Journal

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Jul. 16, 2024 — Tuesday

About Voronoi tessellation and characterization techniques in softmatter. In the article Yang, Zou, and Yu (2002)

They analyse a system with 5000 particles and vary the radius from 100 to $0.1\mathrm{m}$ and analyse the number of edges for each polyhedron face, number of faces for each polyhedron face, perimeter, area of a polyhedron face and perimeter, area and volume of a polyhedron. In a nutshell, they said that the topological and metric properties of Voronoi polyhedra are quantified as a function of particles size and packing density. Edges, vertices, volume, area in terms of the particle size and packing fraction. According to the results of the article, the average face number decreases when the particle size and packing density decreases. The distributions of face number and edges become broader and more asymmetric. On the other hand, the average perimeter and area of polyhedra increses and the distributions of polyhedron surface area and volume become more flat and can be described by the log-normal distribution. Finally, the average sphericity coefficient of Voronoi Polyhedra varies with packing density. [The sphericity, Ψ, of an object is the ratio of the surface area of a sphere with the same volume to the object's surface area $\Psi = \pi^{1/3}\left(6V_p\right)^{2/3}/A_p$].

They mention the following laws: Aboav-Weaire's law and Lewis's law.

In the article Lazar, Lu, and Rycroft 2022 in the section of Stability they state that: When geometric quantities are used for classification purposes, thresholds for the range of possible values must be chosen, on the other hand, topological ones can change abruptly under small perturbations of particle coordinates.

How we can relate the topological and metric properties with rehological properties?

Relation between the interatomic interaction with the geometric properties. I thinkg that there is a relation between the superficial area of the voronoi faces with pressure between two particles.

Thinking about the Lennard-Jones potential in three dimensions, it creates an sphere of potential. It can be computed the pressure in a plane that intersect that sphere.

I think that, that relation, between the potential and the intersecte plane, will help to create a conecction between rehological properties and structural stuff.

$$\vec{P}_{VC} = -\frac{\mathrm{d}}{\mathrm{d}r}\mathrm{LJ}(r)\big|_{r\in R^2}\frac{1}{A_{VC}}\hat{e}_r,$$

where A_{VC} is the area of the shared plane between two voronoi cells and the force is evaluated at that plane. The *VC* indicates, "Voronoi Cell".

Now, this has the same units of the stress tensor.

To introduce the direction of the plane into the pressure, we take dot product with the spherical coodrinate system, an then multiply be the normal vector of the plane,

$$\vec{P}_{plane} = \left[\vec{P}_{VC} \cdot \left(\hat{e}_r, \hat{e}_\phi, \hat{e}_\theta\right)\right]\hat{n}_{plane}$$

Create an histogram of the normal vector. Histogram of the dot product between the normal vector with the cartessian reference.

The better way to analyse the macro caracteristics is an histogram.

About packing density: Using the volumen of voronoi polyhedra. It can be said that a system is jammed, when the mean of the volumens of the voronoi polyhedra tends to a minimum.

About the simulations. 50 simulations with 500 patchy particles took 24 hrs. This is 500 Monomers and Crosslinker. All of them has 50 CL and 450 MO, hence, 200 patches for the 50 CL and 900 patches for MO, hence, 1600 particles in total.

I have no idea how to improve the time of the simulation. Each simulation takes between 27-28 mins.

⭐ Jul. 17, 2024 — Wednesday

Key point of the reunion:

- Start the script for shear deformation

- Keep in mind to vary the following parameters:

    1. Cross-Linker concentration

    2. Size of the box (Packing density)

    3. The energy of the Patch-Patch interaction.

- Analyze the density distibution of the voronoi parameters

- Make and animation, where the color of the particle represent the volume of the voronoi cell and share the script.

- Hint: Directores

About the idea of the normla vector: They do not sees a great future.

The deformation script is done, basically I copy the code from Felipe.

Jul. 19, 2024 — Friday

Yesterday I finich the scripts for the shear deformation and investigate some papers that help me to understad what I'm trying to do for the thesis project.

I found the artilce by Sheiko and Dobrynin 2019 and here are some "main" points:

- Materials response to deformation is expressed by a stress-strain curve measured art controlled strain rate and temperature.

- A set of stres-strain curves constitue the "mechanical phenotype".

- The dependcy of those curves help us to understand the molecular relacation processes, such as conformational tranformation, bond scission and molecule displacement.

- In the article, they classify a material, based on their stress-strain curves, in three categories: Thermoplastics, Biological networks and Synthetic network.

- Feature of interset for the article: Firmness is the stiffeness enhancement in response to deformationa and is one of nature's defense mechanisms preventig accidental organ rupture.

- Solif thermoplastics, the mechanical properties are predominantly controlled by molecular interactions.

- Elastomers, the mechanical properties are controlled by the changes in the system configuration,by unravelling network strands at nearly constant mass density.

- A network architecture is defined by: Connectivity, dimensions and flexibility of network strands.

- The weak dependence on chemical compositions helps to manipulate the mechanical response.

- In the article they focues in the Shear modulus.

- Topological defects: Chain entranglements, dandling chain ends, loops, multiple strands and side chains.

- Search of definitions:

    1. Shear modulus:

    2. Cross-link functionality:

    3. Degree of polymerization: Number of monomeric units (MO and CL)

    4. Kuhn length: A theoretical treatment, developed by Werner Kuhn, in which a real polymer chain is considered as a collection of N Kuhn segments each with a Kuhn length b. Each Kuhn segment can be thought of as if they are freely jointed with each other.

- The softness at small deformations is manipulated by changing the cross-link density.

- Linear chain Networks

    – The cross-linnk density is THE control parameter

- The Young's modulus can be tune by introducing loops and dangles.

- Modify the junctions can controll the network topology

- The cross-link functionality can be increased by adding dendrimes, colloidal particles and microphase domains.

- Their equilibrium characteristics are mostly determined by the degree of polymerization of the chemical network strand.

- Strand entanglements can create a loweer limit for the shear modulus and upper limit for the elongation-at-break.

- Softness can be achieved by solvent swelling.

- Swelling leads to strand extensions and therefore firmness enhacement.

- Dual Networks

  - Networks with permanent cross-links and dynamic cross-links.

  - Permamnent cross-link are responsible for elastic properties and sample shape

  - Dynamic cross-link regulate energy dissipation and strain-rate response.

  - Dynamic networks depen on strain rate, permanent network does not depend on strain rate.

  - At higher rates, physical cross-links do not have enough time to break and behave as permanent cross-links, resulting in high modulus and strength.

  - **To characterize the dynamic mechanical properties of the dual networks at small deformations, evolution of the stress relaxation Young's modulus E(t) during uniaxial extension at a constant temperature is calculated by using a linear viscoelasticity approximation.**

- Network with Brush-Like strands: I didn't read it with detail, beacuse it is out of my scope/comprehension/interest at the moment. It will be great to read it with more knowledge in the area.

Need to check Dealy and Larson 2006 for more information about polymer structures and their characterization.

Now, in the sense, that the curve of strain-stress is essential to characterize the material, I search in lammps how to compute the stres and strin in the simulation. What I found is an page where there explain how to Calculate elastic constants and according to that page, the elastic constants (strain and stress) are related as follows:

$$s_{ij} = C_{ijkl}e_{kl},$$

where the repeates indices impley summation. s_{ij} are the elemnts of the symmetric stress tensor, e_{kl} are the elements of the symmetric strain tensor and C_{ijkl} are the elemnts of the foruth rank tensor of elastic constants.

Then, they state that the elastic constant can be computed at *zero temperature* or *finite temperature* and metiond the following methods for doing it in LAMMPS,

- At zero temperature

1. The C_{ijkl} are estimated by deforming the simulaiton box in one of the six directions using `change_box` command. Then compute the chanfes in the stress tensor.

- At finite temperature

  1. Exploit the relation between elastic constants, stress fluctuations, and the Born matrix. Ray and Rahman 1984

  2. Measure the change in average stress tensor in an NVT simulations when the cell volume undergoes a finite deformation.

  3. Sample the triclinic cell fluctuations that occur in an NPT simulation.

Finally, in the article Clavier et al. 2017 a nice review of the advantages and disadvantages of all of these methods is provided.

So the next week I will check those articles and the examples cripts in lammps.

Possibly, during the weekend's I transfer old entries of multiple daily log in Obsdian, notesbooks, Git and Discord.

Jul. 22, 2024 — Monday

Today I check the examples scripts form Calculate elastic constants, specificly the *Zero temperature* and *Born_Matrix* examples. I understud the methodology. The scripts create a set of particles, then in minimize the system and save that state. Then, a set of 12 deformations are applied, a pair of deformation per basis: *xx, yy, zz, xz, yz, xy*, with positive and negative sign, to change the direction. Then, the stress and pressure tensors are used to compute the strain tensor.

In the *zero* temperature scheme, this is the end of the simulation, meanwhile, this procedure is repeted thru an interval of time for the *Born_Matrix* example.

I want to applied that methodology to characterize the hydrogel, but first, the scripts needs to be converted from reduce units to real units. Also, I want/need to undertad the relations between stres-strain parameters, preassure, stress, the derivatives of the potential energy with stress and strain. Furthermore, I need to seek information about an order parameter to propose.

Taking into account, that temperature is the mean of the velocity of system of particles, we can create a vague relation betweent the "structure" and the temperature. Assuming that a solid or fluid has more bonds between particles than a gas, a gas has a greater temperature than the others. However, how can we stablish a range of temperature o a temperurte in which occurs a transition between solid, to liquid to gas.

If we think that the temperature is a mean, hence we can use the standrd deviation as a tool to identify a transition. When the standard deviation of the temperature is localize, then is in a state, but when the standard deviation is broader, we can stipulate that is happening a phase transition.

Now, here are few point that need to be clarify:

- The temperature is a mean of the particle velocities in a system. To analyze the standard deviation of the temperature, that means to take into account N systems at constant number of particles, volume and energy (NVE).

- The other points I dont remebebr becuase I take another line of thought.

About viscosity, temperature and rheological properties.

The viscosity, temperature and rheological properties are consquence of the composition of the material. The temperature is more related with the internal velocity of the particles, meanwhile, the viscosoty and rehological properties are more related with the relative position between particles.

I undertand the structure of the material, as the relative position of the particles between the, hence, the viscosity and the rhological properties are observables of the strucutre of the material. On the other hand, the temperature is an observable of the velocity of the particles.

It is important to take into account, that the velocity of the particles is affected by the position of the particles and the position of the particles is affected by the velocity of them. Hence, twe can use the hree of them to state phase changes.

In a broad sens, the temperature will help to diffiriantiet between solids and liquid with gasses. The viscosity between solids and gases with liquids and rhologicla properties between liquids and gasses with solids.

Now, with all that in mind, How we can related those properties with specific structures? That a set of parameters will help to kwon that a material has chains in "U" or will form vessicles or chains.

To be honest, I infer that to crespond that, we also need to take into account the compounds and the electronic proporties of their compounds. Becuases, that will help to connect the macro with the micro properties.

About Pressure. Preassure is an external variable. Pressure is the change of momentum over time per area. Now, the temperature is the expected value of the kinetic energy, which is related with the mometum of the particles. So pressure, will help to understad the change of preperties thru time.

The pressure will help to observed the change of temperature over time. This is, because the temperature is directly related with the velocity and mass, such as the momeutm. However, the mass is assume to be constant, even in deformationn, there is no change in mass, only in the surface area at constant volume. So, when the temprature changes, then the preassure register that change in time, because the velocity changes.

However, under deformation, the area also changes, hence, the preassure changes.

Now I need more basic information about SoftMatter stuff, hence I will watching the following videos:
Kent State 2020 course on Statistical Mechanics of SoftMatter

some stuff of definitions:

- Shear Strain: The engineering shear strain (γxy) is defined as the change in angle between lines $\bar{AC}$ and $\bar{AB}$.

- Shear stress (often denoted by τ) is the component of stress coplanar with a material cross section.

- In materials science, shear modulus or modulus of rigidity, denoted by G, or sometimes S or μ, is a measure of the elastic shear stiffness of a material and is defined as the ratio of shear stress to the shear strain.

- Young's modulus E describes the material's strain response to uniaxial stress in the direction of this stress (like pulling on the ends of a wire or putting a weight on top of a column, with the wire getting longer and the column losing height),

- The Poisson's ratio υ describes the response in the directions orthogonal to this uniaxial stress (the wire getting thinner and the column thicker),

- The bulk modulus K describes the material's response to (uniform) hydrostatic pressure (like the pressure at the bottom of the ocean or a deep swimming pool),

- The shear modulus G describes the material's response to shear stress (like cutting it with dull scissors).

Recomendtions of Dr. Tensor, jsjs

- Statistical Physics, A Guenault (Chapman and Hall)

- Introductory Statistical Mechanics, DS Betts and RE Turner (Addison Wesley)

- Introductory statistical Mechanics, Bowley and Sanchez (Oxford)

- Introduction to Statistical Physics, K Huang (Taylor and Francis)

- Statistical Mechanics: A Survival Guide, A. M. Glazer and J. S. Wark (Oxford University Press)

Other references: Statistical Physics, Daijiro Yoshioka, Introduction to the Theory of Soft Matter, Jonathan V. Selinger

⭐ Jul. 24, 2024 — Wednesday

Imporant point of the reunion:

- We are more interested in the curve behaviour.

- Changes in the code: Flip yes, remap x

- Graphs

  - Shear rate vs pressure
  - Sheare rate vs stress

- Oscilatory rheology.

- To charetirize the elastic regime.

- Change shear rate and then viscosity.

- Viscosity in dought.

- Then shearch for yield stress.

- To see the elastic limit.

- For futher simulation: Change the shear rate: Do not let the system to relax.

- Experimentally, not neccecesary you are in a stationary state.

- First we are going to center in the macroscopic propoerties.

- Daniel Bonn.

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