

Introduction to Polymer Physics
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Lecture-03
Motivation to Study Polymer Physics

In the last couple of classes we have discussed the introduction to polymer physics course and we learnt about like how polymers are made very briefly and then discussed about the types and classification of polymers and then finally came to a point on why study polymer physics.

In polymer physics we are looking at the universal features of polymers that are not much dependent on the chemistry. We will elaborate in this lecture on like what exactly polymer physics is composed off and briefly about the history of polymer physics.

As we know from previous class, polymer is a long chain of carbon which is why it is called a macro molecule and that makes it different and flexible. It is flexible because it has many conformations which makes this property not on the chemistry aspect but a property which is more like universal in nature.

Now let us imagine that we have two different kinds of building blocks- one of them is represented by circle and another one is represented by a triangle, and they are forming a polymer chain. For example this polymer chain has many conformations and then each of these take then the amount of the number of configurations that the left one has with circles will be more or less same has the right one will have with the triangles. Now by using the squares we can form a confirmation with the triangles too. So, if we look all confirmations the polymer chain can have starting like two building blocks and the number of confirmations will not depend on what the building block is but it will depend on like how many of those blocks are present here in the chain.

So, in both these cases we have 1, 2, 3, 4, 5, 6 circle blocks and the same thing here we have 1, 2, 3, 4, 5, 6 triangle blocks. So, the number of confirmations will depend on the number of blocks that we have so, as we increase the number of blocks in the circular case or a triangular case we will increase the number of confirmation as well. In the language of physics as the number of confirmations increase the entropy increases and we can say from this entropy is a function of the number of confirmation thus the entropy of the chain will be simply of function of the number of blocks. As the number of confirmations is a function of number of blocks and not exactly like what the block is composed of we have identified that the polymer chain is not dependent on the details of the chemistry where as it is more dependent on like how many blocks are connected together.

This is like one of the examples that if we start to have larger number of carbons they start to have more and number of confirmations and the properties depend on the number of confirmation not the types of building blocks. In this entropy will be the same in different kinds of polymer chains. This is like the basic premise of polymer physics that the behaviours are universal in nature and that is the reason why we see the subject be like a polymer physics not a polymer chemistry as there is a sense of universality in a things how will appear. So, in this particular case we can see two different building blocks which give rise to same kinds of behaviour. So, in general language we can say that we can build models which are referred as toy models that can give the same behaviour as the polymer chain itself.

In this lecture we will elaborate on the one of the properties is we want to look at in polymer physics. For example, let us say if we have like a polymer chain then we are interested in the end to end distance of the polymer chain typically as we know the polymer chain can take many confirmations. We don't talk about the end to end distance of particular confirmation but on the average of the end to end distance over many confirmations which turns out to have much more meaning in many cases. The more relevant is to consider the mean squared average of the confirmation and on that basis we can build a toy models which are referred as random walk

models. the common feature in all these models is that as we increase the number of blocks or the number of segments or the number of this small steps in the model we will see the end to end distance squared which will increase in proportion to the number of the same things, it turns out in many polymer chains indeed. The end to end distance squared is found to be proportional to the molecular weight of the chain or the number of repeat units “ m ” is like some number of segments or units in the in our toy model.

In polymer physics we did not need to look at the the detailed chemistry say looking at each of the carbons and what is happening there what is present inside. For example if we really zoom into particular part of the polymer chain indeed it has some kind of a structure but that is of no particular relevance on how the polymer chain is being formed as long as it possess at certain sets of features. For example this behaviour that we see in many polymer chains is something like this which we referred to as the ideal chain behaviour which we can get from toy models. This is one of the reason for doing polymer physics the other reason is the following let say if we want to look at for purely chemistry point and we want to look at the entire chain of carbons then probably we can look at the detailed chemistry of this particular polymer. We can perform quantum chemistry calculation which amounts to solving Schrodinger equation-the complicated equation. The Schrodinger equation has the solution only for very small molecules like hydrogen. So, as soon as the molecules become complicated we have to go to like numerical solution that is also possible only for small molecules containing 10 or 20 atoms. So, if we talk about anything of the order of 10,000 of atom or 1000 of atom which is a case for polymers it is almost impossible to do any kind of detailed quantum chemistry modelling. This is another reason for doing polymer physics course that the materials which polymers possess are certain universal features. The another reason is that we cannot do the detailed chemistry as quantum mechanics it is not possible today and it is not likely to be possible near future by the computational sources that we have in the world.

There are two basic premise of doing polymer physics- one quantum chemistry which is not possible and second toy models work for many features. These are two essential approaches that are typically followed while doing polymer physics.

One approach is that we start looking at the polymer chain the detailed chemistry and try to build a representation that we called a toy model and then predict the behaviour that we want to predict and then finally compared to experiments to see whether the same behaviour is observed or not. The other way of doing it is will look at experimental result we observes certain Features and then we try to build toy model that give rise to same features and then finally use the toy model to look at other kinds of polymer chains of similar in nature. So, one of them can be like a top down kind of an approach and the other one can be a bottom up kind of approach.

In a case if we start with the detailed chemistry of the polymer chain containing whatever groups represent and then using that we try to build some kind of representation. for example let say in toy model segments now represent for example certain number of carbon atoms. And then we can predict certain features for example end to end distance squared average so, we predict features and then we can do an experimental validation of that feature, and the other approach we forget about the deal chemistry and We get some experimental data then we try to find certain patterns in the data or try to extract certain features from there. So, we observe features and then we build a toy model that also possess the same features and now you see can the two paradigms- in one case we have started from the actual chemistry and try to somehow decrease the number of freedoms try to make some kind of representation that we mix the chemistry that we know and then we try to predict the features that is like a starting from the molecular structure. In the other case we start from say a experimental data in that case it is more like a fitting kind of a exercise where all we need is the models should give you the same value of the quantity or the same kind of an scaling of the quantity that we see an experiments. the advantage we hope in toy model I get from the first step approach or the second approach will also work for other types of system. So, we can use toy models to study similar systems and it is then that this models become useful because if we can get some physical understanding based on these models then we can use that in our design strategy of polymers in devising like a polymers that will give you certain types of behaviour and so on.

Polymer physics helps us to understand why the polymer chains are behaving in a certain way although by a toy model and in second way it can help us design new kinds of polymers. Once we understand what are the basic features of polymer chain that governs these kinds of behaviour, the toy model is not entirely a new idea that is only present in polymer physics as the physics folks will realise that it has many communalities with other toy models such as Ising model for magnetism that again is the toy model. But it gives you the magnetic phase transition excellent model this is the kind of approach that we are following in polymer physics.

Polymer physics is not really a very old field. It started like in twentieth century and we will mainly discuss the work of two or three male scientist in this area. One of them is Paul Flory who was an American chemist. He was in the year 1910 to 1985 he won the noble prize in chemistry in the year 1974. He started as a chemist and worked on a polymerisation reactions and built very nice physical models which were like excellent and gave very simple kind of theory. He was man with great intuition and he has made excellent models of polymer physics which we will discuss some of that in this course.

Then there is a scientist name Sir Samuel Edwards from 1928-2015 he was based in Britain he was the British physicist and Edwards did some of the more rigorous kind of a models that becomes like the modern treatments of polymer physics. And then there was another physics physicist his name was Pierre Gille de Geines he was a contemporary of Sam Edwards. He was a French physicist he also won a Nobel Prize in physics in 1991. These 3 people are the pioneers of polymer physics which we will discuss in this course. Flory made some initial achievements and the pioneer of the basic idea why this toy models should be used in polymer physics. Then Sam Edwards made certain rigorous model that represent the basis of today's polymer physics. And then finally De Gennes added a new component to it which is known as the scaling approach- something that is building on the Flory idea but that becomes useful in a many applications of polymers and it is it has much more sound physical basis.

In next class we will discuss about the random walk models in polymer physics.

