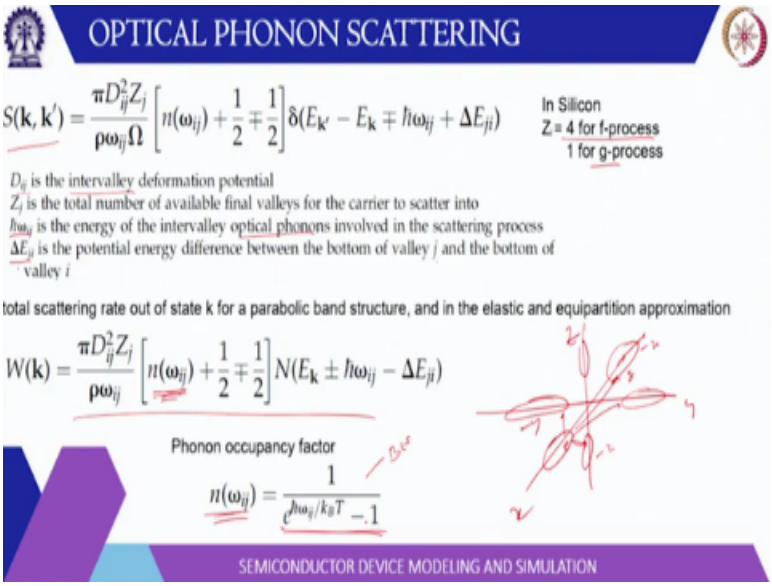


And similarly for optical phonon scattering here we have different intervalley deformation potential. Let us say D ij and Z j is the total number of available final values. So, for example let us consider silicon here. So, if you remember silicon let us say this is x axis this is y axis this is z axis and the values in case of silicon, they are along this at the x there are x values. So, this is basically your x here so in the x direction, there is a y direction and there is a valley in z direction.

So, the electron here can scatter to any value here. So, there are two possibilities one it is scattered from x to - x so that is called g process this cation is called g process. And there is one possibility because there only one such value here. But if it is scattered perpendicular then there are four possibilities + z, - z, + y, - y so this is called f process. So, this is basically D ij is the intervalley deformation potential.

Then Z is a number of variable available, final values for s carrier to s scatter into and of course h bar omega is the energy of optical phonon involved in the scattering process and delta E j is the energy potential energy difference between the bottom of valley j and bottom of i. So, let us say this is value j this is value i. So, what is the difference between their energies so that is delta E j. And then of course if you sum over all the S k for S k, k prime.

Then you get this expression where n is basically the phonon occupancy factor because this scattering is affected by the phonon it is due to the phonon. So, the if higher is the phonon consultation greater is the scattering so at the high temperature there will be more scattering basically. So, this is n and this if you see the phonon occupancy factor, they have different statistic not the Fermi Dirac statistics but this is called Bose Einstein statistic.

So, they use this kind of statistic. This you do not have to remember but understand that how this different scattering phenomena work out.

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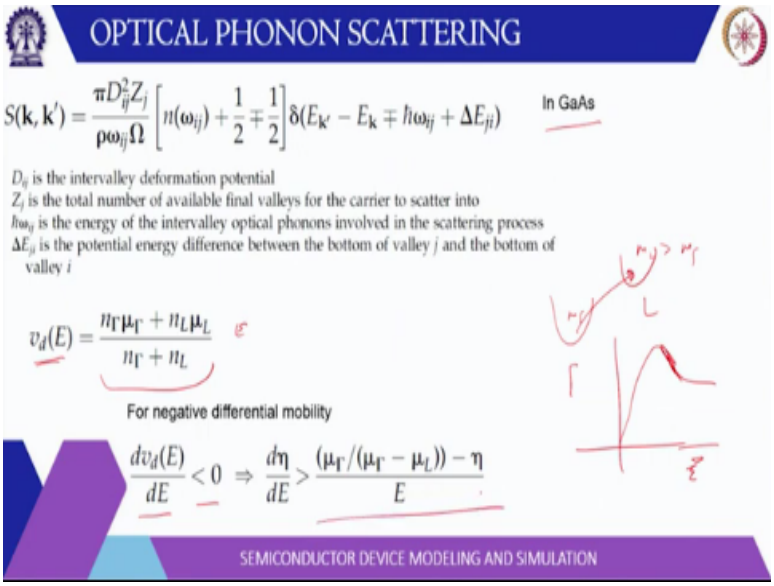


Then of course in case of gallium arsenate there are valleys here. There is a gamma valley, there is a L valley and then there is a scattering here from gamma valley to L valley. And if you recall that the mass is actually more here let us, say m L is more than m gamma this is m gamma. So, that is when these electron go to higher energy state their mobility actually reduces. So, we have this negative differential resistance region with the electric field or the applied voltage.

So, that is dragged here. So, the drift velocity is mu times E and the mu is basically the average of two values gamma valley and L valley. And if you take the derivative dv by dE it should be negative and then we can get the condition for negative differential mobility and that comes out to around that mobility in L should be less than mobility in gamma.

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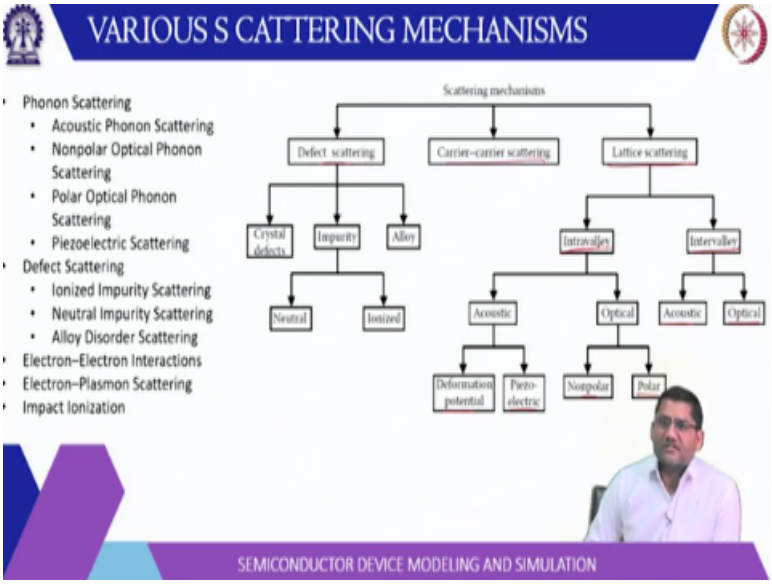


So, here is a summary of different scattering processes. So, there is a lattice scattering then of course within the same valley or they can be across the valley inter valley and intra valley. And then for both there are optical phonon and acoustic phonons and for intra valley there may be some polarity thing may be there. So, there are non-polar and polar and there is a different potential and the piezoelectric scattering are there.

And of course, there can be due to defect scattering so there can be neutral defect and ionized effect. And then there can be carrier-carrier scattering also because at a given position if you have lot of carriers this carrier will also scatter away.

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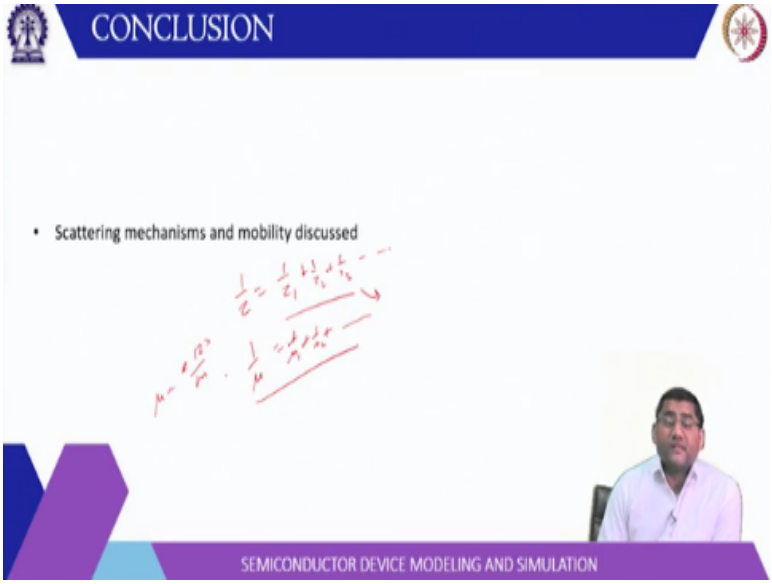


So, we have discussed different scattering mechanism and we have discussed the concept mobility that is arising from this scatting mechanism. So, in summary all this scattering moment mechanism combined together and all the S scattering rate actually combine. So, 1 over tau will be 1 over tau 1 + 1 over tau 2 + 1 over tau 3 and so on and this we can do only if these have same energy dependence.

And if energy dependence is different then of course we have to be little careful and similar applies to mobility because mobility is E average of tau by m. So, this will be one over mu 1 + 1 over mu 2. So, in previous class we discussed this scattering that relaxation time approximation and then in this lecture we discuss different scattering mechanism leading to the different characteristic due to different mechanism and their different temperature dependence. Thank you very much.