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Network in a polymer: Inputs from experimental data

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HIGHLIGHTS

- Polymers are formed when monomers join together to form a chain.
- We study evolution of network in iron acrylate polymer from monomer stage onwards and calculate the probability of degree distribution from Mossbauer experimental data.
- The degree distribution of iron acrylate polymer follows exponential distribution.

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ABSTRACT

Polymers are formed when monomers join together to form a chain. In this paper we study the evolution of a network in iron acrylate polymer from the monomer stage onwards. Our primary aim is to use experimental data to calculate the probability of degree distribution and for this purpose we use experimental Mössbauer absorption spectrum data. We observe that the degree distribution of iron acrylate polymer follows an exponential distribution.

1. Introduction

A network consists of vertices connected by edges. The degree k of the vertex is the number of edges connected to the vertex. The degree distribution $P(k)$ gives a probability that a randomly selected vertex has k links and is used to characterize a network. In recent times, a lot of attention has gone towards the characterization of the topology of complex networks. Earlier degree distribution of networks was confined to random graph theory of Erdos and Renyi [1], but with the discovery of scale free networks [2], small world networks [3] a rich and diverse class of networks has been characterized e.g. networks in superconductors [4], networks in earthquakes [5] etc. Despite the diversity of networks, they follow universal self organizing principles. Random networks follow Poisson distribution, have low average path length and low clustering coefficient. Small world networks have low average path length but high clustering coefficient and may follow an exponential distribution. Exponential distribution has been observed in the topology of transmission lines [6], some river networks [7], earthquakes [8], extensive air showers [9] etc. Scale free networks follow a power law $p(k) \propto k^{-\gamma}$. In this case a small number of preferred nodes are highly connected and the rest of the nodes which are very large in number have fewer connections.

The emergence of a power law in the topology of BA networks [2] is decided by the linear growth and linear preferential attachment. For the limited situation which involves only growth and no preferential attachment, the resulting topology is exponential. In recent times evolving networks have been studied which have features like nonlinear growth and preferential attachment. This has resulted in single models explaining most of the features of the complex network e.g. Krapivsky

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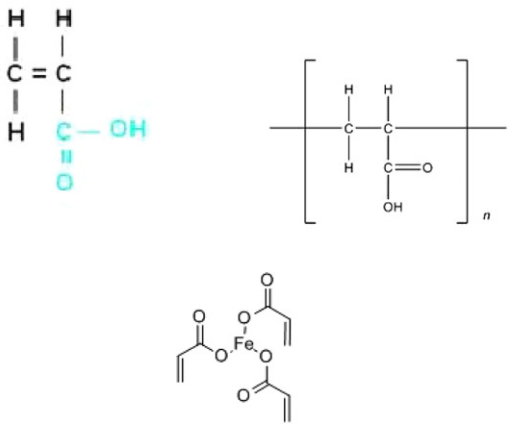

Fig. 1. Displays (left side) acrylic acid, (right side) acrylic polymer and (below) position of iron atom in the iron acrylate polymer.

et al. [10] introduced the concept of nonlinear attachment which results in power law, stretched exponential decay and a star like structure just by varying scaling exponent. Similarly physical network models [11,12] like neighborhood evolving networks can explain power law, exponential decay and transition from exponential to power law as the limiting case of a generalized approach.

In this paper we attempt to explore the polymer network using experimental data. The nature of the data that is needed should be such that it gives some information at various stages of network formation in the polymer. Thus if we can monitor some experimental parameter which varies with the degree of polymerization, then it may be possible to get some information of the network formation from that data. An ideal experimental situation demands that we should have data at each step from the monomer to polymer progression, but it is nontrivial to obtain such data. In order to get some experimental insight we revisit of our old [13,14] experimental data of Mössbauer spectroscopy of iron acrylate [14] polymer. In this experiment the Mössbauer spectrum was recorded at monomer level and also at various stages of polymerization. An area of the normalized Mössbauer spectrum is directly related to the strength of the lattice. From the area of Mössbauer absorption spectrum, recoil free factor and effective thickness can be directly obtained. From effective thickness we obtain a possible number of Mössbauer atoms participating in the polymerization and this number will give us the number of possible nodes in the network.

Polymerization can be brought about by a number of methods. It can be done thermally or passing ionizing radiation through a monomer. Radiations used for this purpose could be protons, neutrons, X-rays and γ-rays. The metallopolymers are studied in the present work, metal ions exist in the substituent group hanging outside the polymer chain. Polymerization was done using ^{60}Co gamma irradiation. The degree of polymerization [13,14] was also monitored by chemical methods and electrical conductivity.

2. Network in iron acrylate polymer

The formation of a polymer starts from a monomer. When two monomers join to form a single unit, it is called as dimer. When another monomer is added to it, trimer is formed. As more and more monomers get added, a polymer is formed. Iron acrylate is a metallopolymer obtained in a chemical reaction when three units of acrylic acid monomer react with ferric oxide to form iron acrylate and three water molecules. The iron acrylate monomer is subjected to irradiation to convert it into a polymer. In these polymers metal ions exist in a substituent group in the portion of molecules pedant to the polymer chain (see Fig. 1).

The effect of the radiation on a monomer is to create a radical. When a radical propagates through monomers a long polymer chain is formed. It has been confirmed through various studies that free radical propagation is the dominant form of chain formation in the iron acrylate polymer. The primary backbone of an iron acrylate polymer chain consists [14,15] of bonds between carbon atoms. The single bond connection between two carbon atoms of a monomer is a link or edge of this network. The whole monomer is a single node and the bond between carbon atoms is a link. The Fe atom in the monomer is responsible for Mössbauer absorption. As more monomers get added to the chain, the polymer becomes more strong and stable and Mössbauer absorption also increases. At the monomer level Mössbauer absorption is low but as the percentage of the polymerization increases, Mössbauer absorption also increases. So the area of the Mössbauer absorption spectrum can be used to get some information which can be related to the nature of the network in iron acrylate.

3. Calculation of number of nodes

In the following we will discuss how we obtained the number of nodes and links for a iron acrylate network. In order to calculate the number of nodes we need two parameters: (a) effective thickness T and (b) recoil free factor f_a. These two