Micro and Nanoscale Energy Transport Dr. Arvind Pattamatta Department of Mechanical Engineering Indian Institute of Technology, Madras

Lecture - 05 Energy Carriers at Micro/Nanoscale and their attributes

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Very good morning, yesterday we were looking in to some of the derivation related to the macro scale heat transfer, close system conduction and also the convective heat transfer transport equations and then we also looked into the constitutive relationships, which are required to close the relation between the heat flux and the temperature. So, we have ones again revised or revisited these constitutive relations in conduction - convection and radiation. I think most of you are quite familiar with them and as I told you that for example, the Fourier's law whatever that is stated as a constitutive relationship as a hypothesis originally by Fourier can be actually shown to derive from the micro scale principles. Now you will also continue with some more constitutive relations.

For example in fluid mechanics, the most commonly used constitutive relation is your Newton's law of viscosity. So, this is also called the Newton's shear stress law. So, what it says that is for a Newtonian fluid, you can relate your shear stress, may be it could be tau x x, tau x y. So, it is a shear stress that stress is a tensor. So, in 2D you have basically 4 quantities of stress, in 3D it is 9 elements. So, any way you can relate for example,

shear stress in the corresponding strain rate right, that is your d u by d y through constant of proportionality which is your dynamic viscosity. So, this is valid for so called Newtonian fluids which follow this particular behavior.

This is another example of a constitutive relationship which is required to solve the Navier-Stokes equation because ones again when we right down the momentum equations we have a everything in terms of stresses and in order to solve them we need this closure problem. So, closure problem for closing, we need this particular constitutive relationship given by the Newton's share stress law. So, this is again another one. So, what is the unit of the dynamic viscosity here? In terms of SI unit kg per meters second in terms of Newton's how do you write it? Newton's second per meter square. So, this is your relationship that you are very familiar with in fluid mechanics. In mass transfer, we are not probably expose too much of mass transfer in our department, but in chemical engineering there very often concerned with mass transfer as important as heat transfer. So, in a case of mass transfer what does the constitute relationship? Fick's law of diffusion, so therefore, you see that this is not a problem only that we have in heat transfer.

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So, every domain has a closure problem and a corresponding constitutive relationship required to close this, so the Fick's law of diffusion. Now we can draw an analogy from your heat transfer and state un equivalent law of diffusion constitutive relationship between the mass flux and what is the corresponding variable instead of temperature concentration.

So, we will have mass flux let us denote this has J double prime, distinguish this from heat flux q double prime; corresponding concentration gradient or species gradient, so this is d m by d x. So, instead of temperature gradient you are replacing this with your concentration or mass fraction gradient and then you have to use the corresponding diffusivities, in case of the Fourier's law you use the thermal conductivity and now you should use the diffusivity, mass diffusivity multiplied by rho so that it is dimensionally consistent with your. So, here your d is in terms of meter square per second. So, this is your diffusivity, mass diffusivity. This is equivalent to your thermal diffusivity alpha that also has the units of meter square per second.

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So, this is your Fick's laws of diffusion and also very important closure required for the mass transport problems. We will also take one example in electric engineering, so that is your Ohm's law. So, how do we state the write the Ohm's law? You can draw analogy between from heat transfer, mass transfer and apply the same thing for Ohm's law. So, now, instead of q or j what and we have? Current density, so let us use the notation again J c for current density or current density flux, double prime, and what is the equivalent quantity to which it is related? Let us say like temperature, mass fraction.

Student: Voltage.

Voltage, can we put it more fundamentally, electrostatic potential difference. So, we have a gradient of electrostatic potential. So, we will say d phi by d x and you have to again put a minus sign because the current flows from a higher potential to lower potential. So, the gradient will be negative, so in order to make sure the current flow is positive from higher to lower it should be a minus sign and the relationship between these two with the proportionality what is the proportionality constant here. So, in a case of heat transfer used thermal conductivity now, we should use electrical conductivity.

So, sometimes we use the notation sigma for electrical conductivity. Resistivity is one over this so, but we will use in terms of conductivity. So, see you in the way that we have you know defined all this constitutive relations they are look analogues, right. So, some flux quantity as a function of some gradient of the fundamental driving potential, in the case of fluid transport it is the velocity gradient, in terms of current it is the electro static potential gradient in terms of heat transfer temperature gradient, mass transfer you have the concentration gradient. So, this is how they are all related and ones again the units of the current density is an ampere per meter square it is like a flux quantity, thermal conductivity is in ohm inverse, meter inverse. So, this is in terms of, see this is your electrostatic potential.

So, therefore, we have looked at some of the classical constitute of relations generally applied for the macro scale transport equations require to solve close the governing equations and solve them. Now we also saw the similarities or analogies between these different constitutive relations and the next question that comes out are these equations applicable at even small scales. So, generally people tend to use state these equations without stating that that is I mean continue ohm approximation and were the validity of these constitutive relations are held, but you a should understand that ones you go to nano scales as we saw defined by the Knudsen number, high Knudsen numbers you cannot ones again use this constitutive relations as it is. In fact, when we do this derivation from the micro scale or nano scale limits we get these equations at the condition that your Knudsen number is small, that is the limiting condition under which we can derive these constitutive relations from the Boltzmann transport equation.

So, now the next thing I want I think all of you to understand is to do a simple scaling.

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I would call this as a scaling analysis or scaling trend or whatever you want to call it, to understand the importance of the ratio of the relative surface to volume forces. So, now, if you take the case of a sphere, so you have a sphere of radius r and if you want to calculate the ratio of volume to the surface area of this sphere, what will be this particular ratio?

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4 by 3 pi r cube, 4 pi r square, r by 3. So, therefore, as your r keeps reducing a corresponding volume to the surface will also keep dropping or in other words your forces now if you look in terms of forces. Now, let us take an example of a surface force a volumetric force and calculate the ratio of those two. So, for example, if you take the volumetric force, gravities classical example of a volumetric force which acts on the entire body, let us take the ratio of gravitational force and what is the good example of a surface force.

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So, assume this we had some kind of a drop or a bubble and outside you have ambience. So, let us say this is your bubble and you have a liquid ambient. So, naturally there are two phases here and therefore, that will be a surface tension which will be balancing the pressure difference across that interface. So, therefore, we can now write, surface force, surface tension force here. So, how do you calculate the gravitational force? You have rho times, gravitational exhilaration times the volume of this sphere. So, you have 4 by 3 pi r cube divided by what about the surface tension force? The surface tension is acting along this perimeter whatever you are looking at. So, the surface tension is defined in terms of Newton per meter. So, you are just looking at the surface area. So, here when you are talking about, you can associate 2 pi r because the unit of sigma is what? Newton per meter not Newton per meter square, so it is associated with just the perimeter, circumference.

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So, therefore, the ratio of this will lead to 2 rho g r square by 3 sigma right. So, now, you can I will give you two values one take the case of radius r equal to 1 meter. So, let us say that this is a big bubble and in ambient liquid, I will give you the property let us say rho is 10 power 3 kg per meter cube and sigma is 78 into 10 power minus 3 Newton per meter. So, you do this for two values of radiant - one is r equal to one meter calculate this ratio. So, let us say that this ratio is sum gamma. So, calculate this ratio gamma for r equal to 1 meter and then reduce the size to 1 millimeter, from 1 meter you reduces the size to 1 millimeter calculate the value of gamma. So, what will be the result for one meter drop bubble?

Student: (Refer Time: 15:55).

So, let us say 8.4 approximately into 10 power 4 right and what about 1 millimeter? So, that is 8.4 into 10 power minus 2. So, therefore, reducing the size of the drop from 1 meter to 1 millimeter, so that is three orders of magnitude we have brought down. The volumetric force, the ratio of the order of magnitude of volumetric force to the surface force has come down by what? Six orders of magnitude, therefore, if we are looking at bubble of one meters they are definitely gravities very very important compared to this surface tension force and therefore, not only for the bubble drop problem. So, if you take two phase flows in also mini channels, micro channels and then you look at the flow pattern in a big channel you will find that it in the big channel gravity is playing a very important role in the flow patterns.

Now, then you go to channel of a millimeter size, gravity is relatively unimportant compared to surface tension and you will find flow patterns are dominated by surface tension force. So, this is a very good example now where you have to know what are the importance of, relative importance of forces. Sometimes when we right down the Naviers-Stoke equation we tend to neglect certain forces without knowing this scaling trend. So, this is a good example to show you that you know that certain forces become suddenly very important at you know different length scales.

So, what we will now do? So, for we have looked at continuum till now, we will go into the little bit into the micro scale nature of the energy carriers responsible for the macro scale transport. So, very briefly I will call this as microscopic picture of energy carriers.

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So, why we are doing this because first we looked at continue ohm and then we looked at transport of heat, we looked at transport of mass and then we also looked at say transport of current and so on. Now what is responsible for this transport? So, that can be understood only into an assuming in to the molecular picture, microscopic picture.

So, if you take for example, heat conduction. So, we talked about, we derived the governing equation for heat conduction and also the closure using the Fourier's constitutive law. But what is happening essentially at the micro scale is that. So, if you take a system or a slab where only conduction is happening or it is a box which consists of gas where only conduction is assumed to happen. You have a high temperature T hot on one end and you have T cold on the other end, and this is filled with gas molecules - plenty of them, this is at still macro scale where continuum approximations are valid.

So, when you are talk about heat conduction here what is essentially happening? The average kinetic energy of the molecules on the hot side is increasing, when you heat the gas on the left side and therefore, the collision average collusions are also increasing on the left hand side and gradually these collusions are transferring the energy from hot side to the cold side. So, this is what is happening at the micro scale and you look at the micro scale picture it looks a little bit more straight forward, but when we write the equation in the macro scale we assume that there is a diffusion right. So, this collective collision and transfer of energy is approximated as a diffusion process and we relate your heat flux and

heat transfer rate to the gradient and temperature and so on. So, this is how we bring out so many approximations, but at the micro scale it is essentially simply collision and transfer of energy from one molecule to the other.

So, now if you are talking about therefore, different medium, different media you have different energy carriers, if you are talking about liquids and gases, so you are talking about essentially molecules which are responsible for this conduction process. So, if you are talking about dielectric solids or semi conductors, which you can assume as insulators or semiconductor. So, most of the crystals fall under this category, in this case the lattice vibrations are responsible for heat conduction because you do not have any media like gas or liquid filling. So, what is responsible for heat conductors or dielectrics. So, only the lattice vibration should be responsible for heat transport and you should understand that these lattice vibrations travel at the speed of sound in the lattice that is the maximum speed at which they travel. So, this can be described with representing them as particles called phonons.

So, as the name suggest you are talking about sound - phone from the Greek root; that means, it something to do with the acoustic speed of propagation of these lattice waves which are responsible for the heat conduction and the corresponding particles which travel at this speed, so they are called photons. So, these are virtual particles; that means, they are mass less and you cannot really dig into a crystal structure and look for phonon somewhere, they are just our imagination. So, really there is only a lattice vibration, but we are associate them with this kind of phonon just like photons if you put a micro scope and try to zoom in you do not find particles in light, they are just a way of understanding because they behaves, seem to behave and nobody knows how this particles look like, what is the mass of this, they are called virtual particles. Whereas electros are physically observed right, you can naturally observe in atomic electrons so they are real particles.

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So, therefore, if you look at the lattice structure, how do you see the lattice structures? So, you have these atoms in a particular solid, you know I have represented these lattice structure by means of these atoms spaced - why am doing this way that these atoms cannot come to close and then just simply sit on top of each other. So, there is certain force acting between these two atoms which is holding this particular crystal structure, you have different structures - FCC structures, BCC structures. So, why this is coming is at particular inter atomic potential is basically resulting in the appearances of the lattice structure. So, if you are therefore, looking at the picture of a semi conductor, so you have these atoms and you also have what somewhere free electronics.

So, somewhere from these atoms some electron as been knocked out the chances are of finding more free electrons and semi conductor are very minimal. So, you will find may be somewhere one or two free electronics floating around. So, they are also responsible for conduction of heat. If you look at metals, in the case of metals what happens? You have abundance of conductional band electron. So, they are all free electrons and they are primarily responsible for heat transport. So, therefore, in case of metals, it is basically the electrons which are responsible for heat conduction. So, if you therefore, measure the thermal conductivity of semiconductor device, semiconductor element and metallic element you will find the huge difference is because of the contribution of electrons in metal and phonons in semi conducted device.

So, therefore, depending on the media you have different energy carriers, right. If you are talking about the thermal radiation we talked about conduction now. So, if you go towards thermal radiation. So, thermal radiation on the other hand is a result of the excitation of the electromagnetic waves right, this is the oscillation of these electromagnetic waves particularly in the band width which is radiated by the sun - which is starting from all the way from UV, visible, infrared and long wave length infrared, so all this together falls under the thermal radiation band.

So, our visible spectrum is very limited you have 0.4 to 0.7 micro meter band, 400 to 700 nano meters this is visible band and that is also the band over which you know the intensity of the black body intensity of the sun, if you say temperature around 5000 Kelvin that is where it peaks and that is where our eyes are also tune to observe in the visible wave length. So, that is where the suns intensity is also peaking. So, the nature has defined devised in such a way that our eyes can tune into seeing objects because sun is emitting maximum intensity in that particular wave length band. So, where as to looking to the UV or IR needs special devises and what are the energy carriers associated now these are again waves. So, therefore, to describe the equivalent particles, virtual particles we use photons.

So, this I have got very interesting history you know I am not going to go over them. So, over a period of time they have evolved different models understanding first as particles then correction to waves and then finally, Einstein comes and says no they are both waves and particles. So, and then that all the electro may not only the electromagnetic waves, but any wave we are talking about electrons, we are talking about phonons, so any wave that is what we will see in quantum mechanics. So, we can always there fundamentally you know quantum level they are all waves and at a larger picture you can use the wave particle duality, use the particle base because classical mechanics can be apply to particles, Newtonian mechanics so that is easier to solve for us. Whereas, see waves requires solving Schrodinger's equation which is computationally very intensive and sometimes unnecessary also, therefore, you have different energy carriers considering the different media.

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Now anyone looking at this lattice structure and the force potential between the different atoms you can actually plot the interaction potential between two atoms. So, you have two atoms, you can actually imagine these two atoms to be separated by means of spring. This is a very simple picture that people usually represent. So, the atoms are usually approximated as a spring mass system, the interaction potential, if they come too close together this spring is going to push them out - they have too far away this spring is going to get compressed. So, this potential is usually used when people do what is called molecular dynamics, they are looking at fundamentally only molecules and there are solving for the forces of interaction in between these molecules.

So, this is the most basic potential that is used, so what happens? So, let us say the potential on the positive y axis is positive potential, negative y axis is negative potential. The positive potential means it is attractive, negative means it is repulsive. So, we can actually for the sake of convenience you will reverse this. So, we will put the negative on the top and then positive in the bottom. So, the repulsion will be plotted on the positive part of the y axis. So, when you are plotting this as a function of the spacing between the atoms.

When the spacing is extremely small you have a very strong repulsion the repulsive potential is negative and I am plotting this like this. Now as the separation between the two atoms increases you know you will find the somewhere they are stable and just standing there and as you keep increasing this, what happens? You have an attraction potential which is coming out. So, this will transition towards the positive potential. So, that is your attraction potential and then that will continue and then it will just read some asymptotic value. So, this part of the repulsive potential is described by the curve which is like this and then it goes to an asymptotic value. So, this is given by A constant by r to the power 12 this is your repulsive potential. The attractive potential is defend by a curve which is B by r to the power 6; this is your attractive potential.

So, this is the behavior of these two curves is generally approximated. So, the overall potential, interatomic potential, so that for r going to infinity this tends to go to zero asymptotical, right. So, the overall potential between the two atoms is generally written as A by r power 12 minus B by r power 6. So, this is the standard form of what we called as Leonard Jones potential. So, very comman potential used in molecular dynamic simulations, so fundamentally you are looking at big system of molecules and you are just solving f is equal to m a, right. So, on that force this represented by this potential here.

So, this spring mass system if you are applying it to that entire lattice structure we have shown, we just shows this atoms hanging in space, but for the sake of looking at the mechanics of them you can assume that they are like connected by a spring mass system which is holding them together at some equilibrium and that is forming the crystal structure.

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So, if they are disturbed from this, they will tend to resist the disturbance and try to come back to this equilibrium state. So, you can basically draw this spring mass between all of these atoms and they look something like this. The equivalent, now you see when you are applying the higher temperature to the left compare to the right essentially what is happenings. So, the vibration due to this spring constant, this spring constant now become a function of temperature, is actually function of temperature. So, the vibration of this atom spring mass system here on the left hand will be higher than on the right hand. So, this will propagate as waves through the crystal. Essentially the vibration of this atoms are propagating as waves which travel at this speed of sound within this lattice structure and that is responsible for transport of heat. Now the equivalent way when you are representing this as particle called phonons is to represent this system with cloud of phonons, phonon cloud.

So, all these are some kind of molecular representation of gases this entire system is now represented by particles, virtual particles of phonons. So, you have two pictures - one you have vibration waves, lattice vibration waves transporting heat; the other picture is collision of phonons this is your particle picture right. So, you can treat this as phonon gas just like your treating gas molecules and you are talking about collision and transport of energy from the hot side to the cold side. So, you can look at both pictures we can derive the corresponding thermal conductivity and so on looking at both the pictures and still you will get reasonable match agreement between in the two.

So, therefore, now you see the analogy we can talk about molecules in gases and liquids and in case of solids phonons which can also be treated like molecules in a box. So, inside you replace the gas molecules with phonon gas understand and similarly in metals electron gas and when you are talking about thermal radiation you have or any electro magmatic radiation you have equivalent picture of photon gas. So, all these are like particle pictures.

So, we will look at; look in to each of them in detail. So, I will give you a kind of a summary, so between the different energy carriers. this will give be a little bit comprehensive so that you can understand some more details apart from the role heat conduction. So, I call this is basic characteristics of energy carriers.

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So, just I want to define certain constant that will be universal constants that we will be using. So, let me define the planes constant h this is 6.6262 into 10 power minus 34 joules second this is your planes constant. Very frequently we will also be using what is called is a modified planes constant denoted like this h cross this is nothing, but h by 2 pi and this is 1.0546 into 10 power minus 34 joule second. We are also using the Boltzmann constant K subscript b 1.38 into 10 power minus 23 joules per Kelvin. So, these are the standard universal constant will be using in this particular course very often so that is why I have giving that up front.

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So, let go to the characteristics. So, I will have different columns here attributes. So, first for phonon, electrons, then we have molecules and what else? Photons, all the energy carriers that we know, these what are the attributes first will define source where do they originate from? What about phonon? So, lattice vibration, electrons from the nucleus, so they are basically freed from nucleus these are free electrons here. So, free from nucleic bonding right molecules are molecules in a medium liquid or gas. So, these are the atoms and photons you can say electromagnetic vibration or oscillation. So, these are electromagnetic waves which are oscillating described by your sinusoidal equation and so on. So, this is your source.

Now, let us look at the next attributes. Propagation media, what about phonons? Now typically the propagation media is solids it could be also metals so, but the most dominant ones are in semi conductors', dielectrics, semi conductors and to a lesser extent in metals. So, electrons and you have molecules, liquids are gases and what about photons you do not need actually a medium for transport. So, either in vacuum or in any participating media and then the third attribute I will call this as all though I have not introduce them, but nevertheless we will just briefly state that here, energy presentation, for energy representation.

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So, how do we represent the energy of phonons is usually by using the momentum or through the frequency. So, we will use that. We use what is called as wave vector denoted by notation K. So, the momentum is actually related to the wave vector we will see that. So, that is nothing but the modified planes constant times the wave vector will be the actual movement, we can also relate the energy to this and we can also write this in terms of frequency.

So, now you see although we are calling this as particles when we look at energy we can represent the energy looking at the wave picture, because wave vector can be attributed only to a wave similarly with the frequency right. So, apart from that photons have what are called as modes, different modes we will see what are those modes in the future classification of phonons. You can have acoustic modes, we have optical modes, we have longitudinal transfers, these are all the waves again, the wave which have to be represented into particle nature. So, modes and polarization because if you talk about waves again electromagnetic waves or any waves we have polarization, direction becomes important right.

Now, similarly if you look at electrons we can also describe this using wave vector and also specific property called spin which is you need to electrons based on the policy exclusion principles, we will again come back to that. Now if you go to the molecules we are primarily talking about momentum of these gas molecules momentum p and then we are also taking about kinetic potential energies of these molecules. For the photons similar to the phonon you have the wave vector or you can also write in terms of frequency and also polarization, electromagnetic waves definitely will have polarization the energy will depend on the polarization. One more last this thing for today, before we will continue this tomorrow this is basically your particle type, this we will do when we work with statistical thermo dynamics, but right now it is good to have an understanding what they represent.

So, when you talk about phonons they are represented by the equilibrium distribution function all the Bose-Einstein distribution function and therefore, these kinds of particles come under the category of Boson. Same with your photon as well, photon is also described by the Bose-Einstein equilibrium distribution function and there also category of Bosons. So, what is the nature of this kind of particles Bosons? So, you have what is called as indistinguishable particles. So, they all look very similar alike and you cannot distinguish them and also any number of these particles can occupy a given quantum state. So, when we do quantum mechanics now you will understand what is this quantum state, after that when we statistical thermo dynamics you will see how the particles can be distributed into this quantum state. So, they are essentially distinguishable particles and therefore, you can put any number of these particles in given energy state.

So, they are the primary characteristics of Bosons. Now apart from that when you talk about electrons what is the distribution function Fermi-Dirac. So, therefore, these are also called Fermions. So, in the case of Fermi-Dirac distribution function the characteristic is that these particles are also indistinguishable, but they obey the policy exclusion principle. So, they have the integer spring plus half minus half and you know only plus half can occupy one quantum state minus half can occupy one quantum state, although they are in indistinguishable it is not like any number of particles can occupy a quantum state. So, you have depending on in the spin. So, particle spin plus half can occupy one particular quantum state minus half and that is the policy exclusion principle, now molecules these are governed by what is called as Maxwell Boltzmann distribution.

You see Bose-Einstein, Fermi-Dirac they are all quantum mechanical distributions, whereas the Maxwell Boltzmann is what is called as classical distribution because when

we are talking about molecules their particles essentially and they are distinguishable unlike phonons photons and electrons.

So, we will stop here tomorrow we will look into some more details of how these distribution functions are represented and so on.

Thank you.