

Foundations of Computation Materials Modelling
Professor Narasimhan Swaminathan
Department of Mechanical Engineering
Indian Institute of Technology Madras
Some Application of MD Simulations

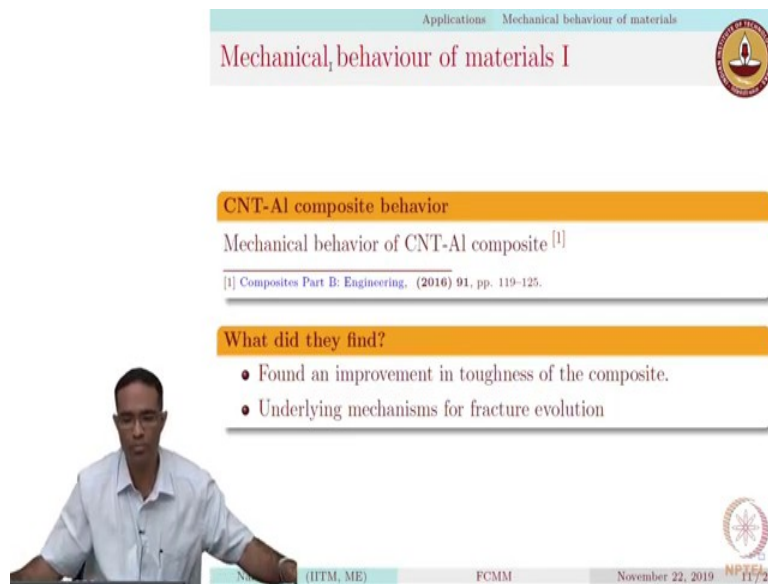
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The screenshot shows a presentation slide with a light blue header containing the text 'Applications Materials' and a small circular logo on the right. Below the header, the title 'Materials types' is displayed in red. A white box with a light blue border contains the text 'Materials' followed by a paragraph: 'Various materials including metals, ceramics, liquids, gases, polymers, composites, biological molecules have all been studied using MD simulations.' In the bottom left corner, there is a video inset showing a man in a white shirt. The bottom of the slide features a navigation bar with the text 'Narasimhan (IITM, ME)', 'FCMM', 'November 22, 2019', and 'NPTEL 10/21'.

Good morning. So, let us continue from where we left of. So, today I just want to introduce a some applications of molecular dynamic 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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Applications Mechanical behaviour of materials

Mechanical behaviour of materials I

CNT-Al composite behavior

Mechanical behavior of CNT-Al composite [1]

[1] Composites Part B: Engineering, (2016) 91, pp. 119-125.

What did they find?

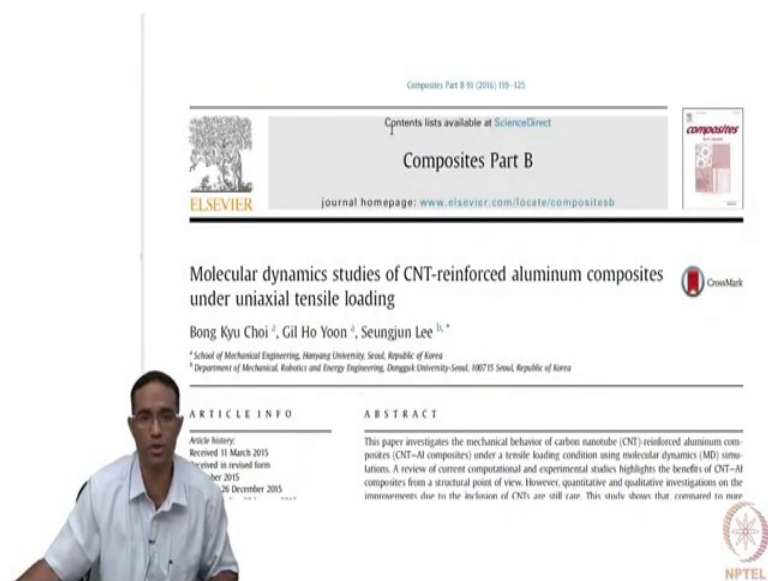
- Found an improvement in toughness of the composite.
- Underlying mechanisms for fracture evolution

(IITM, ME) FCMM November 22, 2019 NPTEL 11/7/21

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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Composites Part B 91 (2016) 119–125

Contents lists available at ScienceDirect

Composites Part B

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Molecular dynamics studies of CNT-reinforced aluminum composites under uniaxial tensile loading

Bong Kyu Choi^a, Gil Ho Yoon^a, Seungjun Lee^{b,*}

^aSchool of Mechanical Engineering, Hanyang University, Seoul, Republic of Korea
^bDepartment of Mechanical, Robotics and Energy Engineering, Dongguk University-Seoul, 00075 Seoul, Republic of Korea

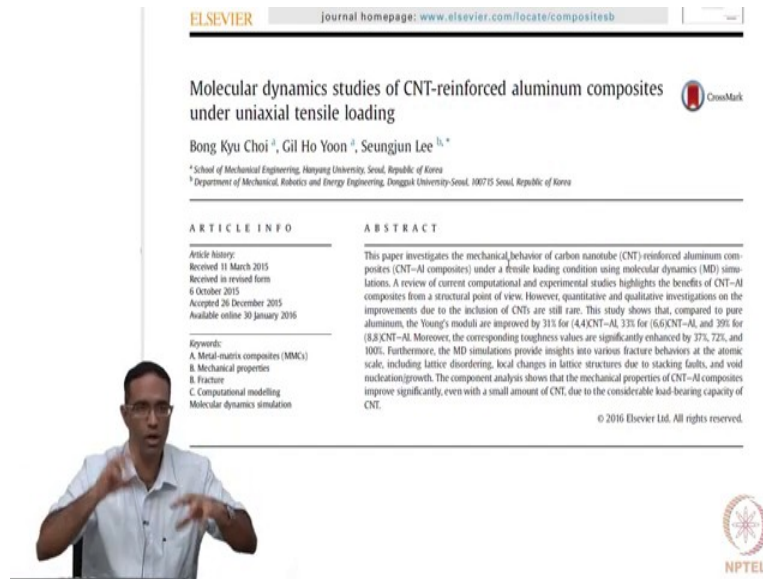
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ABSTRACT

This paper investigates the mechanical behavior of carbon nanotube (CNT) reinforced aluminum composites (CNT–Al composites) under a tensile loading condition using molecular dynamics (MD) simulations. A review of current computational and experimental studies highlights the benefits of CNT–Al composites from a structural point of view. However, quantitative and qualitative investigations on the improvements due to the inclusion of CNTs are still rare. This study shows that, compared to bare

NPTEL



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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120 *KK. Choi et al. / Composites Part B 91 (2016) 119–125*

respectively, compared to the 2024Al matrix [28]. Esawi et al. revealed that CNT morphology played an important role in the dispersion of MWCNT and affected the mechanical strength of the CNT–Al composite. They showed that the Young's modulus of 2 wt % CNT composites improved by 33% compared to that of pure aluminum [29]. Although previous studies reported the effective role of CNTs in enhancing the mechanical properties of metal composites, the level of relative strengthening ranged widely and quantitative agreement has not yet been reached.

Atomic simulations, such as molecular dynamics (MD) simulations, have been widely used to predict the mechanical properties of nano-scale structures. Particularly for the study of failure mechanisms, MD simulations have significant advantages due to the capability of capturing dynamic atomic behaviors. Despite this advantage, investigations and analyses of the mechanical behaviors of CNT–Al composites using MD simulations are still rare. Using MD simulation, Song et al. investigated the effect of a Ni coating on CNT surfaces with regard to the mechanical strengthening of CNT–Al composites [30]. They showed that the Young's modulus of the CNT–Al composite increased with the density of the Ni coatings, because the Ni coating provided an effective channel for load transfer between the CNT and Al matrix. Xiao et al. studied the effects of vacancy defects of CNTs on the fracture behavior of CNT–Al composites [31]. The study illustrated that even a one-atom vacancy defect dramatically reduced the failure stresses and strains. Recently, Silvestre et al. studied the compressive behavior of CNT–Al composites using MD simulation [32]. They reported an increase in Young's modulus due to the inclusion of CNT

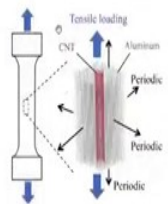


Fig. 1. Schematic of the atomic model for MD simulation, representing the inside of a CNT–Al composite specimen under tensile loading.

2.2. Potentials

Three types of potentials are used to describe the Al, CNT, and Al–CNT interface. For the Al–Al interaction, an Embedded-Atom Method (EAM) potential is employed as follows:

$$E_i = E_A \left(\sum_{j=1}^n \phi_{ij}(r_{ij}) \right) + \frac{1}{2} \sum_{j=1}^n \phi_{ij}(r_{ij}) \quad (1)$$

carburized inner and upper resonances in the matrix increase are summarized in Table 1. The elastic moduli of the three cases for around the upper branch because the CNT is aligned parallel to the loading direction, more effectively supporting the loading. This result implies that the linear elasticity theory (i.e., the macro-scale mixing rule) can be applied to the nano-scale. Thus, the framework in this study can be used to predict the stability of CNT composites with different metal matrices but similar configurations.

To investigate the contribution of the CNT and Al components to mechanical behaviors, we divide the total stress into the stresses of Al and CNT, and the results are shown in Fig. 1. The CNT stresses vary considerably according to CNT diameter while the aluminum stresses rarely change. This indicates that the improved stiffness of the composite is mainly due to the effects of the CNTs. In Fig. 1b, the maximum stress of Al decreases as the CNT diameter increases because the size of the hole in the middle of the Al increases. The hole in the middle acts as a defect. Thus, the enlarged hole weakens the Al matrix, therefore, the maximum stress of the CNT–Al composites increases as the CNT diameter increases due to the strong contribution of the CNT inserted into the hole.

In the region of $0.07 < \epsilon < 0.3$, the curves show a decrease particularly the blue and green ones. A amplified view at around 0.08 strain is shown in Fig. 5. The decreases are due to the stress change of the Al matrix, as shown in Fig. 7b. The decrease in the stress curves represents Al stress slipping on the surface of the hole in the middle of the Al matrix. As a result, the hole is slightly enlarged with an asymmetric shape (Fig. 7b). Simultaneously, the CNT that is initially positioned in the middle of the hole moves to

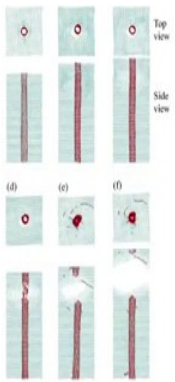


Fig. 5. Snapshots of the MD simulation during the loading process at various strain levels: (a) 0.0, (b) 0.01, (c) 0.05, (d) 0.10, (e) 0.20, and (f) 0.40.

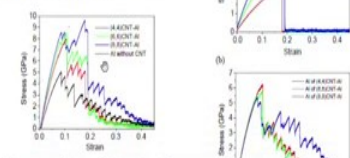


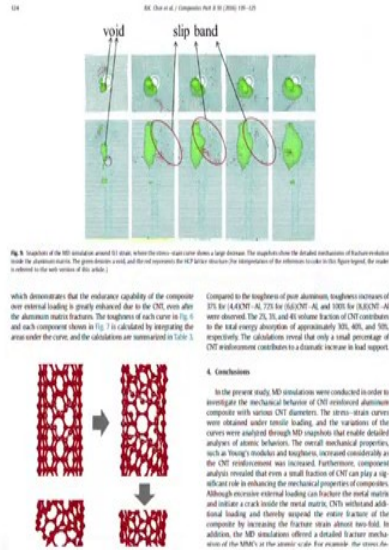
Fig. 6. Stress-strain diagrams for the loading process at various strain levels. (a) Stress (GPa) vs. Strain for CNT-Al, Al-CNT, Al-Al, and Al-Al-CNT. (b) Stress (GPa) vs. Strain for Al-Al-CNT, Al-Al, and Al-Al-CNT.

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.

(Refer Slide Time: 05:43)

Applications Mechanical behaviour of materials

Indentation of nanocrystalline SiC I

New physics during indentation of nc-SiC

Behaviour of nc-SiC is interesting from many viewpoints. Tooling, radiation damage, electronics applications etc. In related works^[2,3], MD simulations of indentation of nc-SiC has shown interesting results, interesting enough to warrant publication in *Science Journal*[2015 IF=34.66].

[2] Applied Physics Letters, (2004) 85, 3, pp. 378-380.
[3] Science, (2005) 309, 5736, pp. 911-914.

What did they find?

Understood new mechanisms taking place beneath the indenter. Could see how dislocations are emitted beneath the indenter. They used about 18.7×10^6 atoms in these simulations.

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So, that was with respect to metals, now I will show you an example with silicon carbide which is essentially ceramic. So, as you all may be knowing, Nano crystalline materials have several interesting properties and Nano crystalline silicon carbide is particularly 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 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 pictures 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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A Crossover in the Mechanical Response of Nanocrystalline Ceramics

Izabela Szufarska,^{1*} Aichiro Nakano,² Priya Vashita²

Multimillion-atom molecular dynamics simulation of indentation of nanocrystalline silicon carbide reveals unusual deformation mechanisms in brittle nanophase materials, resulting from the coexistence of brittle grains and soft amorphous grain boundary phases. Simulations predict a crossover from intergranular continuous deformation to intragrain discrete deformation at a critical indentation depth. The crossover arises from the interplay between cooperative grain sliding, grain rotations, and intergranular dislocation formation similar to stick-slip behavior. The crossover is also manifested in switching from deformation dominated by indentation-induced crystallization to deformation dominated by disordering, leading to amorphization. This interplay between deformation mechanisms is critical for the design of ceramics with superior mechanical properties.

The great interest in nanostructured ceramics originates from the observations and expectations of unique mechanical properties (E , σ) in these materials. Examples include very high hardness, high fracture toughness, and superplastic behavior in normally brittle ceramics. Silicon carbide is of particular interest because of its potential technological applications in high-temperature structural and

are observed both experimentally (1,2) and by means of molecular dynamics (MD) simulations (11,16). In particular, for brittle ceramics such as SiC, mechanical properties such as toughness are essentially determined by soft (often amorphous) GB phases (1,2). Recent experiments (15) of nanovdentation of nanocrystalline SiC (n-SiC) films with grain sizes of 5 to 20 nm have shown “superhardness” (i.e., hardness

18.7 million atoms, which had randomly oriented grains with diameters averaging 8 nm and a density of 2.97 g/cm³ at a temperature of 300 K (16). Structural ordering in GBs is analyzed by means of a partial pair distribution function $g(r)$, which quantifies the probability of finding two atoms at an interatomic distance r . The function $g(r)$ for Si-C pairs is plotted in Fig. 1A (solid line), and it reveals a lack of long-range order, similar to that of bulk amorphous SiC (a-SiC) (dashed line). This is in contrast to a sharp-peak structure of $g(r)$ in a 3C-SiC shown in the inset of Fig. 1A. Visual inspection of the substrate reveals the presence of highly disordered GBs with a more or less uniform thickness. The n-SiC can be thought of as a substrate with two coexisting phases: crystalline inside the grains and amorphous in the GBs. Amorphous GBs were also observed in experimentally sintered n-SiC (17,18).

To shed light on the atomistic mechanisms underlying mechanical response of n-SiC, we indented the substrate with a square-base indenter of size $160 \times 160 \times 72 \text{ \AA}$. Nanoindentation is a unique local probe to measure mechanical properties of materials (19–22). Even though experimental indenters are round on this scale, a square-base indenter helps to maximize the applied stress and the localized plastic flow in the material (23) on length and time scales available to simulation. The ex-



of pores can be as high as 20% (27,28). The crystalline phase within the grains does not yield until the onset of regime 4 at $h = 18.5 \text{ \AA}$. This response is distinct from that of nanostructured metals, in which a dislocation within the grain is nucleated at the onset of substrate yielding (29–31). Discrete plastic events, such as a dislocation glide, take place within the grains in close proximity to the indenter and are reflected in the regular character of the P - h curve. Similar periodic load drops have been observed for the nanovdentation in bulk 3C-SiC. In the case of n-SiC, the load drops are much less pronounced than in 3C-SiC (25), because the calculated load is averaged over a few grains covered by the indenter and the discrete events in a grain are decoupled from those in the neighboring grains. The decoupling from grains not lying directly beneath the indenter is shown in Fig. 2A, in which atoms are color coded by ΔR_{CM} , the total displacement of the centers of mass of individual grains from their positions before indentation. The localization of deformation is much more pronounced in regimes 3 and 4 than in 1 and 2.

The crossover from cooperative mechanical response of coupled grains to discrete intergranular events is shown in Fig. 2B, where we plot the average displacement $\langle \Delta R_{CM} \rangle$ of the grains' centers of mass calculated relative to the previous indentation step. The coupling between grains in regime 1 is manifested as the

The crossover and localization of deformation are also manifested in the rotation of grains.

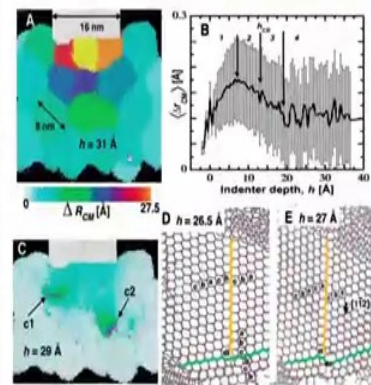


Fig. 2. (A) Grains near the indenter at $h = 31 \text{ \AA}$ (regime 4). Atoms are color coded by ΔR_{CM} , the total displacement of grain's center of mass [CM], relative to the initial system. Decoupling of grains results in




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.

(Refer Slide Time: 08:32)



Applications Mechanical behaviour of materials

Indentation of nanocrystalline SiC I


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What did they find?


Understood new mechanisms taking place beneath the indenter. Could see how dislocations are emitted beneath the indenter. They used about 18.7×10^6 atoms in these simulations.



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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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Physics Letters

Nanoindentation-induced amorphization in silicon carbide


Cite as: Appl. Phys. Lett. **85**, 378 (2004); <https://doi.org/10.1063/1.1774252>
Submitted: 02 February 2004 . Accepted: 01 June 2004 . Published Online: 14 July 2004

Izabela Szlufarska, Rajiv K. Kalia, Aichiro Nakano, and Priya Vashishta

ARTICLES YOU MAY BE INTERESTED IN

Atomistic processes during nanoindentation of amorphous silicon carbide
Applied Physics Letters **86**, 021915 (2005); <https://doi.org/10.1063/1.1849843>

Multimillion-atom nanoindentation simulation of crystalline silicon carbide: Orientation dependence and anisotropic pileup
Journal of Applied Physics **95**, 023511 (2004); <https://doi.org/10.1063/1.1635557>



This is the Nano indentation induced amorphization and silicon carbide.

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of detect nucleation at the initial stages of plastic activity. Therefore MD simulations are expected to shed light on the atomistic pathway to amorphization via nanoindentation.

In this letter we study by means of MD the atomistic mechanisms governing the indentation-induced amorphization of 3C-SiC. At a small displacement a reversible pop-in behavior in the $P-h$ curve is observed, indicating a remarkable elastic recovery of 3C-SiC. This is followed by the plastic regime, in which we observe a series of load drops, which are related to subsurface dislocation activities. We characterize these structural deformations in terms of bond angles, local shear stress and pressure, spatial distribution of atoms, and shortest-path-ring distribution. We demonstrate how the ring analysis can be effectively employed to study nanoindentation damage. Simulation results reveal that the defect stimulated growth and coalescence of dislocation loops play an important role in indentation-induced amorphization.

The potential used in our study is a combination of two- and three-body interaction terms, which include steric repul-

...
 $\approx 2.83 \text{ \AA}$ and all the other are equally spaced by $\sim 3 \text{ \AA}$. The drops of the load correspond to breaking of subsequent atomic layers of the underlying substrate, which in the z direction are separated by 3.08 \AA . The $P-h$ curve also exhibits a shoulder at $h=0.83 \text{ \AA}$. An insight into the nature of this shoulder as well as of the first load drop is brought by performing two unloading simulations [see Fig. 1(b)], in which we gradually remove the indenter from the depths (1)

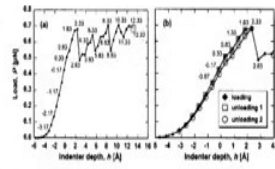


FIG. 1. (a) Load-displacement ($P-h$) curve. (b) Unloading curves from depths (1) $h=1.83 \text{ \AA}$ (squares) and (2) $h=2.33 \text{ \AA}$ (circles).

*Electronic mail: izabela@usc.edu
 0003-6951/2004/85(3)/378/\$20.00

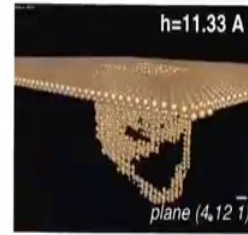
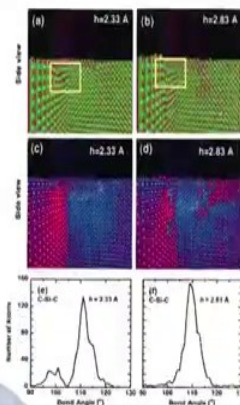


FIG. 3. (c) Ring distribution analysis: atoms with non-ideal rings at $h=11.33 \text{ \AA}$.

surface). In the zinc-blende crystal both of these distributions exhibit a sharp peak at $\sim 109^\circ$ due to the perfect tetrahedral arrangements of atoms. The distributions are significantly broadened in the amorphous phase, α -SiC. In our simulation, bringing the indenter closer to the substrate results in destruction of the tetrahedral arrangements of atoms and in splitting of the single peak in bond angle distribution [see Fig. 2(e)].



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.

(Refer Slide Time: 10:30)

Applications Mechanical behaviour of materials

Understanding diamond machining of Si I

Machining of brittle materials

Si being brittle is hard to machine using conventional techniques. SPDT (Single point diamond turning) based machining seems to be a good option to get ultrahigh surface finishes [4]

[4] International Journal of Machine Tools and Manufacture, (2015) 88, pp. 131-164.

What did they find?

Provided significant insights into several process parameters which may enable improvement in other quantities which control the High pressure phase transformation at the workpiece.

Narasimhan (ITM, ME) FCMM November 22, 2019 NPTEL/2

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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International Journal of Machine Tools & Manufacture 88 (2015) 131–154

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journal homepage: www.elsevier.com/locate/ijmactool

Diamond machining of silicon: A review of advances in molecular dynamics simulation

Sauraj Goel^{a,*}, Xichun Luo^b, Anupam Agrawal^c, Robert L. Reuben^d

^a School of Mechanical and Aerospace Engineering, Queen's University Belfast, BT9 5EX, UK
^b Department of Design, Manufacturing and Engineering Management, City University of Hong Kong, 868C, HK
^c Department of Biomechanical Engineering, University of Sheffield, Sheffield, S10 2TN, UK
^d School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, UK

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ABSTRACT

Molecular dynamics (MD) simulation has enhanced our understanding about ductile regime machining of brittle materials such as silicon and germanium. In particular, MD simulation has helped understand the occurrence of brittle–ductile transition due to the high pressure phase transformation (HPPT) which induces brittle–ductile transition. In this paper, relevant MD simulation studies in conjunction with experimental studies are reviewed with a focus on: (i) the importance of machining variables, undeformed chip thickness, feed rate, depth of cut, geometry of the cutting tool in influencing the state of the deformed silicon to cause HPPT in silicon; (ii) the influence of material properties, rate of fracture toughness and hardness, crystal structure and anisotropy of the material; and (iii) phenomenological understanding of the wear of diamond cutting tools, which are all non-trivial for cost-effective manufacturing of silicon. The ongoing developmental work on potential energy functions is reviewed to identify opportunities for overcoming the current limitations of MD simulation. Potential research areas relating to how MD simulation might help improve existing manufacturing technologies are identified which may be of particular interest to early stage researchers.

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Goel et al. / International Journal of Machine Tools & Manufacture 88 (2015) 131–154

$D = Q^2 + R^2$
 $D \cdot D = 0$ then as follows else the condition is 2D state
 $\sigma = \cos(\theta) \left(\frac{\sigma_{xx}}{\sqrt{1 + \frac{Q^2}{R^2}}} \right)$
 $R_1 = 2 \cdot \sqrt{Q^2} \times \cos(\theta) \left(\frac{\sigma_{xx}}{\sqrt{1 + \frac{Q^2}{R^2}}} \right) - \sigma_{yy}$
 $R_2 = 2 \cdot \sqrt{Q^2} \times \cos(\theta) \left(\frac{\sigma_{xx} + \sigma_{yy}}{3} \right) - \sigma_{yy}$
 $R_3 = 2 \cdot \sqrt{Q^2} \times \cos(\theta) \left(\frac{\sigma_{xx} + 2 \cdot \sigma_{yy}}{3} \right) - \sigma_{yy}$
 $\sigma_1 = \min(R_1, R_2, R_3)$ and $\sigma_2 = \min(R_1, R_2, R_3)$
 $\sigma_{max} = \frac{\sigma_1 + \sigma_2}{2}$
 $\sigma_{min} = \frac{\sigma_1 - \sigma_2}{2}$
 $\sigma_{machining} = \frac{\sigma_{max} \cdot \sigma_1^2 + \sigma_{min} \cdot \sigma_2^2 + (\sigma_{max} - \sigma_{min}) \cdot \sigma_{yy}}{3}$
 $\sigma_{machining} = \frac{\sigma_{max} + \sigma_{min}}{3}$

3.3.4. Calculation of machining stress

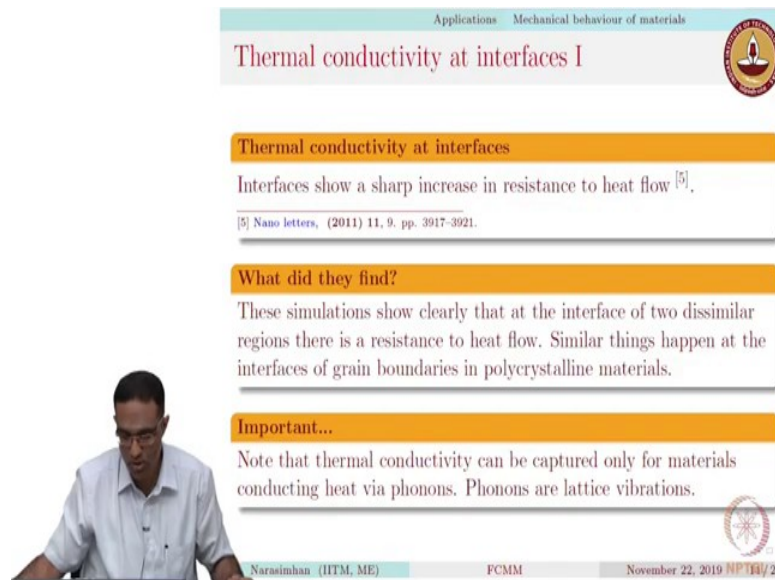
The state of stress acting in the machining zone is shown schematically in Fig. 73 for both 2-D and 3-D stress systems. The instantaneous values of the stress calculated from the MD simulation should always be time averaged. One fundamental problem with the computation of atomic stress is that the volume of an atom does not remain fixed during deformation. To mitigate this problem, the best method is to plot the stresses on the fly by considering an elemental atomic volume in the cutting zone. The total stresses acting on that element could be computed and divided by the geo-calculated total volume of that element to obtain the physical stress tensor. When a stress tensor from the simulation is available, the following equations can readily be used

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.

(Refer Slide Time: 12:38)



The slide is titled "Thermal conductivity at interfaces I" and is part of a presentation on "Applications Mechanical behaviour of materials". It features a yellow header and footer. The main content is divided into three sections: "Thermal conductivity at interfaces", "What did they find?", and "Important...". The "What did they find?" section states that simulations show a sharp increase in resistance to heat flow at interfaces of dissimilar regions and grain boundaries. The "Important..." section notes that thermal conductivity can only be captured for materials conducting heat via phonons. The slide footer includes the name "Narasimhan (IITM, ME)", the course "FCMM", and the date "November 22, 2019".

Applications Mechanical behaviour of materials

Thermal conductivity at interfaces I

Thermal conductivity at interfaces

Interfaces show a sharp increase in resistance to heat flow ^[5].

[5] Nano letters, (2011) 11, 9, pp. 3917-3921.

What did they find?

These simulations show clearly that at the interface of two dissimilar regions there is a resistance to heat flow. Similar things happen at the interfaces of grain boundaries in polycrystalline materials.

Important...

Note that thermal conductivity can be captured only for materials conducting heat via phonons. Phonons are lattice vibrations.

Narasimhan (IITM, ME) FCMM November 22, 2019

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".

(Refer Slide Time: 13:22)

ANO LETTERS LETTER
pubs.acs.org/NanoLett

Thermal transport across Twin Grain Boundaries in Polycrystalline Graphene from Nonequilibrium Molecular Dynamics Simulations

Arun Bagri,¹ Sang-Pil Kim,² Rodney S. Ruoff,² and Vivek B. Shenoy^{1,2*}

¹School of Engineering, Brown University, Providence, Rhode Island 02912, United States
²Department of Mechanical Engineering and the Texas Materials Institute, University of Texas, Austin, Texas 78712, United States

ABSTRACT: We have studied the thermal conductance of tilt grain boundaries in graphene using nonequilibrium molecular dynamics simulations. When a constant heat flux is allowed to flow, we observe sharp jumps in temperature at the boundaries, characteristic of interfaces between materials of differing thermal properties. On the basis of the magnitude of these jumps, we have computed the boundary conductance of twin grain boundaries as a function of their misorientation angles. We find the boundary conductance to be in the range 1.5×10^{10} to 4.5×10^{10} W/(m² K), which is significantly higher than that of any other thermoelectric interfaces reported in the literature. Using the computed values of boundary conductances, we have identified a critical grain size of 1 μm below which the contribution of the tilt boundaries to the conductivity becomes comparable to that of the contribution from the grains themselves. Experiments to test the predictions of our simulations are proposed.

KEYWORDS: Thermal conductivity, polycrystalline graphene, phonon transport, Kapitza conductance

NPTEL

So thermal transport across twin Grain boundaries and Polycrystalline graphene from nonequilibrium 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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Figure 1. Geometry of the ENEMD simulation box. The cold slab is placed at the ends of the simulation cell, while the hot slab is located in the middle of the cell.

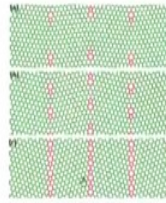


Figure 2. Structure of slab grain boundaries with misorientation angle of (a) 5.5°, (b) 13.2°, and (c) 31.2°.

system. When the heat flow in the structure reaches the steady state regime, averaging over the heat flux and temperature gradient and using the Fourier's heat conduction equation, the thermal conductivity can be obtained from

$$\langle \dot{q} \rangle = k \left(\frac{\Delta T}{\Delta x} \right) \quad (2)$$

in which k is the thermal conductivity and T is the temperature. The brackets, $\langle \rangle$, indicate the average of the quantities over time as well as over the particles in the simulation cell. The above approach for computing the thermal conductivity of a homogeneous system can also be generalized to the case of a system with defects. In the case of grain boundaries, we consider here

single hex ring separates the periodic 5-7 defects. Therefore, more severe grain boundary angles are composed of higher defect densities. The repeating defect pairs can also be thought of as an array of edge dislocations with horizontal Burgers vectors where the five-membered rings represent the extra plane of atoms. In our simulation, periodic boundary conditions are employed both along the direction of heat flow (x) and perpendicular to the direction of heat flow (y). The atomic interactions are defined by a modified version of the Tersoff potential,³⁰ which has been recently shown to yield values of the acoustic phonon velocities that are in excellent agreement with measured data. The potential also provides lattice thermal conductivity values in single-walled carbon nanotubes and graphene that are considerably improved compared to those obtained from the original parameter set.^{31,32}

The atomic coordinates and the overall periodic dimensions of the simulation cell are first optimized using the gradient-based minimization method implemented in the large-scale atomic/molecular massively parallel simulation (LAMMPS) molecular dynamics package³³ in a microcanonical NVE ensemble until the forces on atoms are less than 10^{-6} eV/Å. ENEMD simulations are then carried out on the relaxed structure at room temperature with a time step of 0.5 fs. Before the temperature profiles are computed to infer thermal conductivity, the system is allowed to evolve for 4.4×10^7 MD steps during which the velocities of the atoms in the hot and cold regions are exchanged every 100 MD time steps. After the steady state regime is reached, the temperature gradient through the structure is obtained by averaging over 8×10^7 MD steps. The temperature profiles are determined by dividing the structure into slabs that are approximately 10 Å wide.

First, we validate our approach by computing the thermal conductivity of defect-free graphene. The temperature profiles obtained in our calculations in the case is shown in figure 3b.



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.

(Refer Slide Time: 15:25)

Applications Mechanical behaviour of materials

Radiation damage in materials for reactors

Lithium meta-titanate

Li2TiO3 is a prospective breeder material in fusion reactors. It is not known how neutron damage creates point defects in the material.



(Radiation damage)

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.

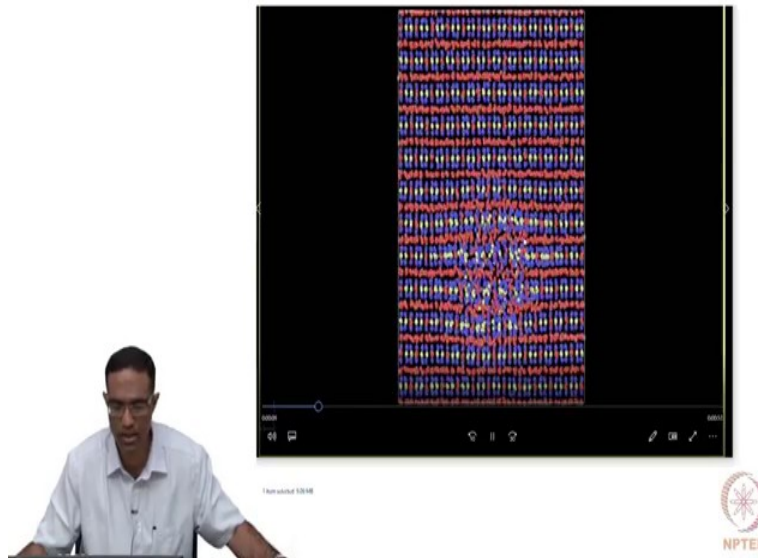
And consequently when they are, when a material is being bombarded with high energy atoms, you create what are refer to as point effects. You may create vacancies, interstitials or antisites. And as these defects actually increase in number the thermo-mechanical properties of these materials are expected 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.

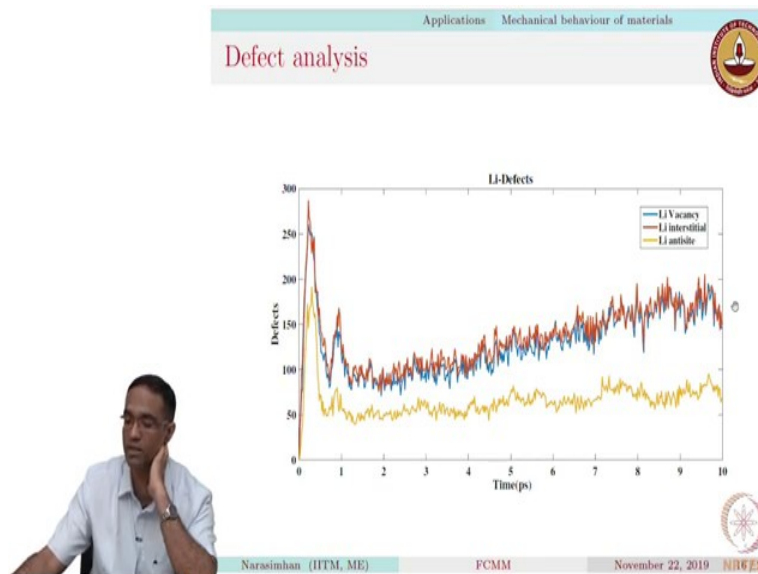
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This is an example of a lithium meta-titanate, lithium meta-titanate and you can see one particular atom moving all of a sudden and creating a small cascade region here. This is a molecular dynamic simulations of this of this particular cascade event 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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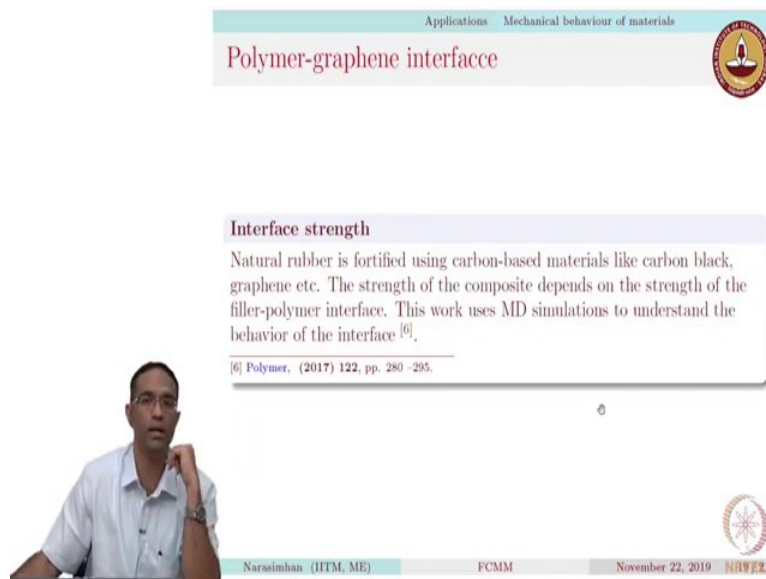


And we can perform some analysis on this to basically see how these point defects are basically evolving with time. So, For example, these are typical kind of plots that you may

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.

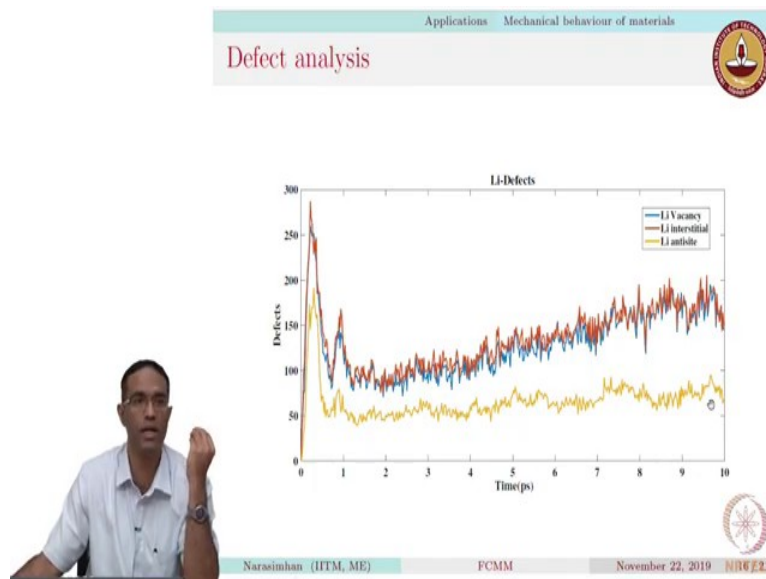
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The slide is titled "Polymer-graphene interface" and is part of a presentation on "Applications Mechanical behaviour of materials". It features a section titled "Interface strength" which discusses the use of MD simulations to study the interface between natural rubber and carbon-based materials like carbon black and graphene. A reference is provided: "[6] Polymer, (2017) 122, pp. 280 -295." The slide also includes a logo in the top right corner and a footer with the name "Narasimhan (IITM, ME)", the acronym "FCMM", the date "November 22, 2019", and the number "11/19/21". A small inset image of a man in a white shirt is visible in the bottom left corner of the slide area.

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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Applications Mechanical behaviour of materials

Radiation damage in materials for reactors

Lithium meta-titanate

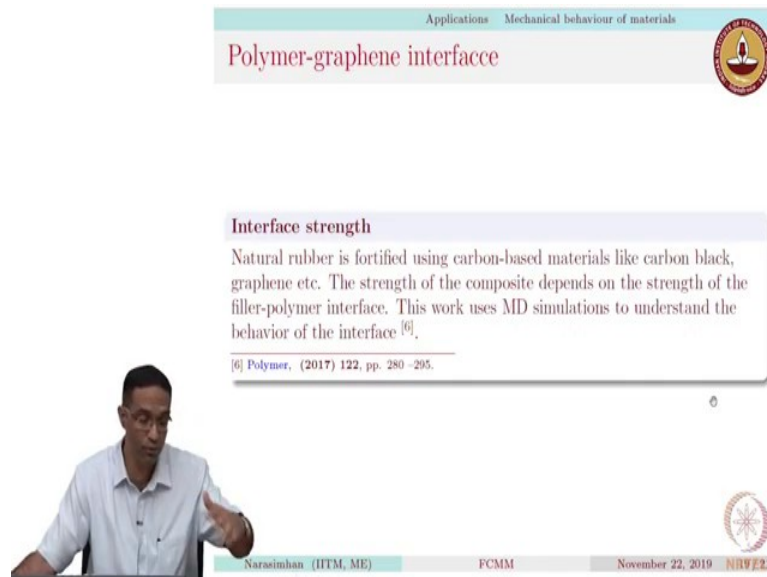
Li_2TiO_3 is a prospective breeder material in fusion reactors. It is not known how neutron damage creates point defects in the material.

(Radiation damage)

Narasimhan (IITM, ME) FCMM November 22, 2019

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

(Refer Slide Time: 19:24)



The image shows a presentation slide with a light blue header containing the text 'Applications Mechanical behaviour of materials'. The main title of the slide is 'Polymer-graphene interface' in red. Below the title, there is a section titled 'Interface strength' in bold. The text in this section reads: 'Natural rubber is fortified using carbon-based materials like carbon black, graphene etc. The strength of the composite depends on the strength of the filler-polymer interface. This work uses MD simulations to understand the behavior of the interface [6].' Below this text is a reference: '[6] Polymer, (2017) 122, pp. 280 -295.' In the bottom left corner, there is a small video inset of a man in a white shirt speaking. The bottom of the slide features a footer with the name 'Narasimhan (IITM, ME)', the acronym 'FCMM', the date 'November 22, 2019', and the course code 'NITF21'. There are also two circular logos on the slide: one in the top right and one in the bottom right.

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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Opening Mode Separation of Graphene-cis -1,4-Polyisoprene

Thumbnail #136



Quasistatic Separation

Thumbnail #136



for all except
intermediate rate
pulling at
0.008 angstroms/fs
which is
0.36 angstroms

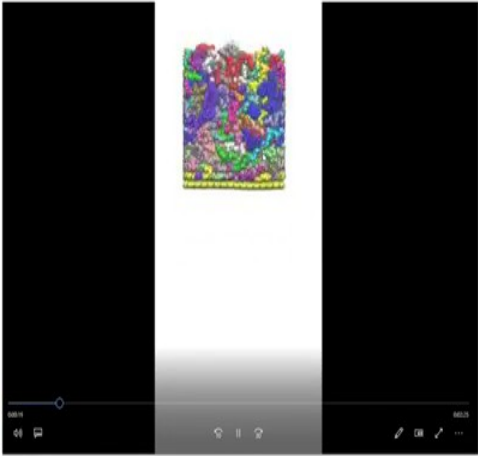
Thumbnail #136



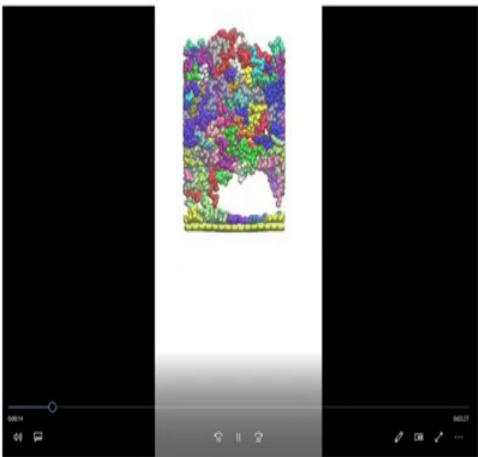


Separation made by graphene between two frames is 0.25 angstroms,

Thumbnail #138



Thumbnail #138



Thumbnail #138





Equilibration of Interface

00:01 00:08

100%

100%

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00:01 00:08

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100%



Initial Assembly: Unwrapped Polymer Network and Graphene

00:01 00:08

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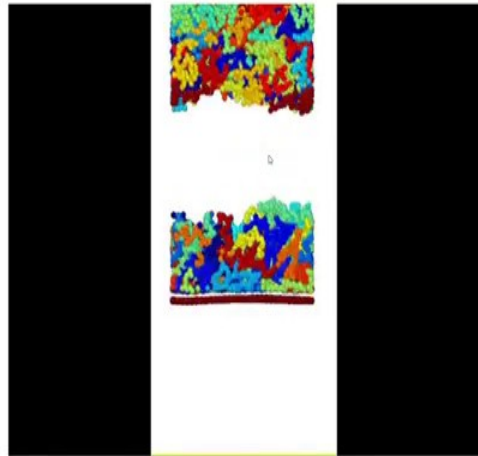
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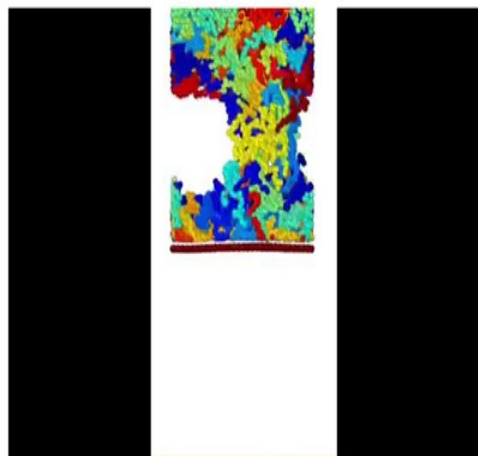
Separation at the Intermediate Rate (0.005 ang/fs)



Thumbnail 01/146



Thumbnail 02/146



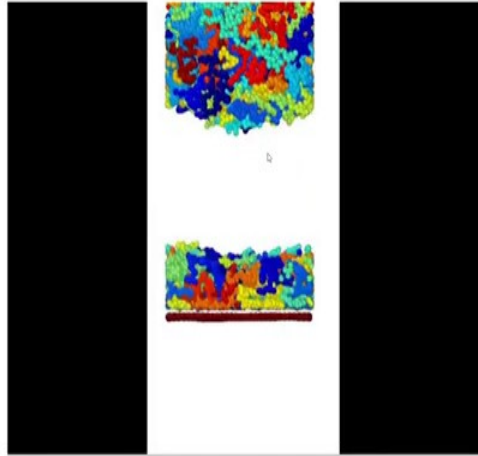
Thumbnail 03/146



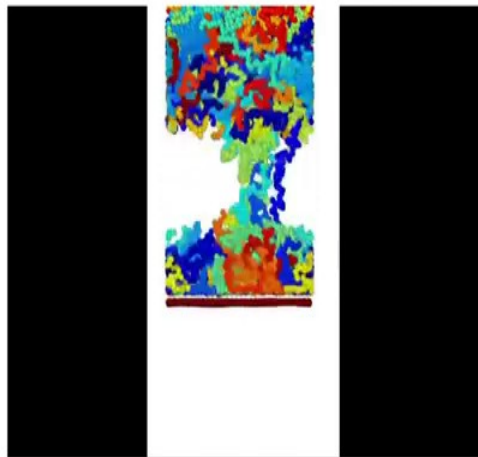
Separation at the Smallest Finite Rate



Thumbnail #138

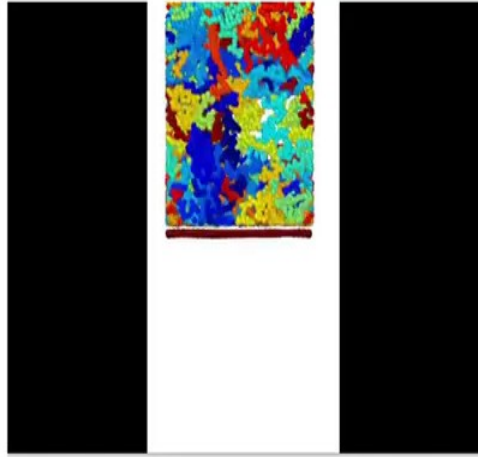


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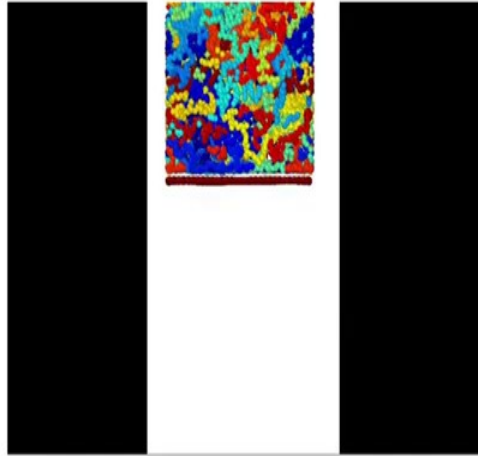


Thumbnail #138





Thumbnail #138

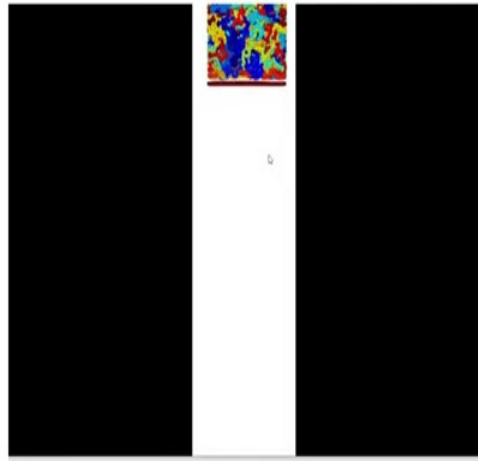


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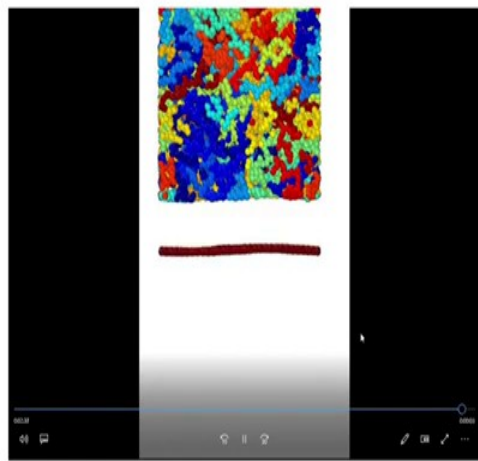




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Thumbnail #138

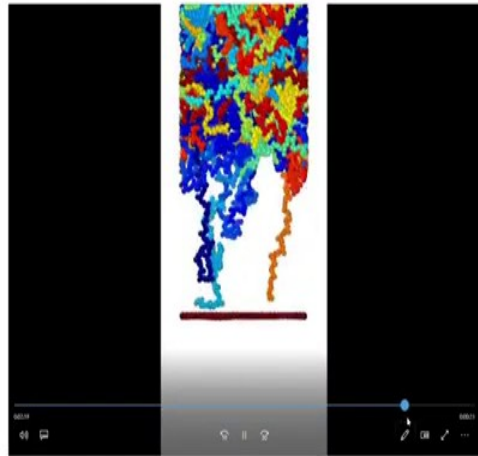


Thumbnail #138





Thumbnail 0/146



Thumbnail 0/146



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.

(Refer Slide Time: 23:10)

Applications Mechanical behaviour of materials

Nobel prize in Chemistry 2016

Molecular machines 2016

Nobel prize in Chemistry for molecular machines. *A tiny lift, artificial muscles and minuscule motors. The Nobel Prize in Chemistry 2016 is awarded to Jean-Pierre Sauvage, Sir J. Fraser Stoddart and Bernard L. Feringa for their design and production of molecular machines. They have developed molecules with controllable movements, which can perform a task when energy is added.*^[7]

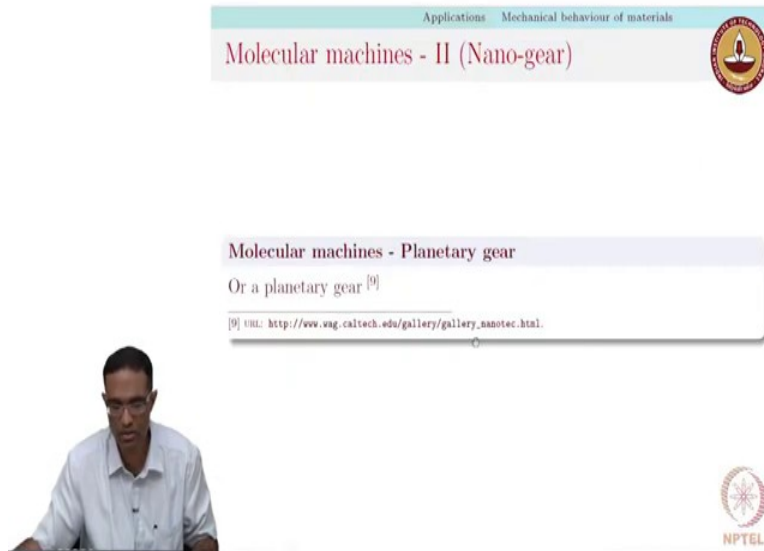
[7] URL: https://www.nobelprize.org/nobel_prizes/chemistry/laureates/2016/.

Arasimhan (IITM, ME) FCMM November 22, 2019 1/20/21

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 Sauvage, Sir J Fraser Stoddart and Bernard L. Feringa 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.

(Refer Slide Time: 23:56)



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.