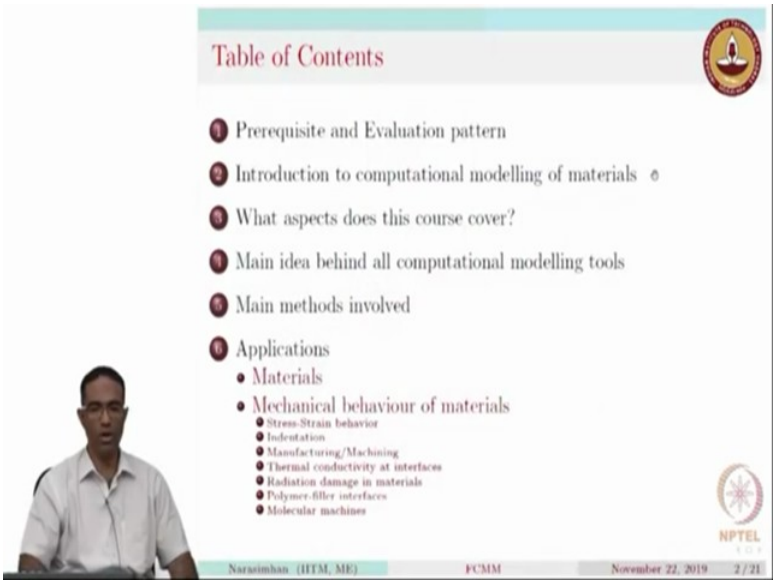
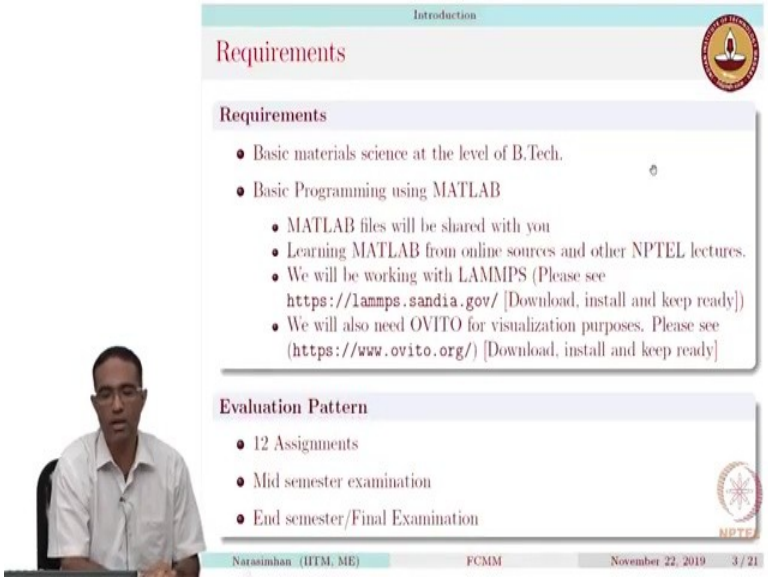
**Foundation of Computational Materials Modelling**
**Professor Narasimhan Swaminathan**
**Department of Mechanical Engineering**
**Indian Institute of Technology Madras**
**Introduction to the Course**

Welcome to the course on foundations of Computational Materials Modelling. So I hope you would have seen the introductory part of the lecture where I gave you a very brief overview as to what we might be doing.

(Refer Slide Time: 0:27)




So, in order to explain some of the details as to what are the various things that you might actually need in the course. We will go through them, we go through some of the introductory material once again. So, I would require that the students who are registering for this course

actually require, have a basic material science background at the level of B.E. or B Tech. They should also have some background on basic programming using MATLAB.

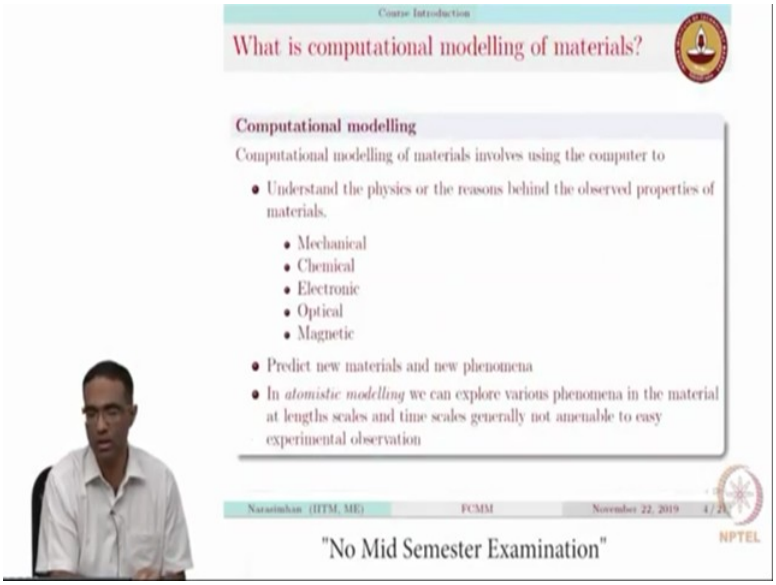
There will be several MATLAB programs that we will be writing in the first part of the course and which involves, which is the basic purposes of this MATLAB, MATLAB programs is to actually create input files or is to create a course so that we can generate various kinds of crystal structures. So I would expect that you have a reasonable experience in programming with MATLAB. If you do not have I am sure that there are several online, if you do not have I am sure that you have several online versions, online tutorials from where you can learn this MATLAB programming and also probably NPTEL lectures.

We will be working with LAMMPS in the third part of this course where we will be teaching you to write very simple input files in order to run some molecular dynamic simulations on gases on metals and also on ceramics. For that you will actually need the LAMMPS code to be on your laptop or desktop. So please make sure that you already have an installed and a working version of this particular software on your computer.

And in order to visualize the results of that is generated by LAMMPS code, you will need something called OVITO which you, which is also freely available, you can simply download and install it on your computer please keep it ready we will not be needing both LAMMPS and OVITO in the first two thirds of the course, but it is a good idea to have them on your laptops and figure out any issues that you have in installing them so that you would not have any trouble later on in the course.

The evaluation pattern will essentially consists of you doing about 12 assignments. This is a twelve week course. So we have planned about one assignment per week. Most of these assignments are expected to be answerable by looking at the slides and some of which you may have to think a little bit like I mentioned in the introductory course. A mid semester examination and then and final examination.

(Refer Slide Time: 03:03)




So with that brief introduction, I would like to start talking about Computational materials modelling in a very broad sense. As the name implies, Computational materials modelling involves using the computer to basically understand the different properties of materials. In particular, it is possible for us to look at mechanical properties, chemical properties, chemical reactions, why certain chemical reactions occur, and why they do not.

Electronic properties are also possible, optical properties and magnetic properties can also be evaluated using computational tools. Not only it is, not only is it useful in understanding physics of the reasons behind a certain observed properties in the materials, it is also useful for predicting new materials and new phenomena which might actually be happening inside the material.

So when you perform an experiment and if you are not usually able to explain why you observe a certain thing, then it is possible that you can conduct some simple molecular simulations in order to try to explain that phenomena or to find reasons as to what atomistic level phenomena is actually causing your observed experimental plots for example. In atomistic, modelling of materials it is also possible for us to explore phenomena at various lengths and timescales, especially lengths and timescales that are not amenable to experimental observation easily.

So, by that I mean that if you want to look at how dislocations are moving in a material or you want to look at the kind of point defects that are going to be generated, when material is being bombarded by ions or neutrons, then such things become hard to observe

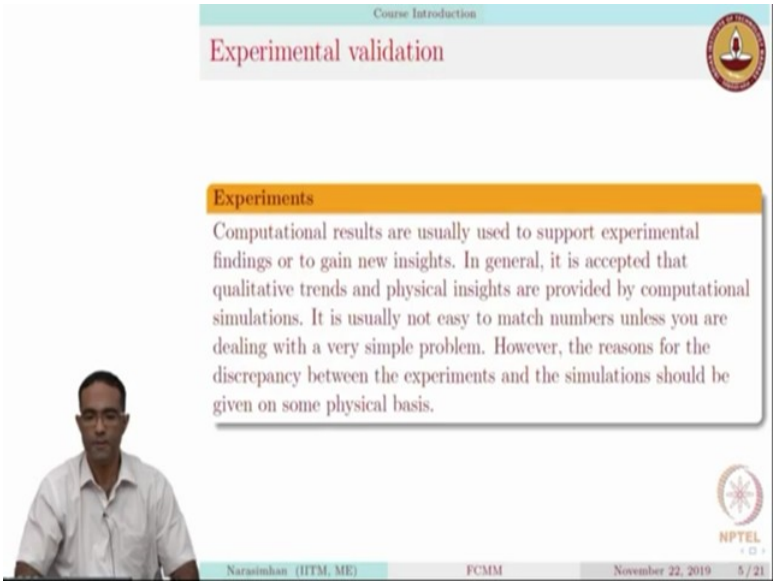
experimentally. Under such conditions it is possible for us to look at how simulate these processes on the computer and, and this helps us gain a deeper understanding at least qualitatively if not quantitatively on what could be actually happening in these materials.

So, of course, that is with respect to both the lengths and timescale, you could be looking at very extremely small length scales that you can really not capture using experiments and molecular dynamics simulations or many atomistic methods are working with systems at the atomistic level and therefore, you would be able to get atomistic level details from these calculations.

So, that is the basic purpose of this course. In addition to that, there are timescales issues also associated with physical phenomena. For example, if you talk about radiation damage in general, you are going to be creating point effects so when a neutron comes and hits a material, it is going to generate point effects in the material and this entire process usually happens in the order of say 10 to 15 picoseconds and it is usually hard to see this using experiment, it is not impossible.

So, molecular simulations helps you understand these processes, even though they are occurring at extremely small length scales and time scales, because the method itself is adapted to actually work in this time scale, you will see more as to what this essentially means when we talk about molecular simulations.

(Refer Slide Time: 06:34)




So, that being said, it does not necessarily mean that experiments are not important, they are extremely important. The discrepancy that you observed in a computational result and

without the experimental must proper be, properly be analyzed and you must be able to give some sort of reason as to why your simulations are not matching with the experts. There could be several reasons for it, but you should make sure that the reasons are as logical as possible, so that your simulation results are at least qualitatively acceptable.

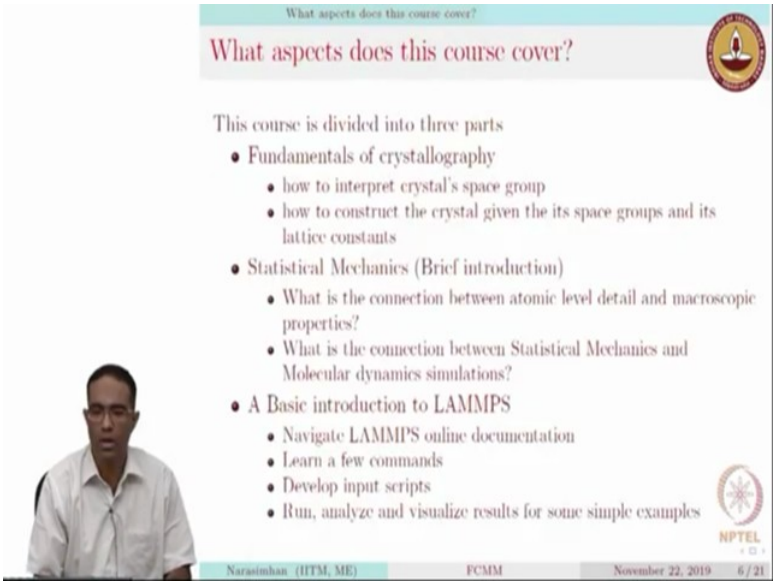
So, but it is usually, that being said I should also mention that it is very hard to expect quantitative the same numbers for many different problems between the computational result and the physical result. For example, when you are trying to calculate the elastic properties of copper, then you generally perform the experimental results a dog bone specimen which is going to consist of a large number of polycrystalline grains.

However, when you are trying to do that, when you try to match these results with the simulations that is performed on a single crystal copper, and you do not expect the same kind of same, same kind of values in the board, you should be able to logically come to that you know one thing is going to consist of large number of grains where the other is going to consist of a single crystal.

A single crystal is probably a little bit more stronger than the poly crystal and the specimen that you are using in your laboratory all probably has a large number of defects and these are not the kind of defects that you have simulated explicitly on the computer. So, you know, you need to be able to draw some logical conclusions based on which you will be able to say that the computational value that I got for my youngs modulus or the yield strength is actually not too bad, okay.

More than quantitative comparisons, we generally use these computational results for qualitative purposes to understand new phenomenon and to explain something that we are not able to immediately see from experiments.

(Refer Slide Time: 08:51)




So, I would like to now talk about what are the various aspects that are covered in this course. This course is basically divided into three, three parts. The first part is called as fundamentals of crystallography and the main objective of this part is to help you interpret a crystal space group. So, we are given a crystal structure and we are told that it belongs to a certain space group, we will talk about what space group means, when we are actually talking about it.

But the first part of the course is essentially meant to help you generate these crystal structures on the computer which is basically the first step in starting to conduct some computational simulation on crystals. So, when, so at the end of the first part given the crystal, the lattice constants of the crystal like for example the A or the angles that is existing between the various lattice vectors and the corresponding space group along with information on what is referred to as the vecof positions which refers to the various positions of atoms inside the crystal structure.

We will be teaching you how to write a small MATLAB script in order to generate these crystal structures and visualize them. And these are obviously not standalone they will actually be useful in the third part of the course, where we will actually use the LAMMPS simulation software in order to perform simulations on these crystal structures.

So, once you understand the first part, the small portion of the last part is actually you can actually start doing that you will be able to generate this crystal structures and in LAMMPS and prepare them for actually further analysis. Then in the second part of the course, we will be dealing with statistical mechanics. This is going to be a little bit of a theoretical portion of

the course, where we basically provide a very brief overview of statistical mechanics just to emphasize its purpose and its connection to molecular dynamics simulations.

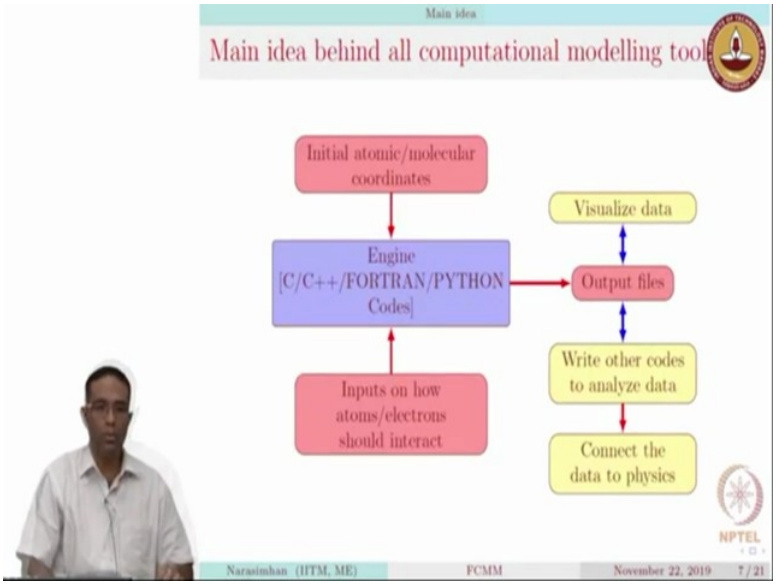
Statistical mechanics is a very deep subject on zone and one can take several courses in order to understand this deeply, but the purpose of having statistical mechanics here is only to see how we can connect some theoretical formulation to some computational technique, basically, the theory of statistical mechanics to the computational technique of molecular dynamics and why I am trying to convince you why molecular dynamics simulations actually work. So, that, that is the reason why we have this brief overview of statistical mechanics.

And then finally, we will have a basic introduction to molecular dynamics, followed by introduction to LAMMPS there we will teach you how to write some simple input files. So, before writing the input files, we will teach you some basic commands that LAMMPS already has and you should be able to generate these input scripts for very simple systems. And the same idea goes on to developing input scripts for complicated systems as well.

So, we hope that once you provide this basic background, you will be able to take it further and do more complicated things with it. So LAMMPS is actually a molecular dynamics simulation software. If you are not familiar with it, if you just Google up LAMMPS L, A, M, M, P, S, there is a two M there that is not a typo, you will be able to get into the website of LAMMPS and try to, you can try to read up a little bit as to what it does. Of course, we will be giving more deeper introduction to LAMMPS when we actually reach that part of the course.

Okay, so we would not be able to run some simulations, analyze some of the data and visualize the results. But that being said, you need to also understand that this is only an introductory course there are so many things that can be done with molecular dynamic simulation software. We will not have the opportunity or the time to explore the entire gamut of problems which can be dealt with using LAMMPS. So, but however, I do believe that the foundations that we provide here will help you understand things on your own by reading the documentation.

(Refer Slide Time: 13:23)




So with that, I think I have covered the basic introduction that we have for this course. Now, I would like to talk a little bit about the general philosophy based on which several computational modelling tools work. Specifically, the manner in which we have is we, the manner in which it works is there is something that I call as the engine which is basically a C or C plus plus or Fortran or a Python program that is written to us, there is written and given to us or we could write them but you know, the purpose of this course is not write codes is to use this code called LAMMPS.

So, imagine LAMMPS or any other computational software to be this engine and you need to provide some inputs to this code. And the basic inputs are two things, one is how are the atoms arranged in the material that you are talking about, so we are talking about atomistic level computational tools. So, we need to provide the positions, velocities or molecular coordinates as inputs to these, to these codes. And then we need to tell how these atoms or molecules are basically interacting with, interacting with each other, these are the two basic inputs that you generally need to provide to this LAMMPS.

And in addition to that, the engine by itself will have certain capabilities where you are able to tell what needs to be done with the input that you have provided. For example, you might want to change the temperature of the system From 10 K to 300 kelvin, how to do that? So, there will be several commands that this, this engine offers or this software offers where you will be able to specify these things in an input file and then you do something called as a running of the input file.

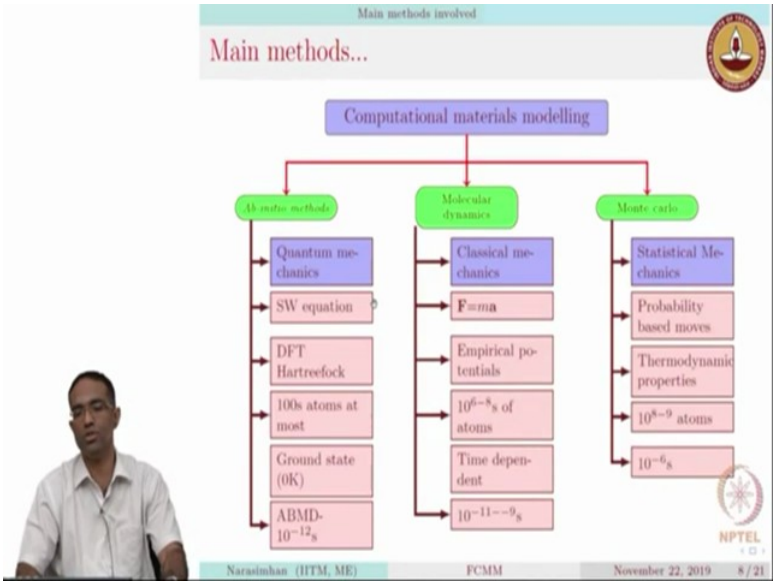
So you run the engine with this input script that you are provided and the engine as actually provides you with some output files. And you will be actually either visualizing the data or you will write other codes to analyze the information that is generated by this engine or the software or the code that you are basically using, okay. But that does not end you have to connect it to the underlying physics that the, that you are looking for, right. So, this is the general idea behind almost all Computational modelling.

So we are talking about a molecular dynamic simulations, then you will have to say give it how the atoms of the crystal structure are actually arranged. Say for example, if you are talking about copper, if you want to analyze copper, you will have to specify the positions of the copper atoms in the unit cell and tell how many times the unit cell is being repeated in the x, y and the z direction so that you have reasonable sized simulation box that would essentially consists of the positions and not always but sometimes the velocities of all the atoms consisting your simulation box which is there in the simulation box.

But it is not just enough to give the positions you also need to tell the system how the copper atoms are going to interact with each other. That means when the copper atoms are coming close together, how is the energy of the system increasing? If the copper atoms are going away from each other, how is the energy of the system changing? So these, this sort of an input is also needs to be provided for molecular dynamics simulations, and this is which is what is our focus in this course.

For other times, types of simulations software, which deal, which deal with, which deal at a much lower scale, for example, Ab initio calculations, where you will also be dealing a little bit with not a little bit you will also be dealing with electronic degrees of freedom in addition to atoms, you also need to talk a little bit about how the electrons are actually arranged around the atom or the ion in some specific manner. And you also need to give some inputs to talk about how these electrons are actually interacting with each other in various ways. So that is not the focus of this course, we will only talk about molecular dynamics simulations here.

(Refer Slide Time: 17:49)




But while, while I said that it is a good idea to know the differences that is existing between molecular dynamics, Ab initio calculations and something called as a Monte Carlo simulation. These are the broad, three broad categories of computation materials modelling, we will be dealing with the central one which is molecular simulations.

So let us start with the Ab initio method. Ab initio means from the beginning. Basically, you have to solve these Schrodinger wave equation in Ab initio methods in some approximate form, okay. So the foundations that is required for you to understand as to how this method works is quantum mechanics, okay. So, density functional theory is an approach by which you can actually solve the Schrodinger wave equation and is a numerical, basically it is a numerical method or technique by which you can actually solve the Schrodinger wave equation.

It is, since it has a large number of degrees of freedom, including both atomistic, atomic and electronic degrees of freedom. You will have, you can probably deal with at most hundreds of atoms in this particular technique. And generally people deal with only the ground state, which is a zero Kelvin or the zero temperature state when they are looking for various properties using these methods and there are methods which combine a little bit of molecular dynamics simulations and Ab initio methods called as Ab initio molecular dynamics. And there since, there is some dynamics since the temperature is not 0 K and there is some finite temperature, the atoms are actually oscillating about their mean positions. And it is possible for you to deal with a timescales in the order of a few picoseconds.

So, in summary, for Ab initio methods, the foundations that is required as quantum mechanics. You solve the Schrodinger wave equation or I, or you use an approximate method, a numerical method such as the density functional theory in order to solve the Schrodinger wave equation because you are dealing with atoms and electrons together, you have a large number of degrees of freedom and consequently the total size of your system will be in the order of may be 100 or 200 atoms.

But several property, for several properties, it is sufficient for you to have these many atoms, for example, the formation energy of an isolated vacancy or the amount of energy that is required to… for atom to make a jump from one lattice to the other. So, for such properties Ab initio calculations provide extremely accurate and reliable calculations in order to get these numbers.

However, like, like I mentioned before, if it is just Ab initio calculations generally people use the ground state of the material, which means the atoms are not at a finite temperature they are not oscillating about their mean position, mean positions. However, methods such as Ab initio MD combines a little bit of molecular dynamics and quantum mechanics or Ab inito techniques where they allow the atoms to actually vibrate a bit.

But even here, the degrees of freedom, number of atoms or the number of atoms and electrons that need to be taken into account is a large number, you generally are not able to deal with more than a few hundred atoms with existing computational resources, and deal with the temperatures beyond a few picoseconds.

Molecular dynamics simulations on the other hand, are classical the word classical often refers to the fact that we solve a Newton's laws, Newton's equations of motion in order to track the positions and the momentum of all the atoms comprising the system. You do not use, you use what is referred to as empirical potentials, which is to be viewed as some sort of a nonlinear spring that is connecting the atoms together, so that the, the entire system stays together.

So you need to connect them in some way so that they are staying together. So, these are called as empirical potentials or inter atomic potentials. Because we do not have electronic degrees of freedom associated with molecular dynamics simulations in general and we are solving the classical, we are solving the classical Newton's equations, it is possible for us to

deal with a huge number of atoms, for example, people have done from million to hundred million atoms simulations using a molecular dynamic simulations.

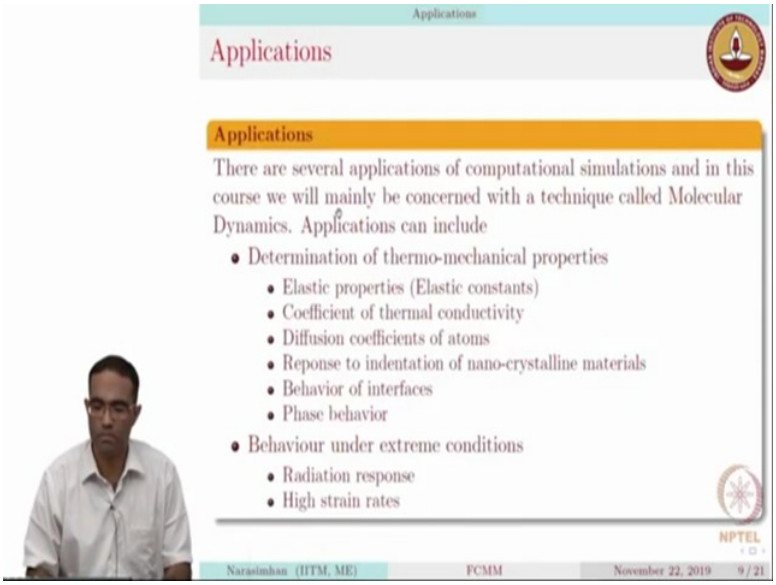
Molecular dynamics as the word implies dynamics it is time dependent, which means you can capture the finite temperature behavior of the systems. So, if you are going to simulate a piece of copper at 300 Kelvin, you will actually see these atoms vibrating about their mean positions at the temperature.

So, since the number of degrees of freedom was a little bit more, can be handled a little bit better than what Ab initio handles, so it is about ten power minus eleven to ten power minus nine seconds can usually be captured using molecular dynamics simulations that is close to a nanosecond which is still on the higher end. So is usually typically the timescales or the order of few hundred picoseconds for molecular dynamics simulations.

For Monte Carlo simulations, the foundations is still a statistical mechanics, of course you need some statistical mechanics, also to understand molecular dynamics simulations. But instead of explicitly moving these atoms based on by solving Newton's equations, they are based, the moves of these atoms are based on some probability. And it is possible for us to get several thermodynamic properties of the system.

And because you are not explicitly integrating the equations of motion like you do in molecular dynamics, it is possible for you to have a slightly larger number of atoms and explore slightly larger timescales in Monte Carlo simulations in connection with atomistic calculations. Monte Carlo simulations can also be used for several other things. So, these are the main classifications of various tools that are generally used for computational materials modelling.

(Refer Slide Time: 24:29)




There are several, so, let us now talk a little bit about before going into talking about how we actually build these crystal structures or how statistical mechanics connects the microscopic properties of matter and why to macroscopic properties and why molecular dynamics simulations work. It is a good idea to take a look at some examples of, from existing research articles to see how people have used molecular dynamics simulations in their research work and what sort of information they are able to get by conducting MD molecular dynamics or MD simulations, so to speak.

So, molecular dynamics simulations can be applied for a wide range of, to get ideas on wide range of properties, some of them are determination of thermal mechanical properties such as the elastic properties for example, you could get the elastic tensor, elasticity tensor of a given piece of copper or any other metal for that matter and get the elastic constants of the material. So, instead of performing an experiment you may be actually able to conduct a simulation to get a ball park value for these, for these constants which may be used in finite elements simulations for example.

You can get the coefficient of thermal conductivity of a given material provided certain conditions are satisfied, you can get how fast atoms are actually diffusing in a given metal, in a given material and this is extremely important to understand concepts such as a segregation and several other issues and material and also require these diffusion coefficients are basically you can actually look at inundations. So, I will show you some examples in a little bit what sort of inundations studies have been carried out in order to understand how certain

ceramics behavior, behave when they are subjected to inundation. Now nano crystalline ceramics behave in your, when they are, when they are subjected to Inundation.

Then you can also talk a little bit about or obtain information on phase behavior, what different phases of a given materials can exist and what are the conditions under which one phase can actually transform to the other and understand the thermodynamics of these different phases is also possible using molecular dynamics simulations.

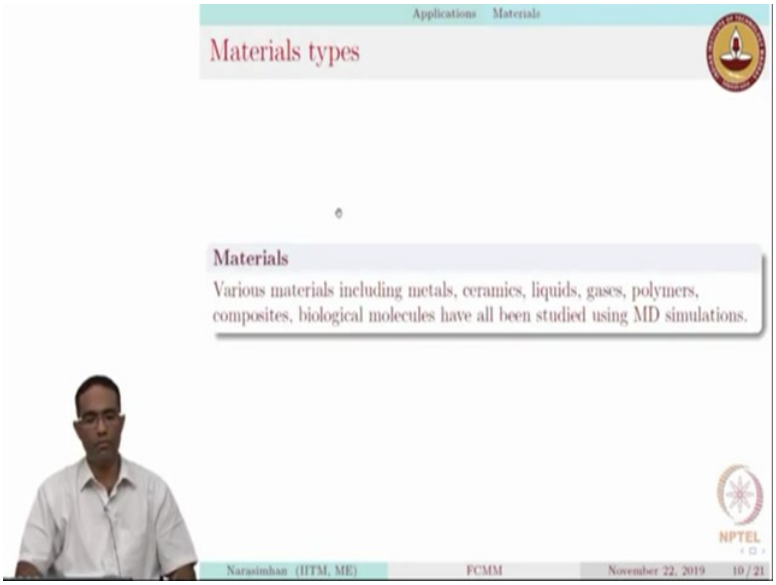
In addition to these properties, we also can study extreme conditions. One of the examples that I have already gave you is looking at a radiation damage behavior of materials. So, radiation damage. So, for example, if you look at materials being placed in the nuclear reactor they are constantly subject to radiation. So, when I say radiation damage, it essentially means an ion or an atom or a neutron coming and hitting the material say the structural material which is holding the nuclear fuel for example.

And this particular material, the atoms in this particular material displace from their original positions because of this bombardment and a large number of point defects like vacancies interstitials are going to be generated and over a period of time, these vacancies and interstitials actually degrade the materials properties.

So, radiation response is one very effective is a good example where molecular dynamics simulations is extremely useful because the timescales in which the point effects are actually generated and the timescales in which molecular dynamics simulations function are compatible. So, these results could actually be very useful to get an insight as to what is happening at the atomistic level.

Then you can also perform high stranded experiments that are usually not possible in practical situations. You can pull the systems at various rates, for example, and to get how strain rate is actually affecting the mechanical behavior. However, one should understand that the strain rates that are generally obtained and molecular dynamics simulations could be unrealistic and one needs to make a very careful, one needs to perform a very careful analysis to connect the results that is obtained from molecular dynamics simulations to experimental data, right.

(Refer Slide Time: 29:10)




So, that being said, various types of materials are currently being, you can, are being researched when it comes to molecular dynamics simulations, people have looked at metals, ceramics, liquids, gases, polymers, proteins, composite materials etcetera have all been studied using MD simulations. This course will generally look at some examples of ideal gases, metals and a simple example which uses ceramic.