Foundations of Computational Materials Modelling
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Lecture 16
Introduction to Statistical Mechanica-I

Good afternoon, So let us, before we start the new topic where I want to discuss a little bit about statistical mechanics, I think I said that we would take a look at this construction of the monoclinic units cell by choosing lattice vectors slightly different manner, and see if the, the unit cell that is going to be produced or the crystal that is going to be generated looks exactly the same.

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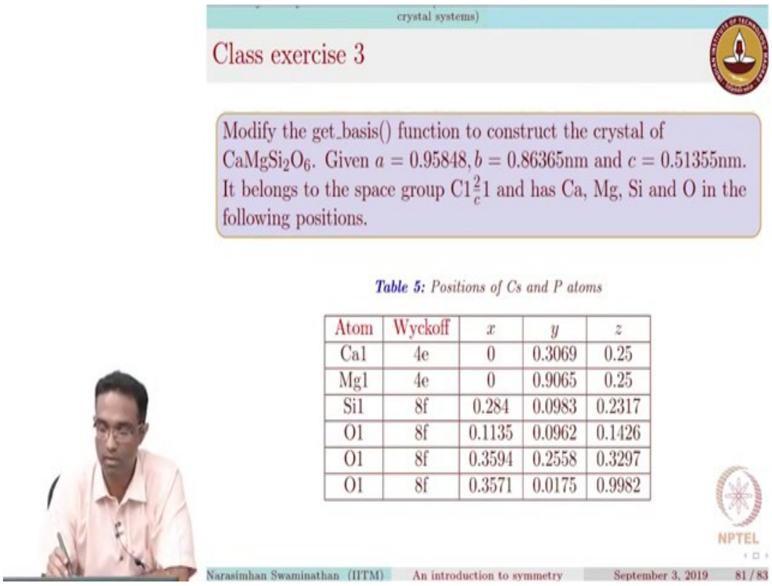

crystal systems)

Class exercise 3

Modify the get_basis() function to construct the crystal of $CaMgSi_2O_6$. Given $a = 0.95848, b = 0.86365$nm and $c = 0.51355$nm. It belongs to the space group $C1\frac{2}{c}1$ and has Ca, Mg, Si and O in the following positions.

Table 5: Positions of Cs and P atoms

Atom	Wyckoff	x	y	z
Ca1	4e	0	0.3069	0.25
Mg1	4e	0	0.9065	0.25
Si1	8f	0.284	0.0983	0.2317
O1	8f	0.1135	0.0962	0.1426
O1	8f	0.3594	0.2558	0.3297
O1	8f	0.3571	0.0175	0.9982

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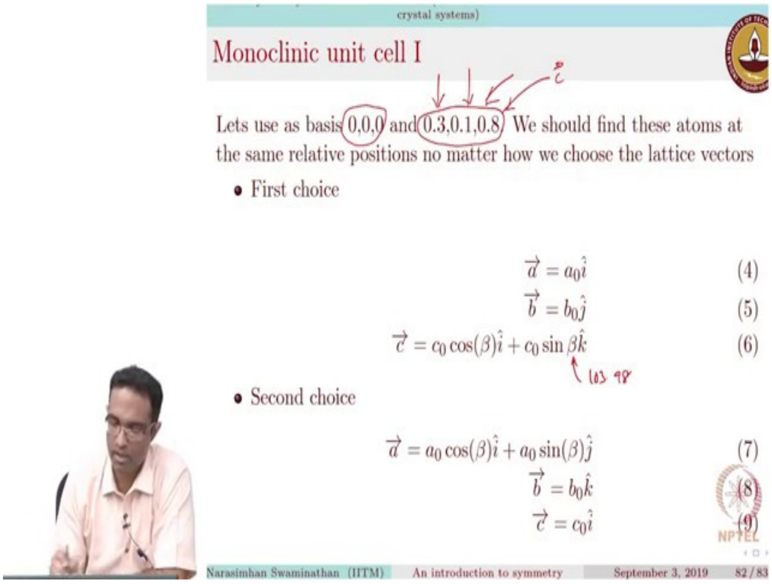

crystal systems)

Monoclinic unit cell I

$\hat{c}$

Lets use as basis 0,0,0 and 0.3,0.1,0.8 We should find these atoms at the same relative positions no matter how we choose the lattice vectors

- First choice

$$\vec{a} = a_0\hat{i} \quad (4)$$

$$\vec{b} = b_0\hat{j} \quad (5)$$

$$\vec{c} = c_0\cos(\beta)\hat{i} + c_0\sin\beta\hat{k} \quad (6)$$

103 98

- Second choice

$$\vec{a} = a_0\cos(\beta)\hat{i} + a_0\sin(\beta)\hat{j} \quad (7)$$

$$\vec{b} = b_0\hat{k} \quad (8)$$

$$\vec{c} = c_0\hat{i} \quad (9)$$

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So, what I am going to do now is so this is a problem that we were dealing with. We were dealing with the CaMgSi2O6 which is having the monoclinic which for which the monoclinic crystal system is appropriate. So, we have the lattice constant a, b and c given to us.

And how do we actually choose the lattice vectors and we know beta our beta should be given here okay beta is for this problem the beta was some 103 point some 98 or something like that if you look at the MATLAB file you will know it. So, the first what we are going to do is we are going to not generate the entire crystal structure.

I am going to I am going to choose two basis atoms one at 0,0,0 the other one at point 3 point 1 and point 8 and show you that no matter how I choose my lattice vectors, the position of this point related to a, b, and c This will correspond to the a lattice vector, this one will correspond to the b lattice vector and point 8 is going to correspond to the c lattice vector.

So, no matter how I choose my lattice vectors, I will show you that this will be in exactly the same spot, relative to the a, b, and c. So, first what I am going to do is I am going to choose my a along the.

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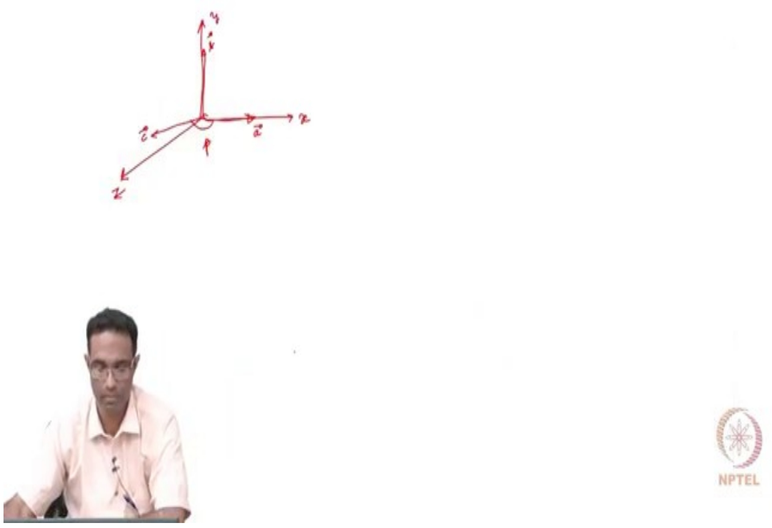

So, this is going to be our coordinate system. The first choice is having a along x axis. So, this will be my a vector and then the c vector was somewhere here it was actually on the x-z is a plane with included angle beta and this is our b vector. So, now, I have constructed this structure.

So, this is the first one this is actually the unit cell which was constructed using these basis vectors. So, as you can see, so the b is pointing in the same direction as Y, you can see here the b is pointing in the same direction as y, a is pointing the same direction as x and the c vector is actually in the x is the plane case in the x is a plane and you will be able to see it only if I rotated it.

$$\vec{a} = a_0\hat{i}$$
$$\vec{b} = b_0\hat{j}$$
$$\vec{c} = c_0\cos(\beta)\hat{i} + c_0\sin\beta\hat{k}$$

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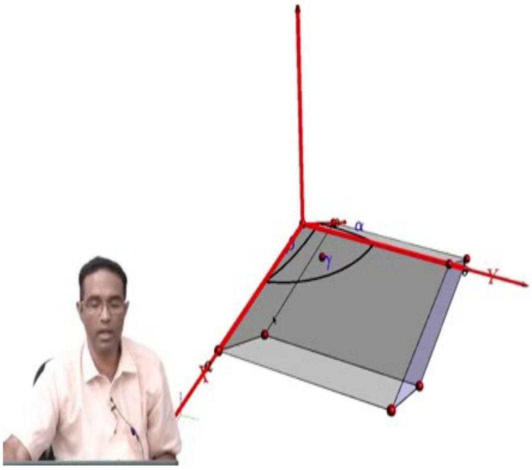

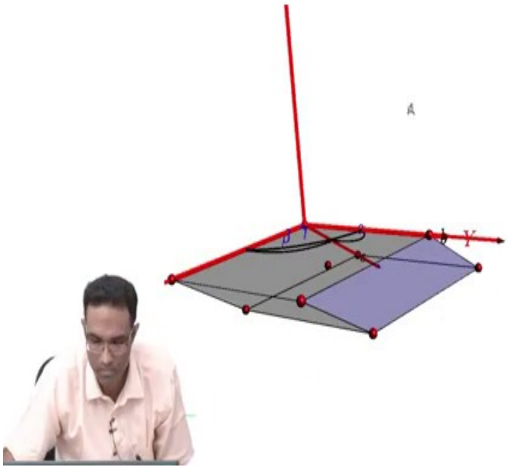

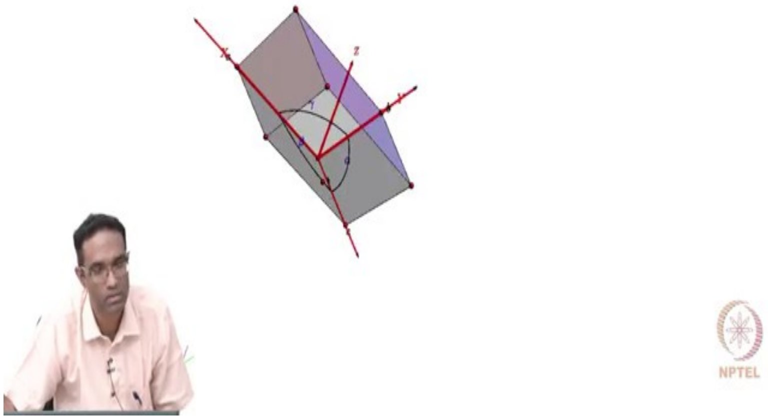

So, this is actually c vector and it is in the x is a plane. So, now the question is if you look at it from the b axis you should see the, the obtuse plane and so, what I wanted to show is this is the point that we are dealing with this red color point that you can see can you see this point here, that is the internal point is these are the corner point which correspond to the basis 0,0,0 whereas this internal point is the point which corresponds to point 1, point 3, point 1, point 8 we need to keep it in mind so that we can check these things.

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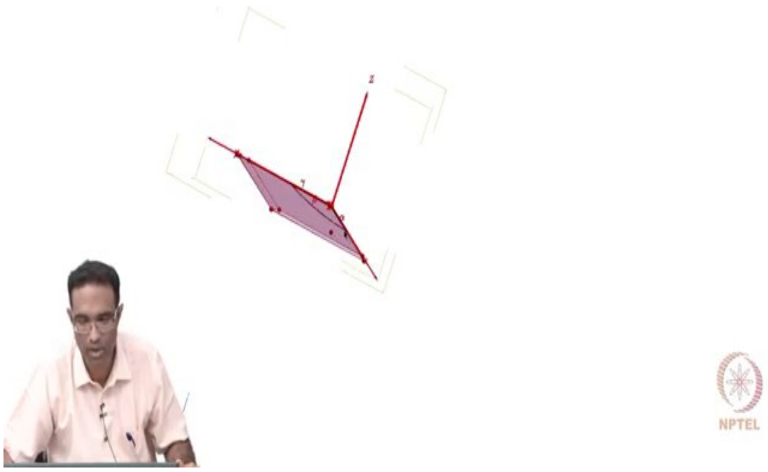

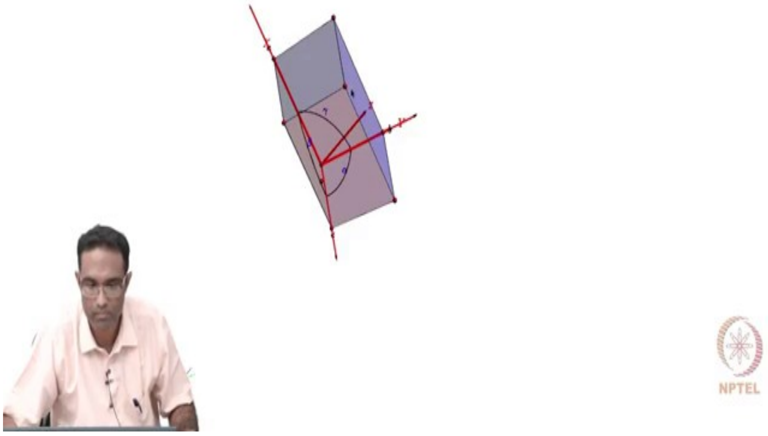

So, let me looking at from the b axis, so this is going to be your c, and this is located at point 8 c, so this would be this distance would be point 8, so it is kind of closer to the length of the c and this distance will be how much point 3 a and this is a and if you wanted to see the corresponding distance in b you rather rotate it in such a way that the b is perpendi….along the plane of the page.

Very slow…, so this point right here would be at point 1 b, from here if you measure the distance to this point it will be point 1 b. So, I am not able to move it here because it is exceedingly is slow. Now, similarly figure to have used a different choice of the lattice vectors. In this case I have made the a vector lie along the x-y plane a cos beta. So it is going to look more like this is still z.

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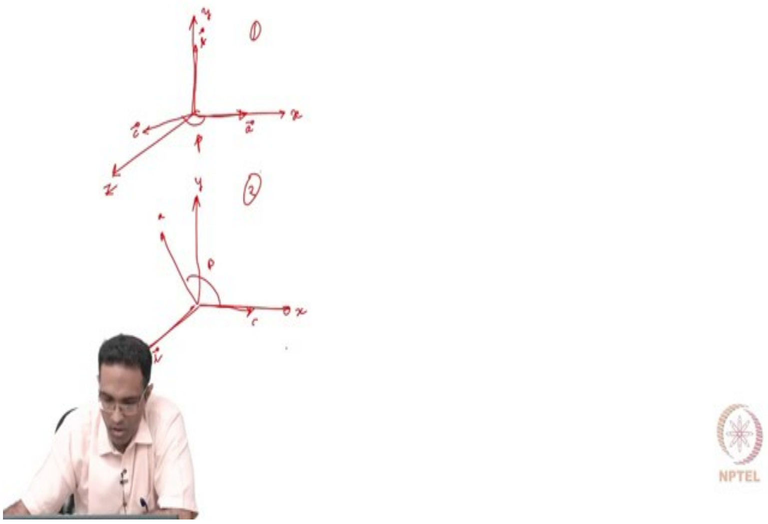

So this would be our c vector, this will be my a vector and that would be the included angle beta a is actually lying in the x-y plane, and z is correspond to the b vector. So, I have just chosen the lattice vector slightly differently when compared to what we did in the previous choice. This was a first choice, and this is the second choice.

$$\overrightarrow{a} = a_0\cos(\beta)\hat{i} + a_0\sin(\beta)\hat{j}$$
$$\overrightarrow{b} = b_0\hat{k}$$
$$\overrightarrow{c} = c_0\hat{i}$$

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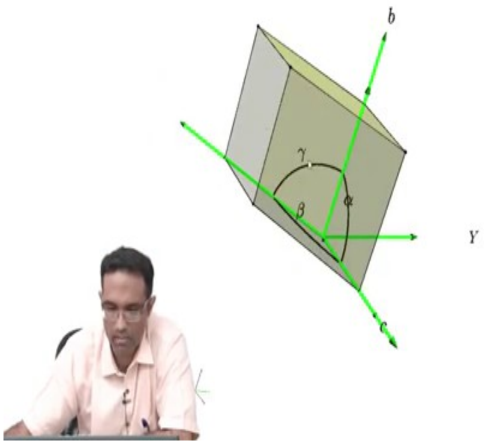

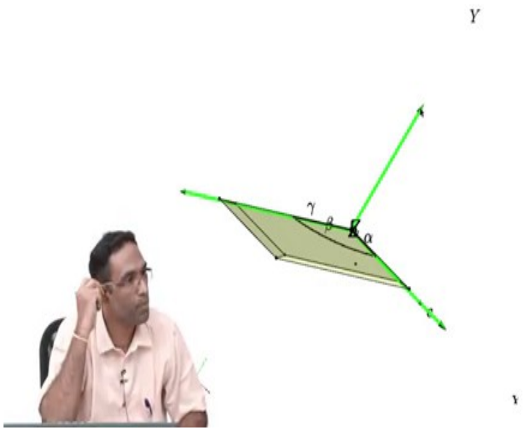

If you look at this as well, if you look at this as well, it is possible for us to see that. So, my b is about the z axis. I am viewing it from b and I am able to see the obtuse plane and then this is my c, this is my c direction and clearly this is this distance is point 8 right it is kind of closer to the end of c and this distance is how much point 3, this distance is point 3 because this is going to be along a and if I view it would from the if it all this thing lets me yeah, so, this one this one is b right this is 0.1. So, no matter how I actually choose this the coordinate system how I choose the lattice vectors with respect to the coordinate system. It is possible for me to generate the same crystal as long as I am careful.

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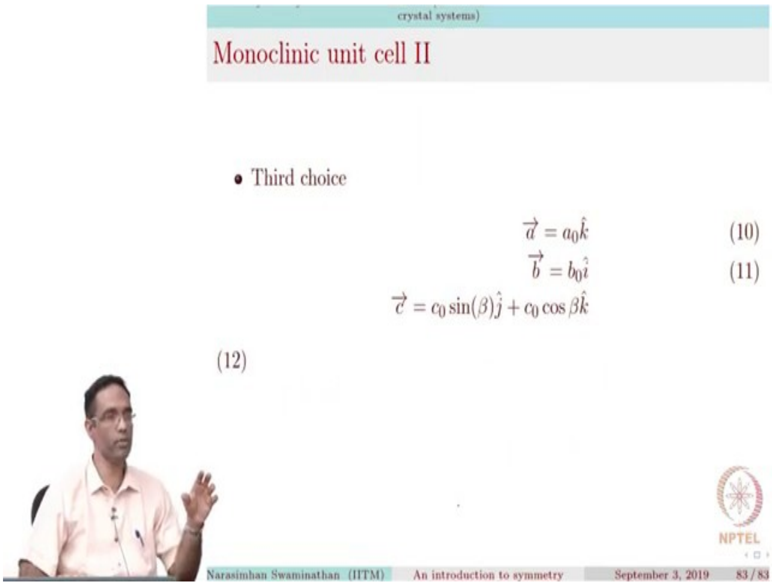

crystal systems)

Monoclinic unit cell II

- Third choice

$$\vec{a} = a_0\hat{k} \quad (10)$$

$$\vec{b} = b_0\hat{i} \quad (11)$$

$$\vec{c} = c_0\sin(\beta)\hat{j} + c_0\cos\beta\hat{k}$$

(12)

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Remember we need to associate a with the x fractional coordinate be with the y fractional coordinate is it with the c sorry and is it with c is it fractional coordinate with the c vector? So we need to associate a with x, b with y and c with z as long as you are consistent there it does not matter how you are going to choose these lattice vectors, so this is important.

For monoclinic crystal systems this can this can get a little bit confusing when you are generating your crystal structures. So this is the third, in the third choice I made a point the z direction b point in the x direction whereas c is going to now lie in the y-z plane, c is not going to lie in the y-z plane.

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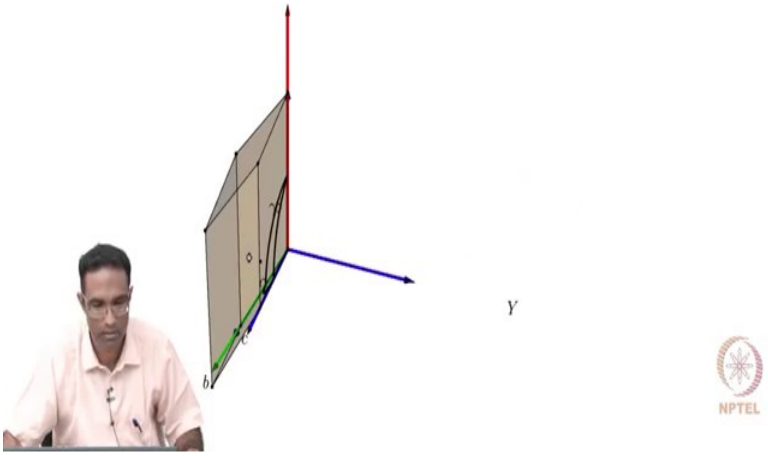

So, in that case also, if you take a look at it, you would still make you would still have this particular fractional coordinate lie at the correct spot with respect to each of the three axis. There would be no inconsistency, so consequently any general position if you are going to generate it would lie at the appropriate spots it may it may not look the same.

You might have to make some additional effort to make sure that the crystal system look the same if you are using different set of lattice vectors. When you use the MATLAB code that I just gave you, it is it is not really apparent. That is why I had to use this to demonstrate this. But when the lesson is, as long as you are consistent with associating your a vector with x, b vector with y and c vector with z, and choosing these lattice vectors in the Cartesian coordinate system will not really affect the manner in which your crystal is actually built.

But the other, the other, the other ones are pretty straightforward orthorhombic or tetragonal all these things are straightforward, because they have not include angle of 90 degree and it is quite obvious how these crystal structures should be generated. But for some of these things, it can be a little bit confusing.

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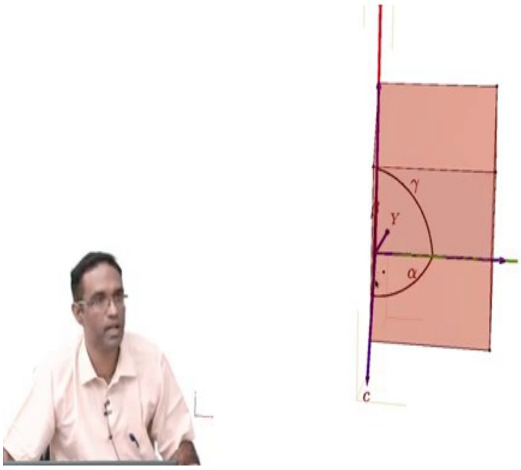

So, this is viewing it from the b axis, this is beta and about the c it is closer to point 8 and about a is closer to point 3. So, this would be point 3, and then if I rotate it further, you can make sure there it is just point 1 in the z axis along the b along the b axis of the b lattice vector.

Student: is it similar saying the reference axis and crystal axis you said about?

Professor: Yes the similar to saying that the reference axis the Cartesian coordinate system x, y z axis and the crystal a, b, c axis are different and you can…

Student: you can choose your reference in any way you want

Professor: In any way you want, you can choose your reference in any way you want. Yes, that is what that is a point that this exercise basically demonstrates why it is obvious for the other crystal systems. This can get a little bit confusing, so I thought it might be useful for us to take an example and show that it does indeed not change things quite a bit. Any questions before we proceed?

Student: Please adjust the mic

Professor: But you have any questions so far and what? Ok, Good… So, now I am going to start doing something the next part of the course, where we start talking a little bit about statistical mechanics statistical mechanics, like I mentioned in the previous class is a subject by itself and you can take several semesters worth of courses to understand this course, very deeply.

Our purpose in this course is not really that our purpose is to talk a little bit about statistical mechanics to show you that it is because of the framework of statistical mechanics that molecular dynamics simulations actually work and some of the expressions that are used to actually calculate properties of materials, after you have conducted a molecular dynamics simulations are in fact, coming from the framework of statistical mechanics.

So it is a good idea to actually know some of these basic principles when we are trying to run the molecular dynamics simulation, so that we know what this simulation is actually doing. So, that was that is that is the goal of this particular module of this course. So, I will not go in great detail discussing all the results of statistical mechanics, but hopefully just provide enough ground so, that when you are actually looking at some expressions that people are have used in order to obtain properties of materials, you should actually know that these are coming from statistical mechanics and there are rigorous ways by which these can be derived and you should know how to use these expressions to calculate these properties and not necessarily always have to derive them from the fundamentals, may not be always possible. So, that is the goal of this part of the work.

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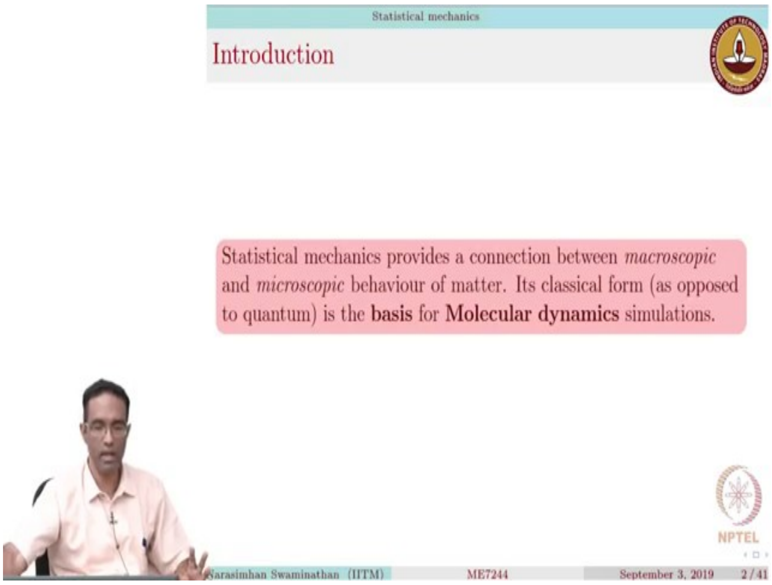

Statistical mechanics

Introduction

Statistical mechanics provides a connection between *macroscopic* and *microscopic* behaviour of matter. Its classical form (as opposed to quantum) is the **basis** for **Molecular dynamics** simulations.

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So, many of you might already have some introduction to statistical mechanics or statistical thermodynamics per say. Right enough in your in your material science courses they might have dealt with it in some detail. So, some of this might be a little bit repetitive, so bear with me.

So, overall statistical mechanics provides a connection between the macroscopic properties of matter and the microscopic constituents of matter. So, what does macroscopic means and microscopic means is something that we can we will come to in a little bit in more detail, but to give you a, to give you some idea you can say that, temperature is basically a macroscopic property of a given system.

Pressure is a macroscopic property of a given system. So, is Gibbs free energy enthalpy and all these things, all these thermodynamic. When you think about thermodynamics, there is nothing, no more information that is available to you, as to how that particular quantity is actually related to the things that actually make up the system. So, if you have atoms making of the system thermodynamics is not telling you how the positions or the velocities of these atoms is actually related to temperature or pressure or Gibbs free energy or enthalpy. The idea of statistical mechanics is to provide this connection that’s it and it is it can be quite involved in trying to see how this is obtained.

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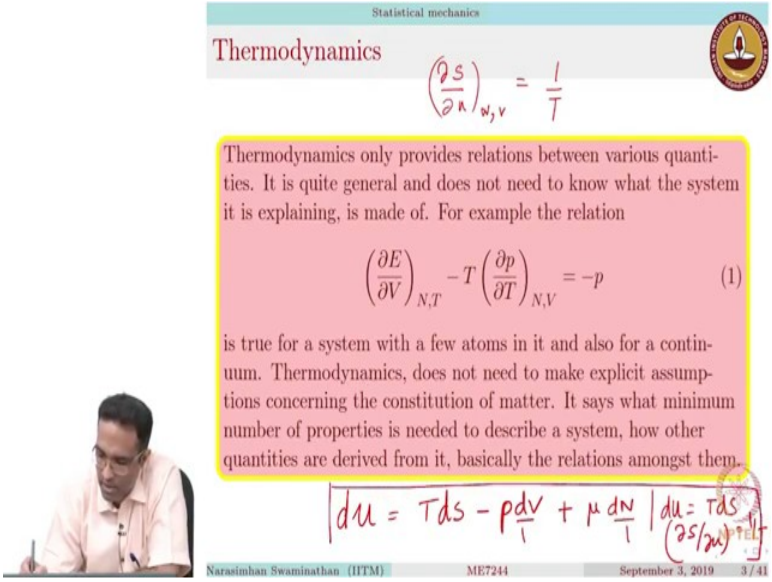

Statistical mechanics

Thermodynamics

$$\left(\frac{\partial s}{\partial u}\right)_{N,V} = \frac{1}{T}$$

Thermodynamics only provides relations between various quantities. It is quite general and does not need to know what the system it is explaining, is made of. For example the relation

$$\left(\frac{\partial E}{\partial V}\right)_{N,T} - T\left(\frac{\partial p}{\partial T}\right)_{N,V} = -p \qquad (1)$$

is true for a system with a few atoms in it and also for a continuum. Thermodynamics, does not need to make explicit assumptions concerning the constitution of matter. It says what minimum number of properties is needed to describe a system, how other quantities are derived from it, basically the relations amongst them.

$$du = Tds - p\underset{1}{dV} + \mu \underset{1}{dN} \quad du = Tds \quad (\partial s/\partial u)$$

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So, thermodynamics like I mentioned, it just provides the relationship that exists between various thermodynamic quantities right. So, you all have seen several such relationships, for example, it tells you that maybe the rate of change of entropy with respect to the internal energy at constant number of species and volume is equal to what is it? dou S by dou u maybe 1 over T.

$$\left(\frac{\partial s}{\partial u}\right)_{N,V} = \frac{1}{T}$$

How would you how would you do you all seen this thing plus what? What else will come here? Material science students?

Student: chemical potential, nu dN

Professor: Chemical potential, our nu dN.

$$du = Tds - p\underset{1}{dV} + \mu \underset{1}{dN}$$

So, we need to know a little bit of this thermodynamics if you want to appreciate statistical mechanics, somewhat. So, now if you wanted to look at what is, so let us, let us, let us try to write down this relationship. So, you see that I am keeping volume as a constant, and this number of species as a constant, so I am going to say du is equal to TdS or dou S by dou u when volume and number of species of the material is kept a constant, I get this thing called one by T, which is temperature.

So, this is classical thermodynamics right classical there must have studied it in mechanical engineering or material science all of you would have studied these equations at some level, some of you might have looked at chemical potential, some of you might not have looked at chemical potential that is the only difference.

So, thermodynamics is not doing anything beyond this and this is another relation, this is another relation is interesting to look at dou E by dou V at constant N and T minus temperature times dou p by dou t at constant N and V, nothing but the negative of pressure it is possible for us to prove this relationship as well, let us not worry all this is how this comes along you can prove it.

What is important for us to notice it does not really thermodynamics is does not really worry about what the system is actually now made of. This relationship holds true whether it is consisting the system as one atom of two atom or hundreds, hundreds of atoms. This is a relationship that thermodynamics can give you and it does not make any expli… assumption concerning what the constituents of matter are.

So, it only says what minimum number of properties are required to describe the system. You all must have seen that, if you have can you can somebody highlight that the minimum number of properties that is required to describe the system. So, we always talk about things like what is it called?

Student: Gibbs face

Professor: Gibbs face or Gibbs face rule. So, if you have one single phase a single constituent system, you need only three things to actually describe that system, either N, V, E or N, P, T or something like that. So, those are basic thermodynamics, we will not go into that we will assume that some of that is known to you all. So, if you know that you can basically derive other quantities that are there in thermodynamics, so that is thermodynamics.

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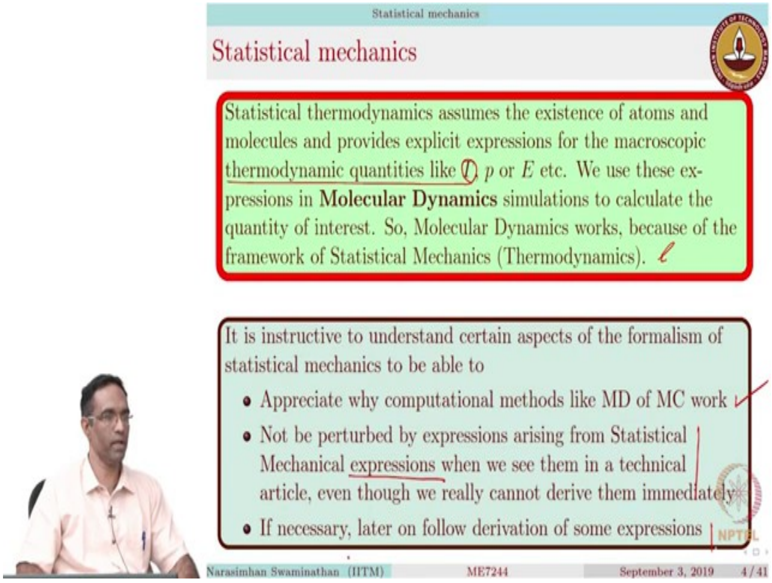

Statistical mechanics

Statistical mechanics

Statistical thermodynamics assumes the existence of atoms and molecules and provides explicit expressions for the macroscopic thermodynamic quantities like T, p or E etc. We use these expressions in **Molecular Dynamics** simulations to calculate the quantity of interest. So, Molecular Dynamics works, because of the framework of Statistical Mechanics (Thermodynamics).

It is instructive to understand certain aspects of the formalism of statistical mechanics to be able to

- Appreciate why computational methods like MD of MC work
- Not be perturbed by expressions arising from Statistical Mechanical expressions when we see them in a technical article, even though we really cannot derive them immediately
- If necessary, later on follow derivation of some expressions

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The statistical thermodynamics is not doing that, it is going to assume the existence of atoms and molecules and it can provide explicit expressions for the macroscopic thermodynamic quantity like temperature, pressure, or energy, etc and it is these expressions that we are going to use in molecular dynamics simulations to get these properties. For example, if you have a system comprising of a large number of atoms at a particular temperature T, and all of them are interacting with each other through some in some way, then let us say it is not interacting with each other.

So, maybe an ideal gas, argon gas is that inside this room and the entire room is actually isolated from the surroundings. So, it is an isolated system and if somebody asked you, how would you calculate the internal energy of the system, what would you do? How would you get? What would be an expression that you would instantaneously write down? In order to tell me that instantaneous kinetic energy, the internal energy of the system is nothing but the sum of the kinetic energy of all the molecules.

Assuming that there all not interacting with each other. So, that very statement is connecting this concept called internal energy to something that is associated with each and every atom that is there in this box, it is connecting the velocities of each and every atoms in this box to the macroscopic thermodynamic quantity called energy. So, it is in this spirit that statistical mechanics is capable of providing you with expressions for the macroscopic thermodynamic quantities from the microscopic constituents of matter.

So, like I mentioned at the beginning of the class, the goal is to be able to appreciate why computational methods like MD and MC are working, how we can use these expressions once we run MD simulation this is very important. So, this not be perturbed by expressions arising from statistical mechanics expression, arising from statistical mechanics expressions.

When we see them in a technical article, it is not always possible to re-derive all the equations of statistical mechanics to be convinced that these can be used, it is impossible it is probably not possible. So, we need to be able to at least know where these expressions could have come from and how we can actually use it without knowing its detail derivation.

If necessary, we should be able to follow some derivations as well. So, these are this is actually the spirit with which I am want to present the statistical mechanics portion of this course. There are more deeper courses that you can take in statistical mechanics and I think you should probably take them if you want to learn more.

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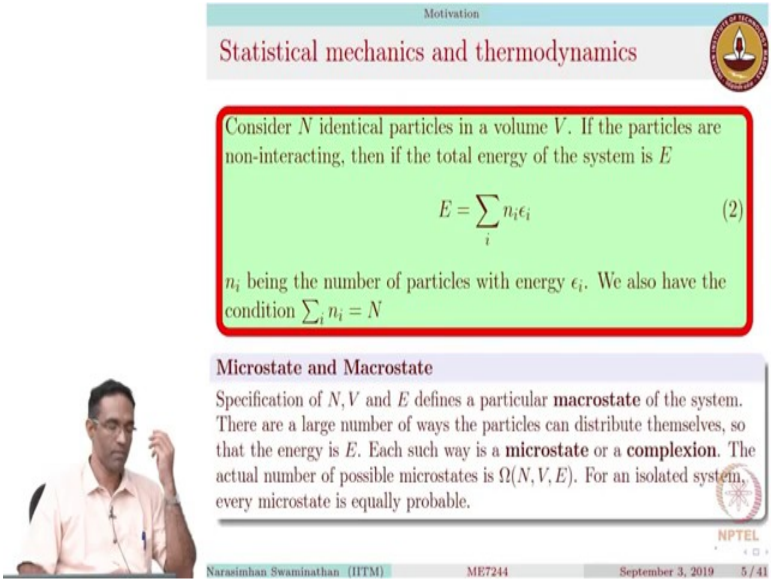

Motivation

Statistical mechanics and thermodynamics

Consider N identical particles in a volume V. If the particles are non-interacting, then if the total energy of the system is E

$$E = \sum_i n_i \epsilon_i \qquad (2)$$

n_i being the number of particles with energy ϵ_i. We also have the condition $\sum_i n_i = N$

Microstate and Macrostate

Specification of N, V and E defines a particular **macrostate** of the system. There are a large number of ways the particles can distribute themselves, so that the energy is E. Each such way is a **microstate** or a **complexion**. The actual number of possible microstates is $\Omega(N, V, E)$. For an isolated system, every microstate is equally probable.

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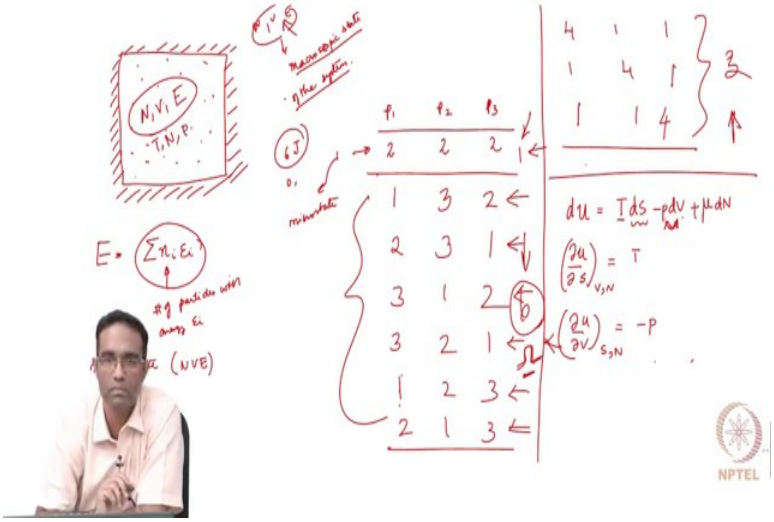

So, let us start a little bit with some basic ideas of statistical mechanics. So, let us begin with considering a volume V. Suppose we have a volume V and it is completely isolated I always like this isolated things makes things very easy and it consists of N particles, this entire volume is V and this entire thing is in energy E there are N different particles here.

So macroscopically, macroscopically we are actually specified the system completely, like right now, I just said that a thermodynamic system can be specified completely using these three using three variables of three things. So, N, V and E completely specify the macroscopic state of the system, microscopic state of the system.

However, at the microscopic level, the possibilities of specifying something called as a microstate is just huge. So, what that essentially means is the energy E of the system can be realized in so many different ways. Specifically, the total energy E is nothing but n i times epsilon i, where n i is a total number of particles with energy epsilon i.

$$E = \sum n_i \varepsilon_i$$

So, you can just add them all up and you can get this energy. So, there is now it should be apparent that there are so many different ways this energy E can be reached, the particle each of the particles can be put in different energy levels, so that the total energy of the system is E.

So, the in order to illustrate this, let me take an example just to see what this means, let us say that our particle does not contain more than or the number of particles is this three, so there is p1, p2 and P3 are the particles, they are identical in every aspect, but I can distinguish them that means I can one is maybe marked with some yellow color and other one is with blue color the other one was red color.

And the total energy of the system is something like 6 joules and I am going to say that they cannot take energy 0 or any decimal energy all integral energy is only they can take these particles, just for the sake of illustrating what these many ways of getting this energy E means. So, one way of getting this 6 is, have all of them have the energy of 2 Joules, 2 plus 2 plus 2 6 that is one way, yes.

Student: This of … Are you considering only kinetic energy, no interaction between particles?

Professor: No, in this system. So, the question is in this example am I looking at.

So, now if I want to look at some other way by which this particular energy of 6 Joules is reach one other way say maybe 1, 3 and 2, 2, 3, 1, 3, 1, 2 is there anything else 3, 2, 1 maybe and so on 1, 2, 3 1, 2, 3 then what is it?

Student: 2 1 3

Professor: 2 1 3 huge, large number of ways, quite a few number of ways in which you can have one particle at energy level 3, one particular energy level 2 one particular energy level 1. Then is there anything else that I can do?

Student: 4 1 1

Professor: 4 1 1 then 1 4 4, then?

Student: sir…..

Professor: 1 4 1 is that it?

Student: 141

Professor: Sorry this is 1, this is 1, then this is also 1. Anything else? Any other possibility?

Student: both are the same….

Professor: No, is there any other way by which I can get 6 joules from three particles? 5 1 0, No, because I am not allowing that. So, when we saw this distribution, we saw that there are different ways of getting some energy. There are different ways of realizing this macro state. There are different ways of realizing this macro state. Each of the state is called a micro state. This is one microstate, this is another microstate, this is another microstate, this microstate one particle as energy 3, other particle as energy 2, other particle as energy 1, this one is 2 particles of energy 1 and one and one particular has energy 4.

It is very clear that there was one particular state which had the maximum possible number of ways of achieving it. For example, this 1 3 2 combination, you had 1, 2, 3, 4, 5, 6 ways of achieving that whereas, whereas only three ways of achieving this and only one way of achieving this. So, if this were a real system, if this were a real system, then the likelihood of you at any given instant of time, the likelihood of you observing it in this micro state is higher than the likelihood of you observing it either and this or this microstate.

Yes or no? So it happens that when you have extremely large number of atoms like what happens in a real material, when the number of atoms or the number of molecules of the degrees of freedom that you are dealing with is in the order of 10 to the power 23 moles of atoms then there is going to be one specific microstate, which is so large number this number, this is called as the microstate or the total number of microstates or the complexions number of complexions.

Number of ways you can actually achieve this particular microstate, when you have a large number of atoms, this number is going to be so large that you are going to be seeing it when you examine this system. 99.99999 percent of the time you will see that all the other systems all the other complexions or other microstates do occur, but they occur very rarely and you hardly observe them.

But that does not mean that the system cannot take that microstates all the other microstates are also equally probable they are going to occur. But you will observe this because this occurs very, very frequently. This is an example of three particles, some energy 6 Joules of energy, we just took it just to illustrate basically, this was done to illustrate two terms one is a macro state and microstate.

The micro state is in commensurate with the applied microstate, each of these each of these are the same macro state N, V, E the energy is 6 Joules they are not it is not differ. So, there are microstate, each of this is a microstate and then what you specify is a macro state. The macroscopically using thermodynamic variables, what you specify is a microstate and the ones that you specify microscopically by looking at the number of ways you can actually achieve this macro state is called as a microstate or number of complexions.

Student: we need to specify the pressure and temperature from this system why NVE is sufficient?

Professor: So why is N, V and E actually sufficient and you do not need pressure and other things. So, the question is why is just three sufficient, so that is actually a deep question, we need to look at Gibbs phase rule to actually answer the question, we will consider that for a single phase material with consisting of one type of atoms, one type of species, it is enough if you have just three, three variables specifying the state of a system, but look let us look at it from basic thermodynamics you have seen this expression du is equal to Tds minus pdv plus mu dN, have you seen this before? Yes.

$$du = \underline{T}ds - pdV + \mu dN$$

So, what is dou u by dou s at constant V and N? It is temperature. So, in this expression it is viewed as if this ds is a controlling variable and the corresponding thing that turns out or comes out of it is actually the temperature. In this expression with u that dv is actually the controllable variable and the pressure that comes out of it is actually the result of it. So, dou u by dou v, at constant entropy and, N is actually minus pressure. So, they are conjugate variables.

$$\left(\frac{\partial u}{\partial s}\right)_{V,N} = T$$

$$\left(\frac{\partial u}{\partial V}\right)_{S,N} = -P$$

You do not specify both pressure and volume at the same time specifying one, will automatically determine what the other ones through this relationship. That is the answer for it. If you are going to specify everything like for example, it is possible N, V, E you cannot do it independently, you cannot do you cannot specify the temperature here independent of the entropy of the system. You cannot specify the N independent of the chemical potentials of the system. You cannot specify the pressure independent of the volume of the system they are all related.

Student: Incomplete questions

Professor: Although macroscopically are specified a certain set of parameters N, V and E responsible to achieve this through in many ways as possible to achieve this through many ways and each such way is actually called the micro state corresponding to a given macro state of the system.

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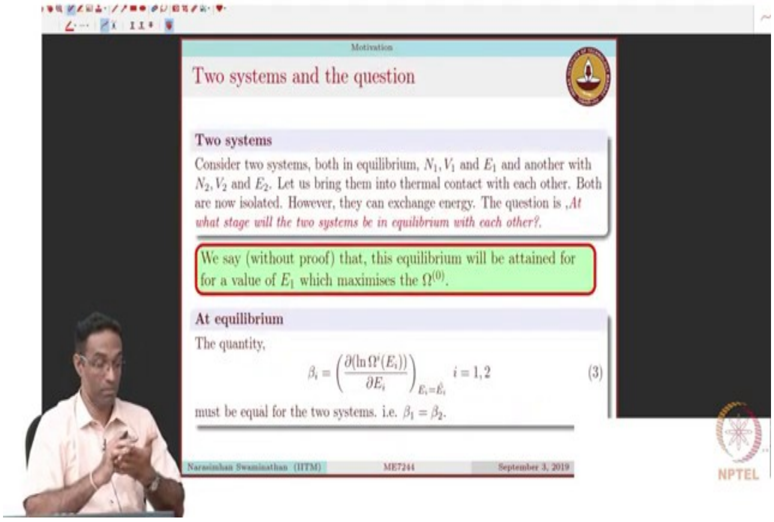
Motivation

Two systems and the question

Two systems

Consider two systems, both in equilibrium, N_1, V_1 and E_1 and another with N_2, V_2 and E_2. Let us bring them into thermal contact with each other. Both are now isolated. However, they can exchange energy. The question is ,*At what stage will the two systems be in equilibrium with each other?*.

We say (without proof) that, this equilibrium will be attained for for a value of E_1 which maximises the $\Omega^{(0)}$.

At equilibrium

The quantity,

$$\beta_i = \left(\frac{\partial(\ln \Omega^i(E_i))}{\partial E_i}\right)_{E_i=\bar{E}_i} \qquad i = 1, 2 \qquad (3)$$

must be equal for the two systems. i.e. $\beta_1 = \beta_2$.

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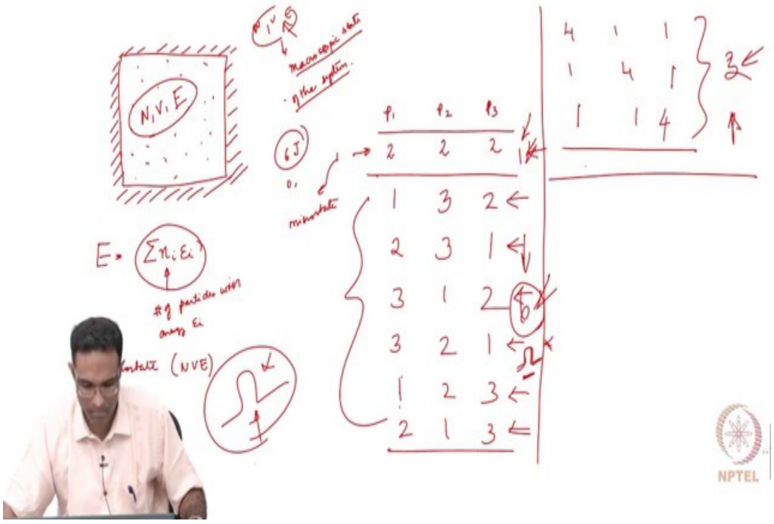

Now, the question is, the nice thing about the statistical thermodynamics is if you knew this Omega the number of ways you can achieve this particular given microstate, if you have an explicit expression for that, it apparently seems to be sufficient for you to derive the entire thermodynamics of the system.

Now, how instead of worrying about how to calculate this omega which we will come to in maybe one or two classes, I would like to show you how if you knew this omega, this and making only one single postulate, we will show that the entire thermodynamics will actually follow from it.

You will be able to see all the expressions that you signed thermodynamics based on this omega instead of the thermodynamic parameters, all the thermodynamic parameters can in turn be obtained from this omega and omega is nothing related to thermodynamics it is related to the number of ways, this thing can actually reach a certain energy number of ways you can arrange this system so, that a particular energy is obtained.

So, Omega is actually a number is some large number, of course, it depends on your N, V, E. But it is, it is going to turn out to be a number at the end. Some large number for a system that is comprising of a large number of atoms. So, in this case, this was all these were omegas where the total number of complexions that you can actually obtain in order to reach a particular macro state. So, what we will do now in order to show that is as follows.

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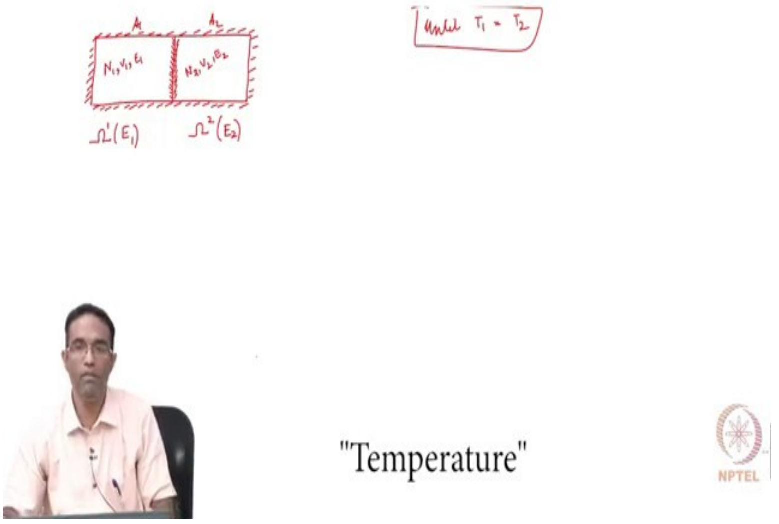

"Temperature"

So, we will consider a system, there are two systems here. So, this one consists of N1 V1 and this has energy E1, this is N2, V2 and energy E2 and both of them are isolated from the surroundings and for now, they are also isolated from each other. So, we say that so, clearly from our previous discussion, we can say omega1 N1, V1, E1 is a total number of ways the system here the A1, this is the A1 system and this is the A2 system which are both isolated.

The total number of ways A1 can have this macroscopic state, total number of ways, so here N1 and V1 actually do not matter it is only the energy that is going to be of importance to us. So, we will not necessarily write them. Omega2 is the total number of ways the A2 system can actually have the macroscopic state N2, V2 and E2.

Now we are going to do a small experiment what we are going to do is we are going to say that this central wall that is right here is going to make both the system A1 and A2 come into thermal contact with each other, they are going to come in thermal contact with each other but the number of the species do not move around or the volume does not change, it is not a piston move with piston, it is just something that allow the exchange of energy alone.

The question that we now ask is, when will the exchange of energy stop? Something is different about these two because of this energy has to flow what is it?

Student: Temperature.

Professor: Temperature, there is something different about it. Because of this the energy has to exchange and that thing that is different is what is going to drive the energy to move from one system to the other, and it will happen according to classical thermodynamics until when, until there temperatures are equal, so until T1 is equal to T2 this exchange of energy is going to happen.

$$T_1 = T_2:$$

So, this is from thermodynamics we already know it, that is a known proven statement from thermodynamics. So, there is nothing we question about it. So, we want to see if we can have such a relationship or if a relationship similar to this can be attained without actually invoking temperature