Foundations of Computation Materials Modelling
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Some Application of MD Simulations

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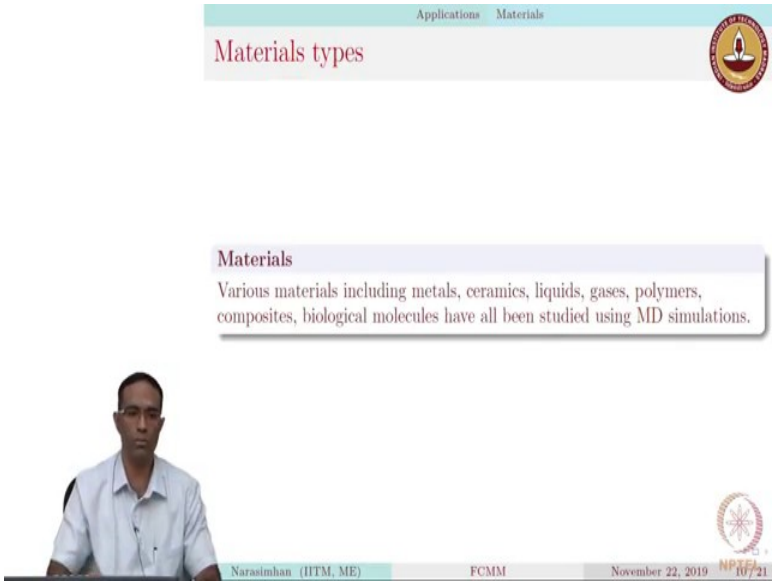

Good morning. So, let us continue from where we left of. So, today I just want to introduce a some applications of molecular dyna mic simulations just to tell you in what way this particular tool has been used for various research activities. So, the first, these examples that I am going to show you are from research articles, IIT Madras has an subscription to some of these articles and these various figures and tables and videos will be shown in order to just introduce you to the kind of things people have done using molecular simulations.

However please note that it is not required for you to actually have these articles in order to answer question in the assignment or in the exam this is just to give you a flavor of how what sort of things people can do with the molecular dynamic simulations.

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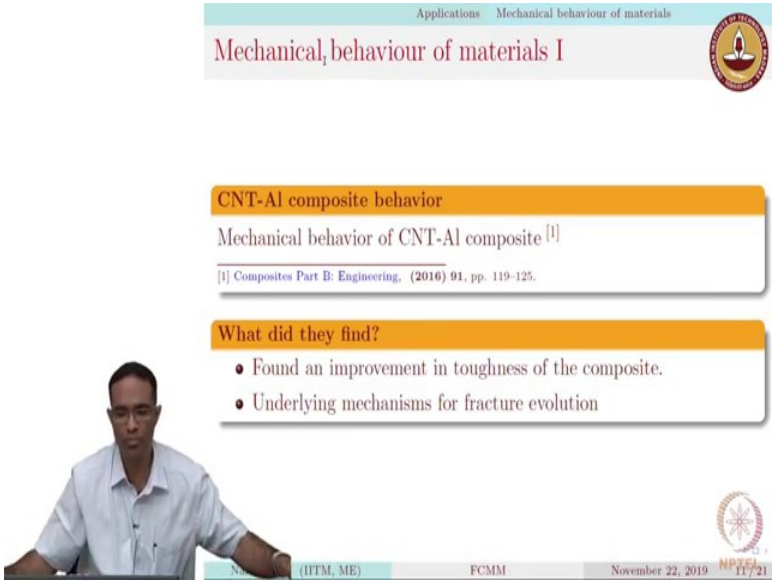

So, the first example that I am going to show concerns the mechanical behavior of CNT aluminum composite. So, it is very clear it is very clear that carbon Nano tubes have played a very important role in improving several properties of materials and mechanical properties is one of among them and in this particular article which is there in composite B the authors have actually use molecular simulations in order to see what happens when you put carbon Nano tubes inside an aluminum matrix and examine the toughness and the elastic properties of this composite material.

So, it is a good idea to actually take a look at what they have done. So, I am going to just open up the article from that.

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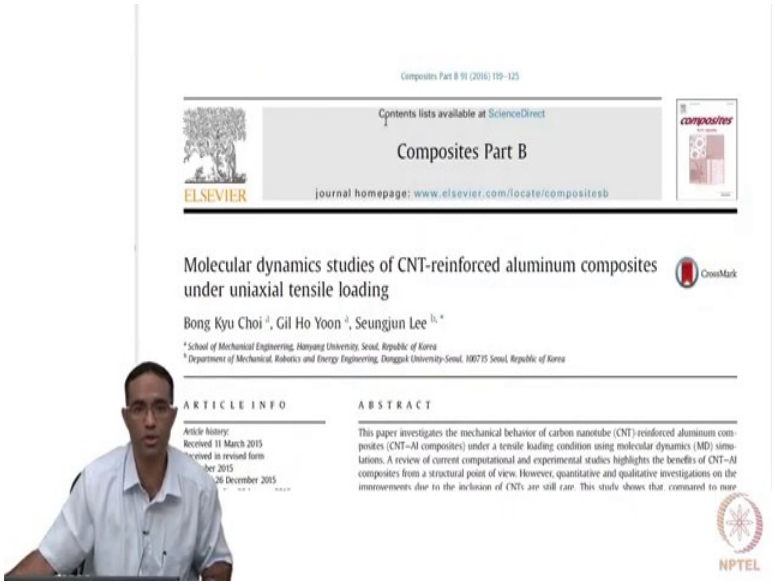

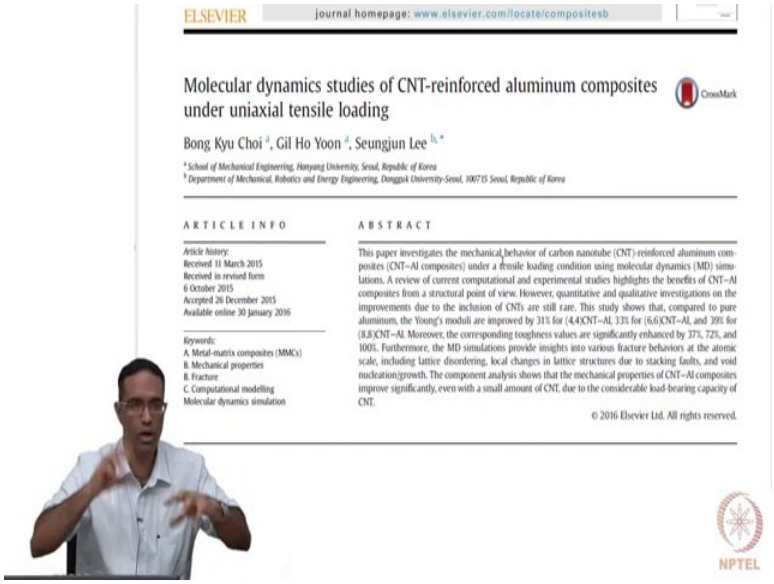

This is the article here. So if your university actually has the subscription to this Journal please take a look at this particular article it is extremely interesting. So, the paper basically investigates in a mechanical behavior of the composite material where they put carbon Nano tube they want to put carbon Nano tubes and in aluminum matrix and change the type or size of the carbon Nano tube, perform an axial test to examine in the mechanical properties, in particular young modules and the toughness of the composite material.

So, if you take a look at the abstract the brief in brief the what if they find after they performed this analysis they were able to conclude things such as saying that the Young's modulus of the composite material improved by nearly 31 percent for a particular type of carbon Nano tube 33 for the other and nearly 39 for the third different types of carbon Nano tube. They also found that the corresponding toughness values of these composite material was significantly different, when compare to the aluminum itself.

So, in this manner molecular dynamic simulations can be used in order to examine the mechanical properties or the qualitative feature exhibited by materials when different modifications are actually done to that.

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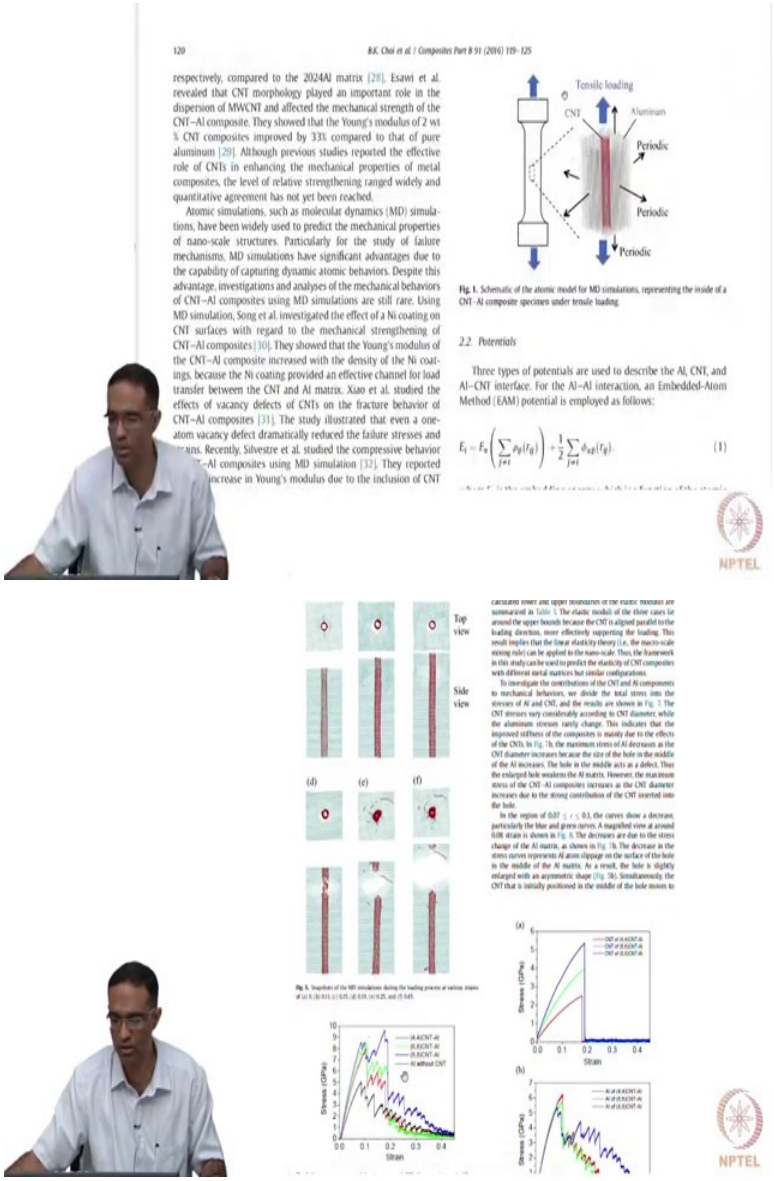

So, in brief what did they do, they basically simulated a small portion of a dog bone specimen, a dog bone specimen is basically an example you do not really do the entire dog bone specimen in MD you do a small portion of it. So, assuming that this is the small portion that they have taken and you see the behavior right here in figure 1 where the carbon Nano tube is right in the center and it is surrounded by the aluminum matrix.

So, they have to give proper interactions existing between the carbon Nano tube material just basically carbon and the aluminum atoms and of course between aluminum and also between the carbon atoms and once they are able to once, they give this sort of interaction and the perform a tensile test using molecular dynamics simulations. You are essentially able to plot something that looks like a stress strain diagram for various combinations of carbon Nano

tube and aluminum and conclude or what happens to the elastic properties and what happens to the overall toughness of the entire material.

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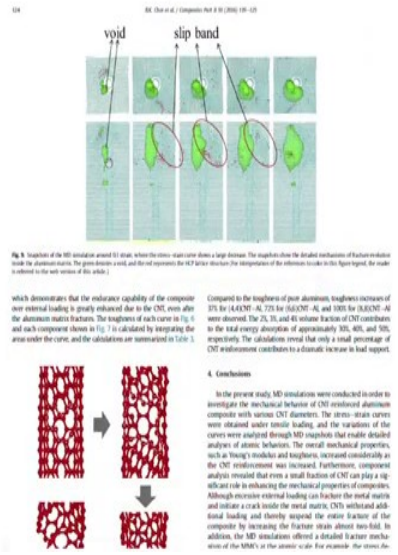

Not only do they actually have these conclusions on Young's modulus and the toughness but if you look at figure 5 and also figure 9 here, they are able to say something about the fundamental mechanisms that is actually governing the matrix failure when they look at the atomistic behavior of the material. So, they are able to show that there are void that are going to be formed and slip bands that actually are generated when such and how these thing vary in the presence of this carbon Nano tube are also discussed.

So, in this manner it is possible for us to look at atomistic level features in order to explain some of the observed macroscopic properties such as changes in the Young's modulus or changes in the elastic, or changes in the toughness of the material. So, this is one application where we talk about the mechanical property variation. So, now let us look at something else.

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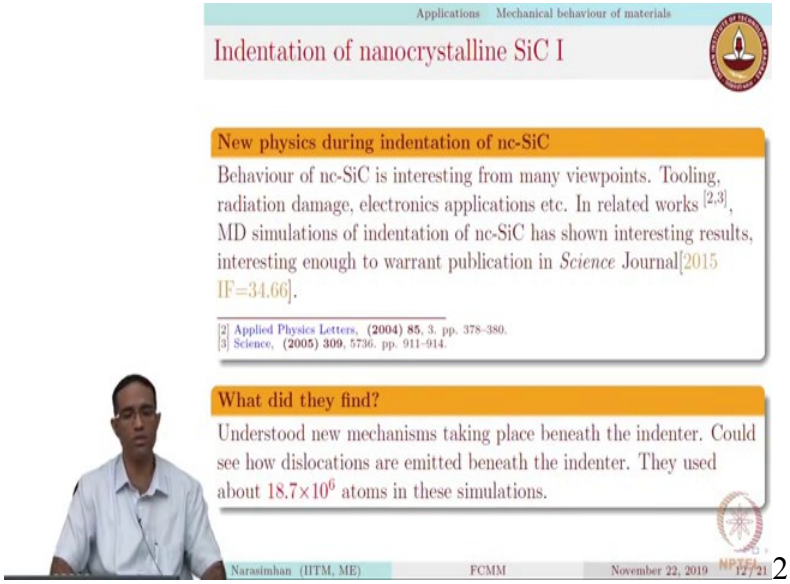

So, that was with respect to metals, now I will show you and example with silicon carbide which is essentially ceramic. So, as you all may be knowing, Nano crystalline materials are have several interesting properties and Nano crystalline silicon carbide is particular interesting because it has, it is expected to have high resistance to something called as radiation damage, further more it is useful for electronic applications and is also used for as a tool in order to, for machining purposes.

Now when you have Nano crystalline silicon carbide some of these properties are expected to be enhanced. So, in related works which is there in these two articles “Applied Physics Letters” and “Science” MD simulations of Nano crystalline silicon carbide have shown very interesting results and they..., it is not..., that the previous example that we saw was a single crystal aluminum and you had piece of carbon Nano tube in between but this particular “Science” paper actually deals with constructing Nano crystalline silicon carbide. So, I will show you a few picture from paper, they have several different grains in their samples in their MD simulation each grain consisting of atoms, array of atoms which are oriented in different directions and they perform an indentation test on this sample and they try to understand the load displacement response and conclude on various fundamental physics as far as this particular material is concerned.

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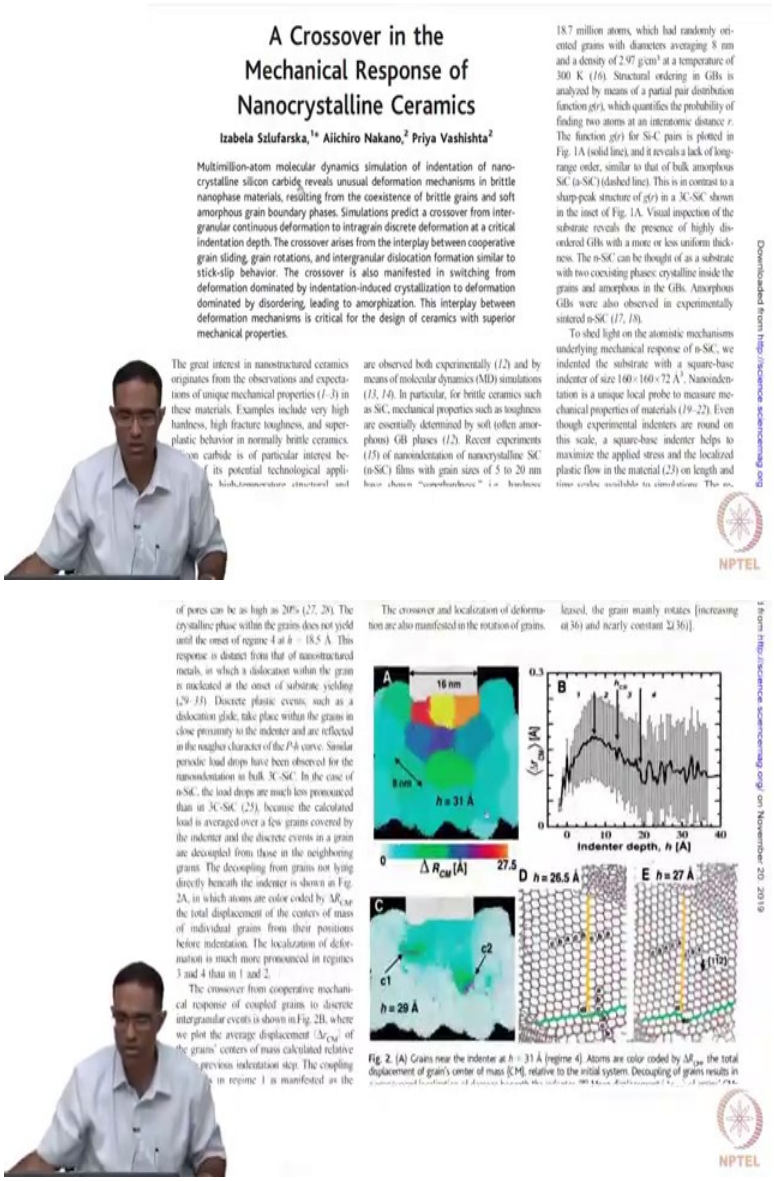

So, let us take a look at this, this is a paper, "Science" paper. So, I will show you some pictures which is representing the kind of simulation system that they are using. So, these are the, this is your Nano crystalline silicon carbide and they have used several different grains each of this grains are actually colored differently and you can see the indenter right here, I am pointing to the indenter over here and when they performs indentation you get a low displacement graph and from this low displacement graph, it is possible for us to look at several features of the material.

So, good idea to actually take a look at this book if you are having subscription to if you are able to get hold of this particular paper, you can take a look at this article. So, in this manner, it is not just a single crystalline material that one can actually deal with in molecular

simulations, but it is also possible to construct Nano crystalline materials and look at their behaviour.

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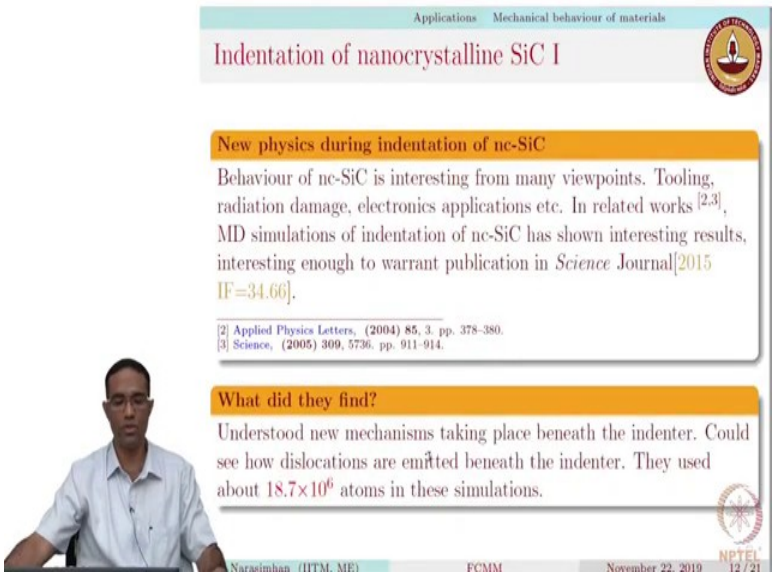

So, in this article primarily they found that there are new mechanisms that are taking place beneath the indenter and they could see how dislocations are actually emitted beneath the intent. Of course this dislocation emission is more clear in the "Applied Physics Letters" paper.

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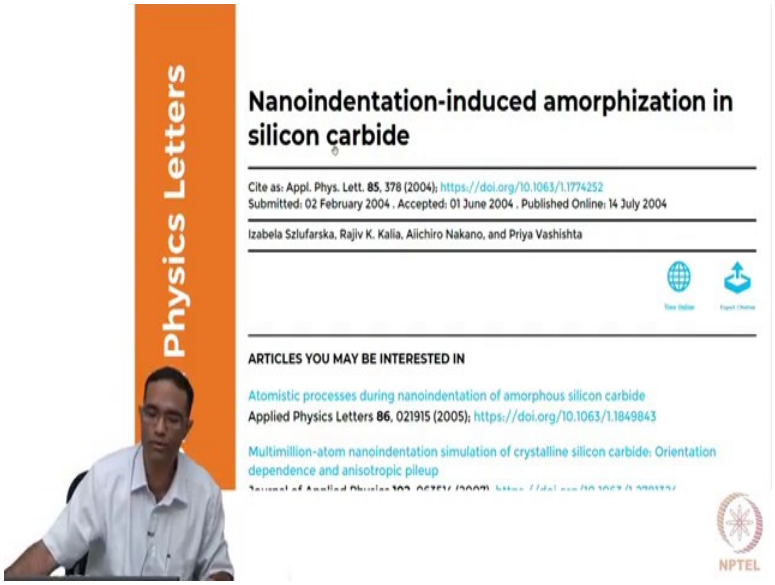

This is the Nano indentation induced amorphization and silicon carbide.

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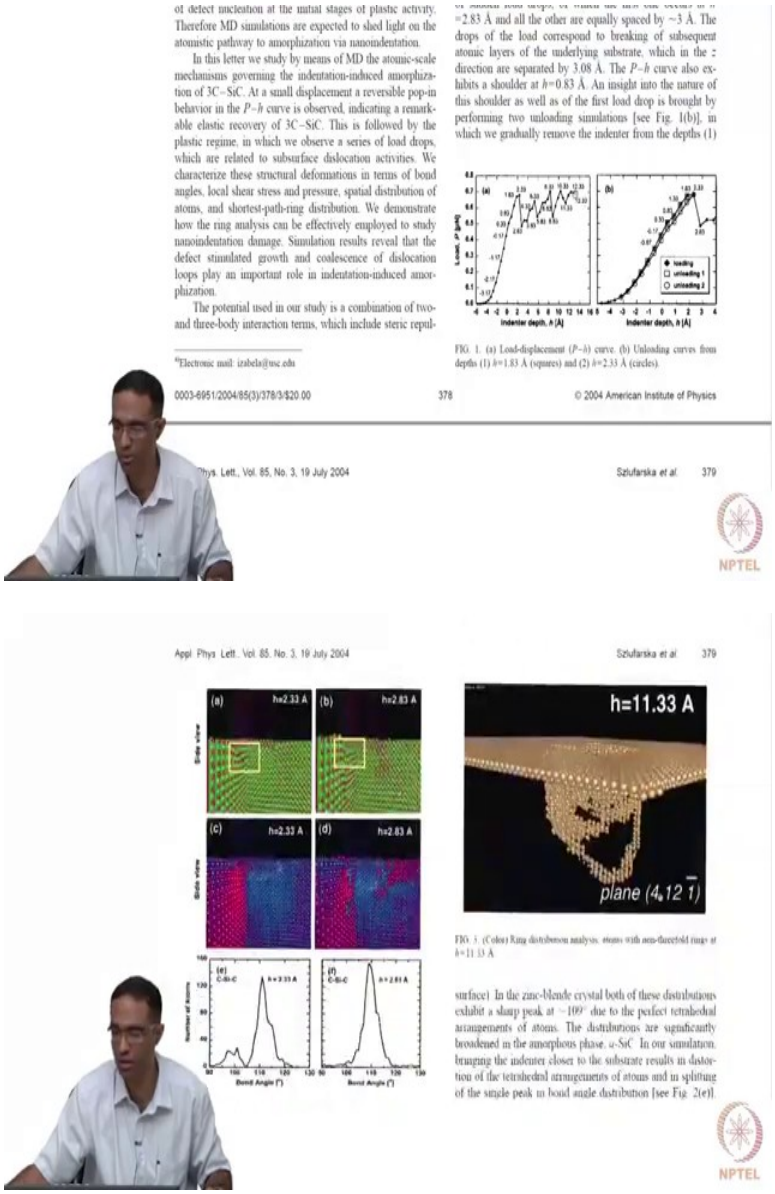

So, this is the load displacement plot with they have and this is of course not really a Nano crystalline material that they have used, they have used a single crystalline material but on performing indentation they have marked these atoms which are deviating from their normal behaviour, and they are able to look at the manner in which these dislocations are actually emitted beneath the indenter when they intended ceramic materials such as silicon carbide.

So, this is an example showing the mechanical behaviour of ceramic material. And another thing that I would like to point out is that the "Science" paper that I just discussed here uses, uses atoms in the order of about 20 million for performing these simulations as you can see some their grains are quite large in the order of about eight Nano meters. So, actually quite large when you consider this to be atomistic simulation.

So, the total number of atoms that they had were about 20 million atoms which is huge. So, Some of these simulations can be expect to take a very long time to actually complete and therefore you must be careful enough to set your input files in a manner so that if a job dies in between you should be able to restart it from the point where it actually stopped. So, some of these things are extremely important and another example that I would like to point out is in manufacturing.

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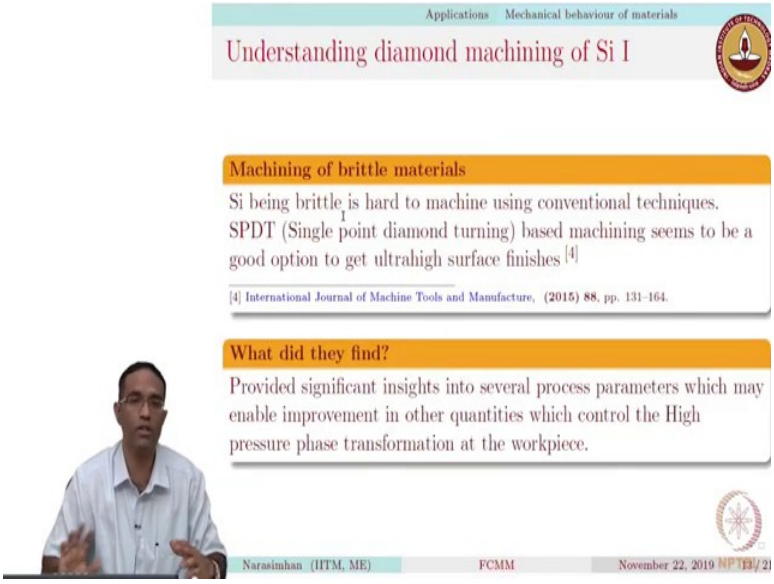

So, like I mentioned in the previous class what is important about MD simulation is to see if you can get some qualitative insights into the material behaviour and not always worry about the matching of the numbers between your experience and your simulations. So, one such example is actually machining of brittle material. So, silicon being a brittle material, it is hard to machine using conventional techniques, just it's too brittle.

A single point diamond turning based machining operation seems to be a good option in order to machine and get ultrahigh surface finishes in these materials. So, there is a paper here "International Journal of machine tools and manufacture". So, this is just to point out that molecular dynamic simulations is also being used in manufacturing area. So, it is not restricted to Material Science or mechanical engineering or in determining just thermodynamic properties, but it has been extended to several other areas as well.

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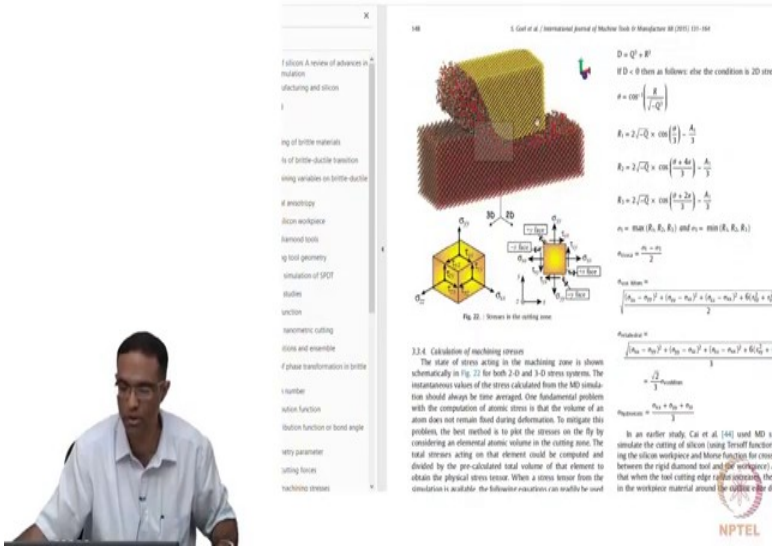

So, we can take a look at this paper here, which is there in the international journal of machine tools and manufacture. There is a lot of stuff which you can actually take a look at but mainly I would like to point out to this particular figure here where they have the substrate which is made of which is basically silicon and this is your Diamond Tool and that is essentially machining is entire material right here.

And the based, of course it is important to know what they find out. So, they found out that various process parameters can be changed in order to improve the manner in which the, the high pressure transformation takes place beneath the indenter which can actually enable improvement in other quantities that are related to manufacturing. So, of course these examples are very qualitative.

I do not intend to actually go through the entire article and tell you exactly what they did. This is just to provide a brief overview of what in what applications molecular dynamic simulations have actually been used by various people, by various researchers.

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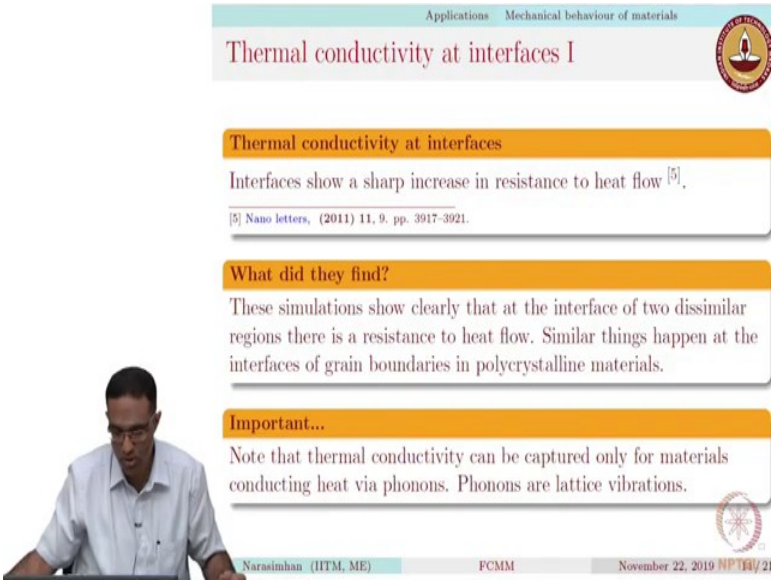

Another example, so, we saw some examples on mechanical behaviour we saw an example where MD simulation have come of use in manufacturing or in machining operations. Another example where it can be used in the thermal area is to determine thermal conductivity at certain interfaces.

You can determine the thermal conductivity of some materials even in the bulk phase. But what is interesting in this particular article that I am about show is a manner in which the presence of some interfaces change the manner in which heat flow or causes a sharp increase in the resistance to heat flow. So, this is actually from a paper "Nano letters".

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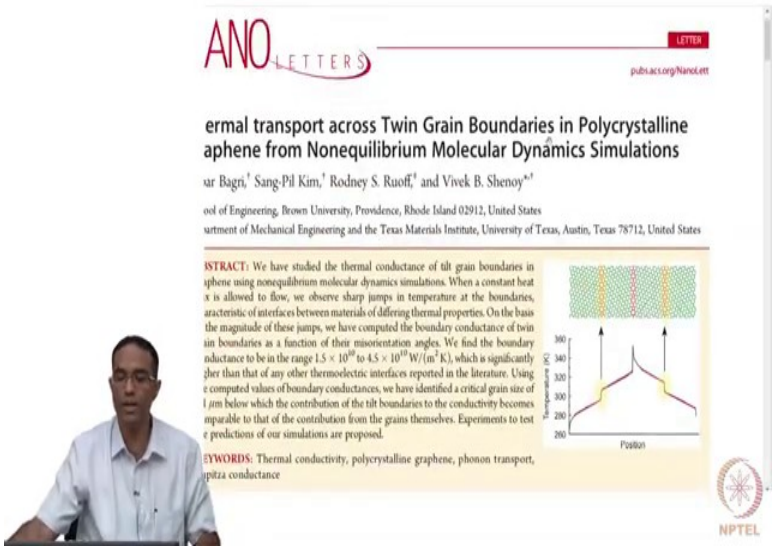

So thermal transport across twin Grain boundaries and Polycrystalline graphene from non-equilibrium molecular dynamic simulations. So, if you just take a look at this paper right here this figure right here in the abstract. So, they built atomistic models of graphene so this all graphene right here. And you see that the orientations of this side and the orientations of this side orientation of this side, orientations of this side are all different. Consequently You have some sort of a mismatch, between this differently oriented graphene sheets and it is interesting to know what happens when heat flows in such material. So, this is a plot of the temperature verses position across the, this distance and they see that there is a linear variation and temperature of position here. So, you can take the slope of this to relate that to your thermal conductivity, but at this particular point where grain boundary is existing, there is a sharp jump.

There is a sharp jump basically, indicating that there is some sort of a higher resistance to heat flow at these grain boundaries. It is possible, this has also been done not only on graphene sheets but also on other bulk materials with grain boundaries. So, it is possible for us to find out thermal conductivity as well. So, you can find a thermal conductivity of materials using molecular dynamic simulations.

And there are several different approaches to do that in this they have actually taken a direct approach where they maintain different temperatures in different regions in order to obtain that jump in the temperature profile and hence evaluate the thermal conductivity.

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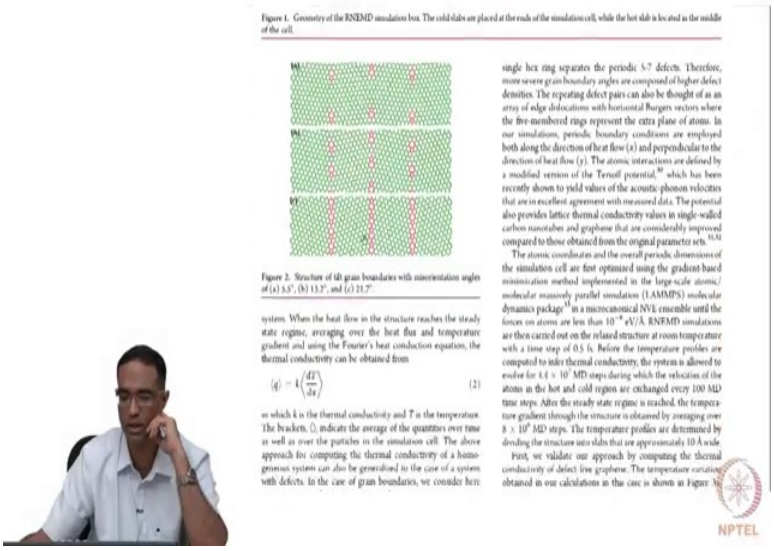

So, you can take more detailed look at this particular paper. If you are interested in calculating these aspects for your research work. So, that is an example where you calculate thermal conductivity with MD simulations.

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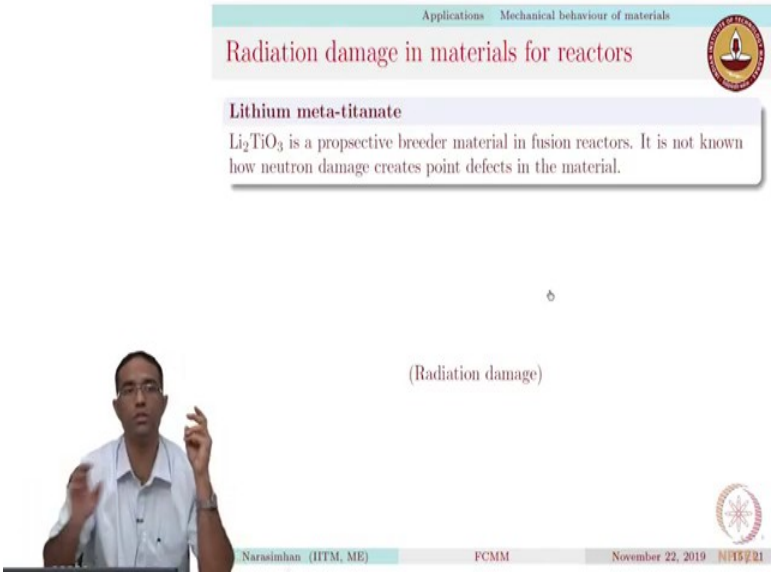

Another example where we have that we have molecular Dynamic simulations is in radiation damage of materials. So, in radiation damage, what happens is we are talking about materials which are used in nuclear fusion or fission reactors and simply because of the fact that there is a lot of activity in these reactors; ions, electrons and neutrons may actually bombarding the structural materials in these reactors.

And consequently when they are, when a material is being bombarded with high energy atoms, you create what are refer to as point effects. You may create vacancies, interstitials or antisites. And as these defects actually increase in number the thermo-mechanical properties of these materials are expected to degrade over time. So, it is interesting to know, how many such defects are going to be produced in the material.

So this is clearly an atomistic level phenomena and furthermore the time scales over which the cascade happens the process happens where the atoms coming and hitting and creating a few defects in material is actually in the same order of magnitude as it happens as you can track as you can capture using MD simulations.

So, this entire process generally happens in the order of a few tens of picoseconds in the real system and MD simulations are excellent and capturing phenomena that happens in few tens of picoseconds like I mentioned in the previous class. So, MD simulation is perfect for actually capturing these events which are referred to as primary damage events and I will show you some videos which.

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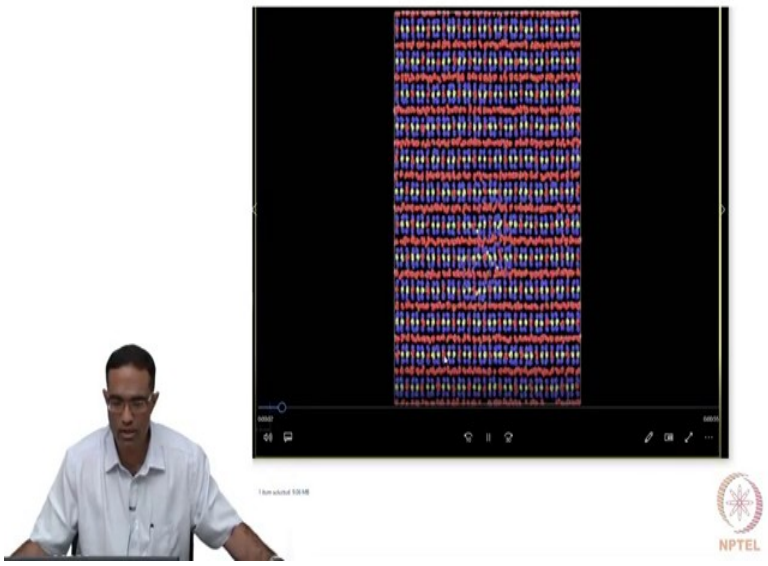

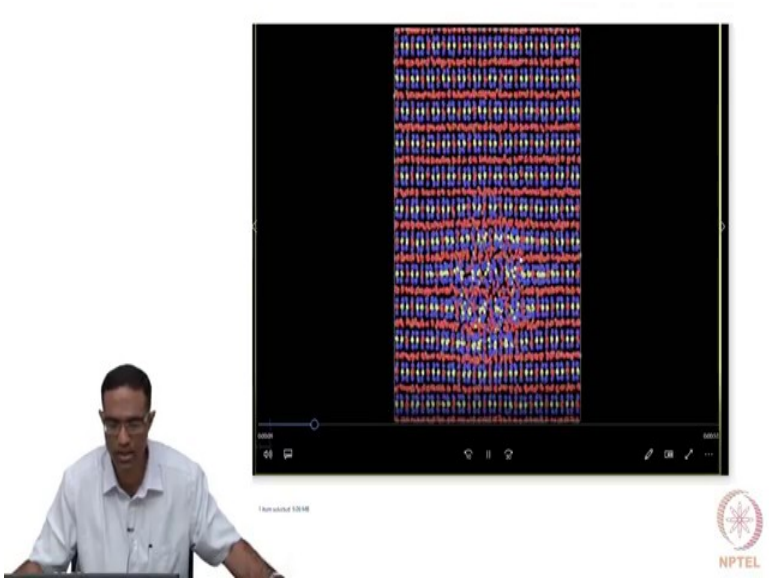

This is an example of a lithium meta-titanate, lithium meta-titanate and you can see one particular atom moving all of a sudden and creating a small cascade region here. This is a molecular dynamic simulations of this of this particular cascade event in lithium meta-titanate and it creates, wait you, you wait long enough and after some time you create a small region which consists of Point defects.Whereas the remaining regions surrounding it still crystalline or perfect crystal and what we are interested in is looking at how these point defects are evolving with time. And what is at the end of the cascade, cascade means the process by which the atoms getting bombards this particular material to create point defects.

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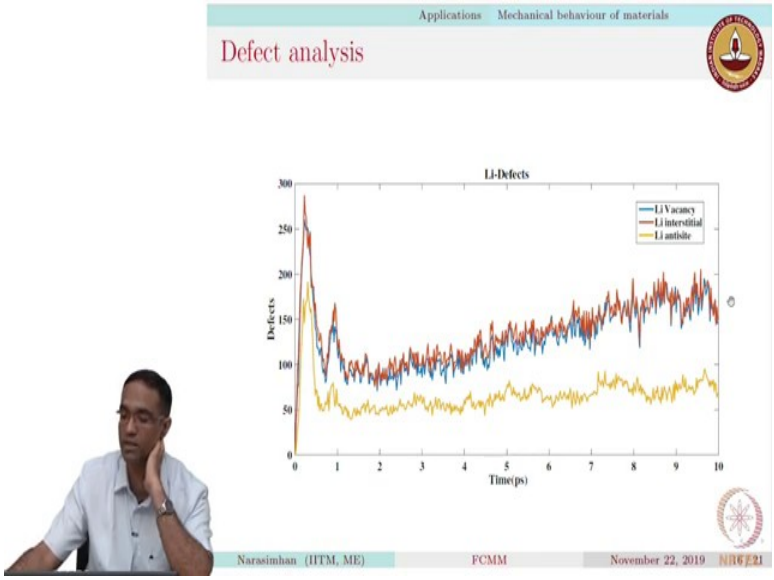

And we can perform some analysis on this to basically see how these point defects are basically evolving with time. So, For example, these are typical kind of plots that you may

get when you are looking at how these defects are actually generated over time. So, we see that the total time scale over which this entire simulation has taken place is about to 10 picoseconds and you can see some defects which are usually you just still increasing even after the cascade is completed.

Whereas some of these defects such as lithium anti sites are kind of settled down to more or less or constant value.

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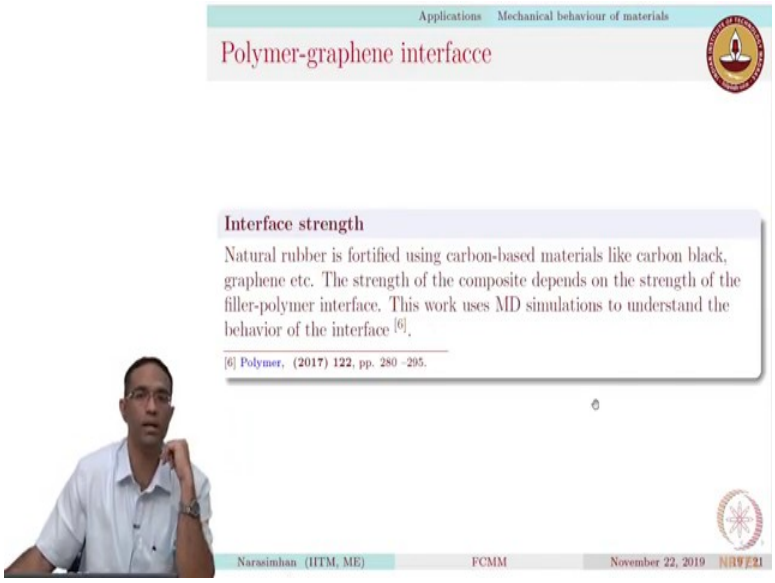

So, some of the results of this simulation is also you could also take it to a higher level calculations and perform further analysis on them.

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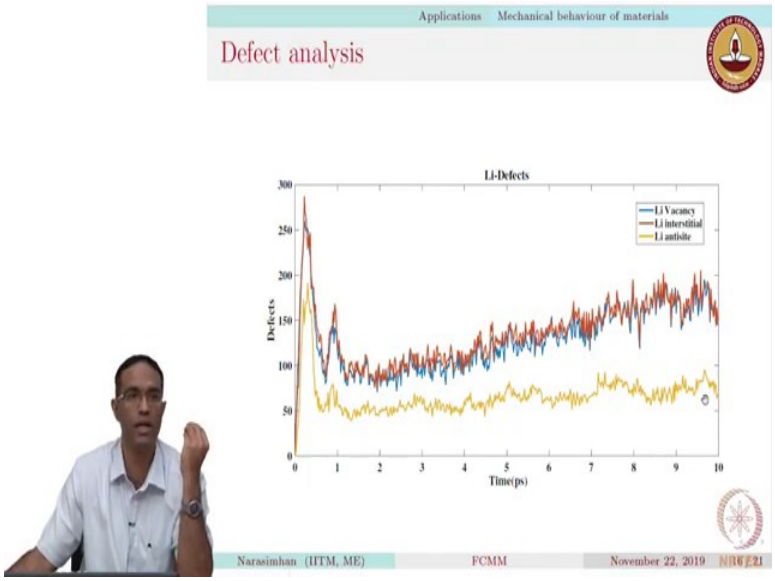

For example, the number of defects that is being generated during primary damage may serve as an input to something called as rate theory model where you could try to analyse what happens at even longer time scales when the defects begin to actually defuse.

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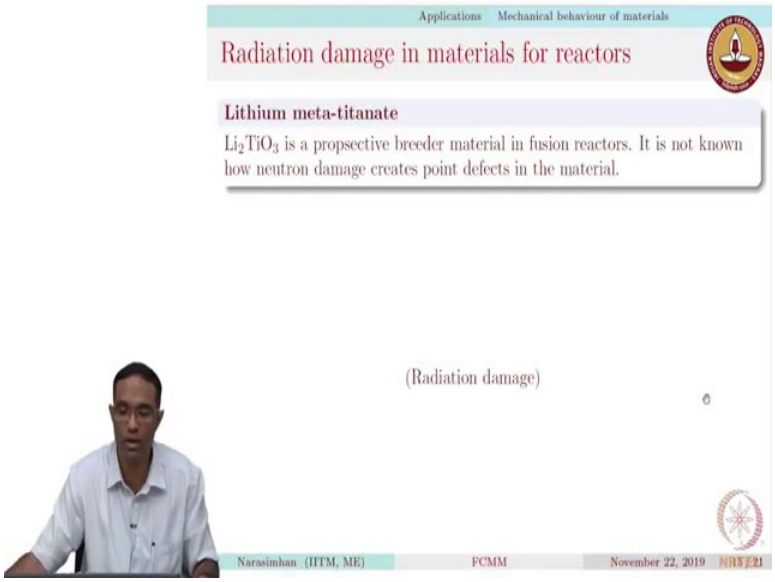

So, this is an example, another example where MD simulations have being used of late.

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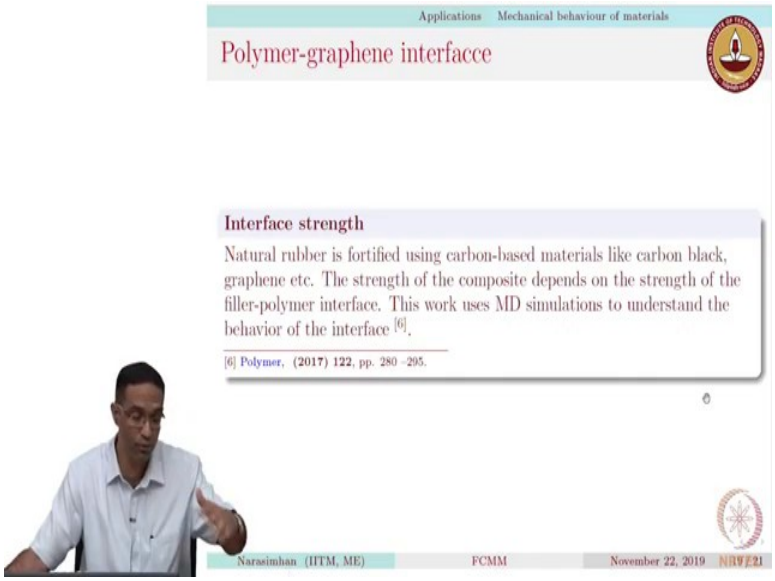

Another example now so far we are seeing some metal, some ceramics and so an example in manufacturing, but molecular dynamic simulations are also used in polymer simulations. And also protein simulations to understand various mechanisms related to protein folding and so on and so forth. One of the applications that we were interested in our group is looking at how natural rubber is generally fortified using carbon-based materials such as carbon black and its strength is generally affected by the strength, the carbon black has with the polymer surface.

So, in this work the carbon black was generally was modelled as a graphene sheet and a polymer was placed on top of it and we performed an extension experiments in order to understand how the system behaves at various rates of pullings. So, what was the interface strength at various rates of pulling and where the failure actually took place.

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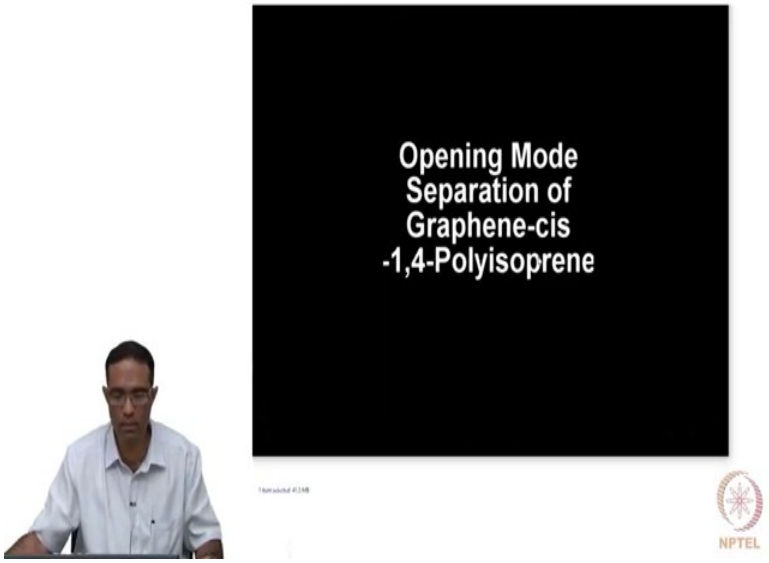
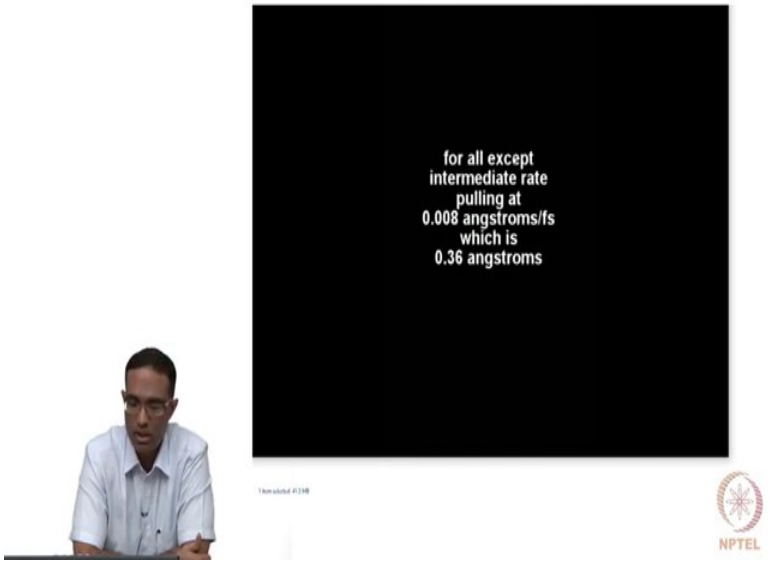
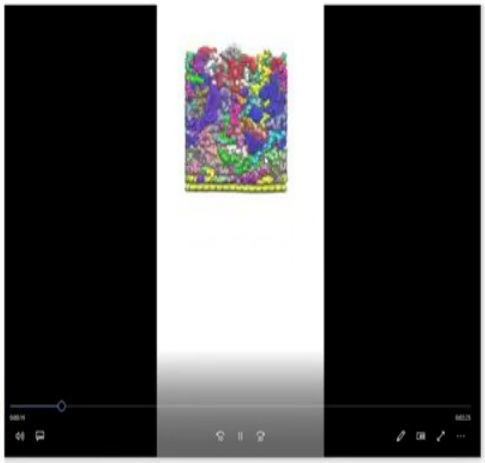
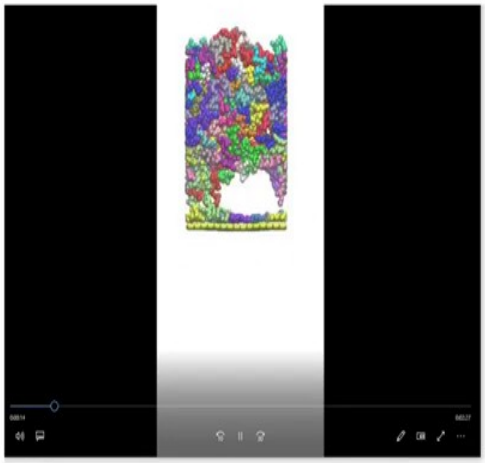


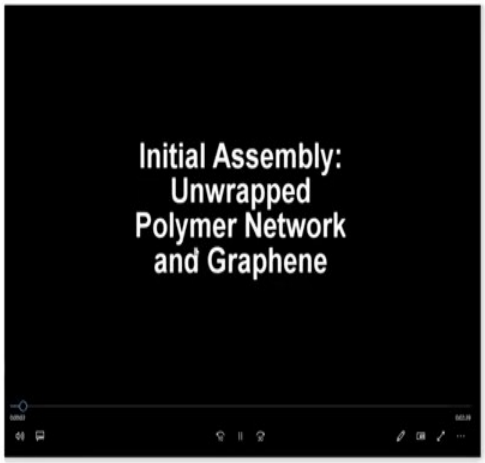



Separation made by
graphene between
two frames is
0.25 angstroms,






Equilibration
of Interface


Initial Assembly:
Unwrapped
Polymer Network
and Graphene


Separation at the
Intermediate Rate
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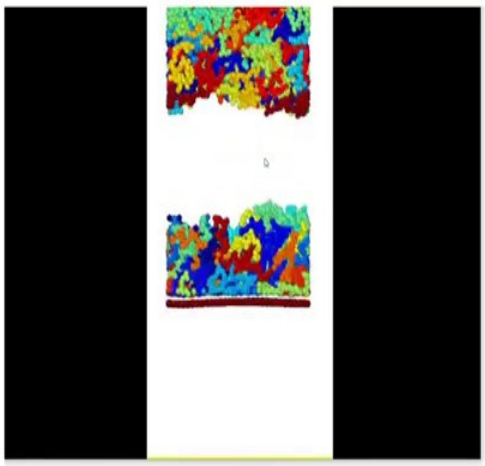
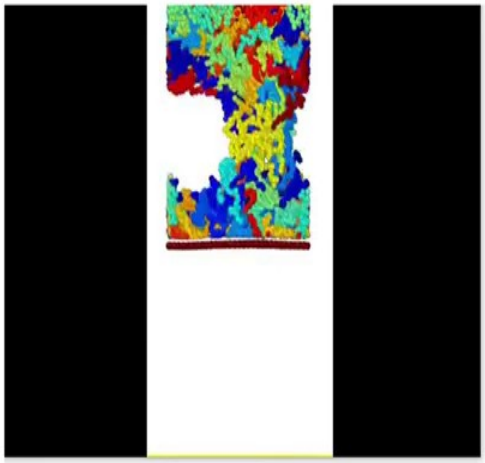
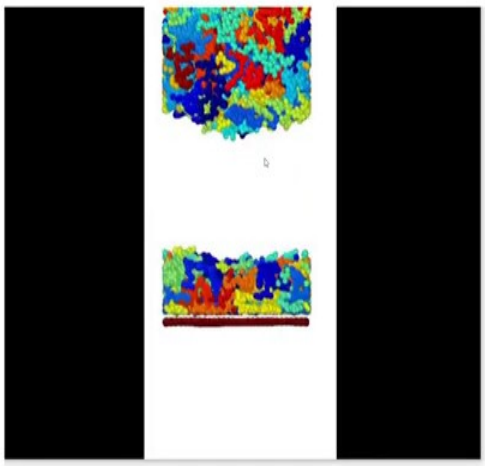
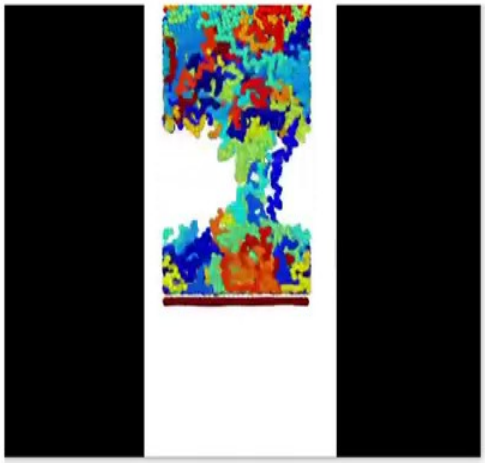
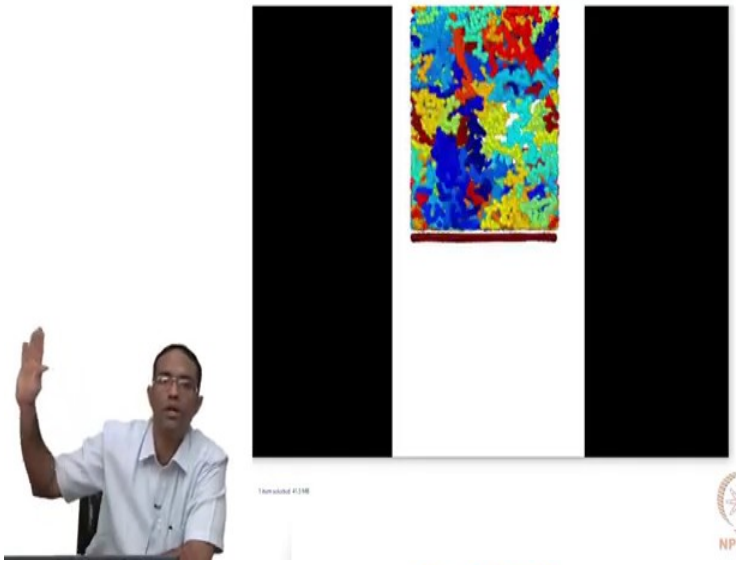


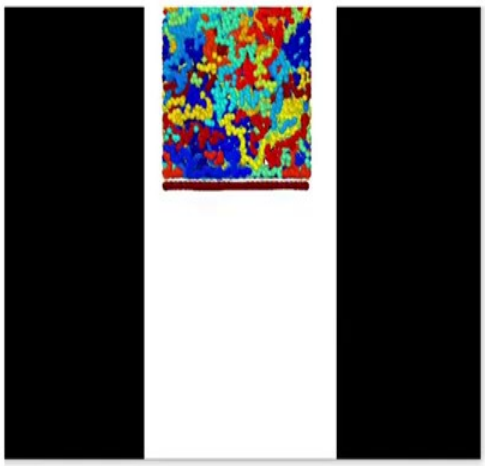


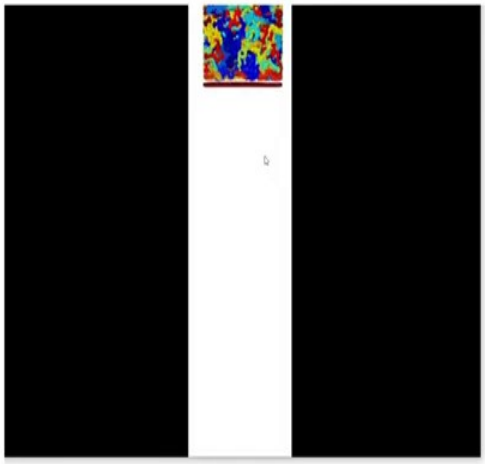

Separation at
the Smallest
Finite Rate

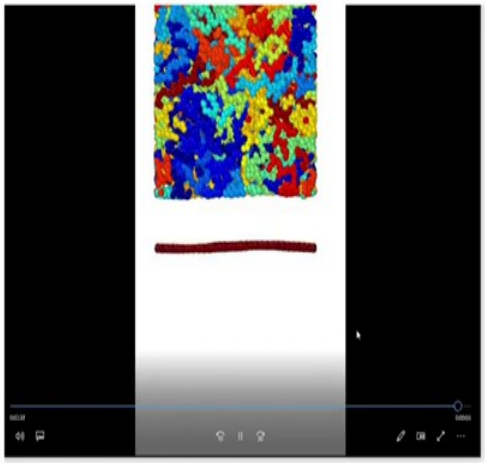




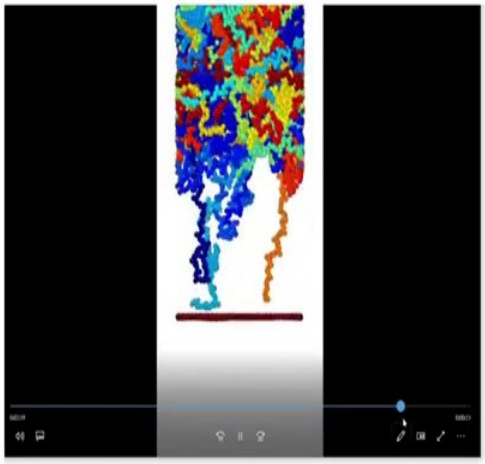









Rapid Separation



So, I will show you some examples of that. So, this is an example where we show opening mode of separation of grapheme, initial assembly of the unwrapped polymer do you see the polymer network that is right there right on top of it and the graphene sheet, which is there in yellow. That is how we started off the simulation and then we perform a small equilibration where the polymer and the graphene sheet both come together and you can see all these polymer items being vibrating.

In the next step, we made we separated the polymer from the graph feature at various rates. So, this is at extremely slow rate. So, the rate at which you are actually seeing this being pulled on the rate at which the simulations are being performed and may not look the same things have been rescaled so that the video appears in a reasonable within a reasonable time. So, this is at some specific rate and you see the power failure is happening somewhere in the middle of the polymer.

This is at somewhat at intermediate rates and that is the behaviour that you see with chains being pulled to a longer extent, slightly faster separation now at intermediate rates you see that there is more polymer chains that is being stretched. And some of them still being connected to the graphene surface over here. So, depending upon the rate at which you pull the polymer you see different behaviour, and that is what is being captured by these simulations.

And at extremely high rate this is at somewhat at intermediate rates and at extremely high rate what you see is the polymer does not have enough time to actually respond to the speed with which the graphene has been pulled and it behaves like a rigid block. Some of these concepts are very, are appropriate when you look at the visco-elastic behaviour of these polymers and qualitatively they match, so this is the behaviour that I would like to talk about when we this is what I wanted to talk about when we that I wanted to show the behaviour for the polymer material.

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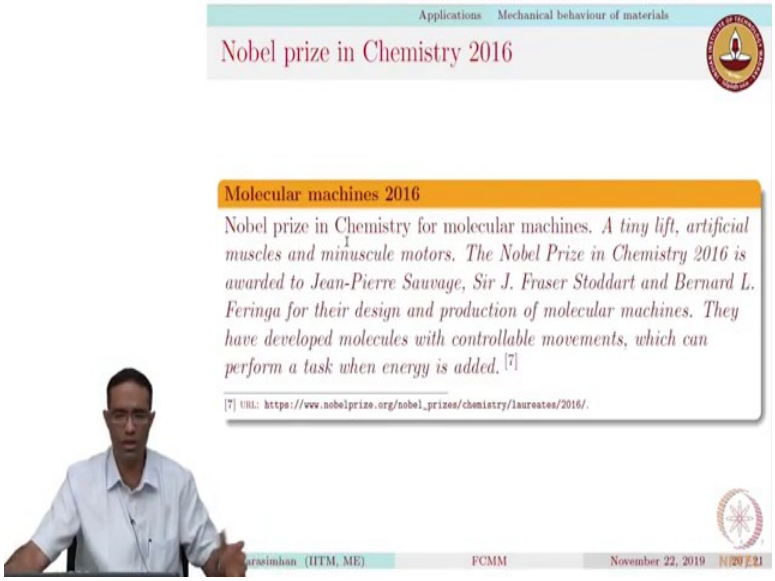

Another aspect that might be interesting is to look at molecular machines. So, Nobel Prize in chemistry for molecular machines was given in 2016. So, the nobel prize in chemistry was awarded to Jean-Pierre Savvage, Sir J Fraser Stoddart and Bernard L. Ferniga for the design and production of molecular machines. So, some of these machines have also been simulated on the, are also there on the internet.

You can find a few examples where molecular dynamic simulations are actually showing these behaviour. For example, I just wanted to show you some examples from the internet where people have made molecular simulations of this molecular machines.

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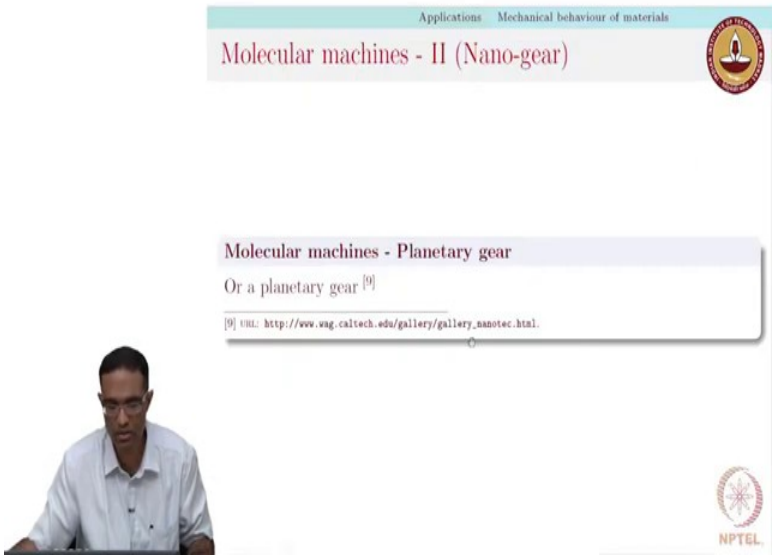

These examples can actually be found on this website right here. So, please take a look at this website. You will be able to see some very nice examples of molecular machines which have been built using molecular simulations, molecular dynamic simulations such as a planetary gear and is also fluid pump if I am not mistaken. So, these are some of the examples that I just wanted to give just to motivate this course and tell you how molecular simulations are actually useful.

Of course, the range of applications extends far beyond the simple examples that I have just pointed out so far and in this course being an introductory course, they may not be doing all these advanced applications. We will just learn how to perform some simple molecular dynamic simulations and connected to some physics that we are all familiar about but once you know that performing some of these calculations must also not be very hard, and we must be able to pick it up very quickly, with that I would like to conclude this class and thank you.