Dr. S. Sivaram talks about the future of the science of polymers materials which is now entering a second wave increasing the importance of 'convergence research'.

Dr. S. Sivaram
CSIR Bhatnagar Fellow
Polymers and Advanced Materials Laboratory
CSIR - National Chemical Laboratory, Pune

Material Science of Polymers
What Lies Ahead?

The Progression

Polymers were the product of post war renaissance in the chemical industry driven by the promise of inexpensive petroleum derived feed-stocks. The fifties and sixties saw the introduction of many polymers that changed the face of human civilisation. From early curiosities polymers became an indispensable part of our daily life, and so ubiquitous, that we no longer realise how addicted we are to polymer materials! Today, the world produces in excess of 250 million tonnes of polymers, providing livelihood to billions of people and has a business value exceeding USD 1.5 trillion per annum.

This progress is truly spectacular if one considers the fact that the science of polymers is less than 100 years old and emerged only in 1920. It took another 20 years for the science and engineering to mature before the first commercial products began to emerge. World War II provided the impetus and beginning 1940, the world witnessed in rapid succession, the introduction of several new polymers which transformed all walks of human life, be it shelter, clothing, transportation, human health and hygiene, energy, information technology, communication, sports, leisure and entertainment.

The rapid rise of a new industry in the early fifties spurred, both, academic and industrial research. Polymer science began to emerge as a new interdisciplinary subject, taught in universities around the world, melding seamlessly the disciplines of chemistry, physics and engineering. A new breed of scientists and engineers emerged to work in academic research and in large industrial R&D laboratories in the area of polymer science.

Since the early nineties, the world has seen far less revolutionary discoveries in polymer science. The entry barriers for a new polymer in the market has increased, driven by the relentless forces of globalisation, easier diffusion of technologies, issues of sustainability, pressure from regulatory agencies and rapid commoditisation. Most companies that pioneered discovery driven product development in polymers have exited the business. This has resulted in major downsizing of the research efforts as well as opportunities for employment to those trained in this discipline in the more developed parts of the world. The manufacturing geography has progressively shifted to regions of consumption, namely, China, India and the Far East. Manufacturing companies in these regions have been content to exploit the economies of scale in a market that is underserved, rather than push the frontiers of science and technology.

So it is pertinent to ask, what is the future of this science in an environment where industry is probably not challenged anymore by a compelling need for discovery and innovation to protect or grow its bottom lines? It should be recognised that more than any other branch of science, the growth of the science of polymer materials was intimately intertwined with the growth of the polymer industry. Consequently, it is only natural that many practitioners of this branch of science feel a little orphaned now. Is there an emerging science, industry or an unmet application need which needs greater attention now? What lies ahead for the science of polymer materials?

Issue of Sustainability

This is one of the most discussed issues regarding polymer materials. I believe that the issue is a little overstated. We consume less than 10 per cent of the global output of oil and gas for the manufacture of polymers. This apart, converting hydrocarbon to useful materials with substantial value addition makes eminent sense. It is the combustion of the hydrocarbons to generate electricity and in the engines of the automobiles which is unsustainable. Consequently, the feverish activity to shift the resource base of the polymers from hydrocarbons to carbohydrates (biomass) is not entirely founded on good reason. In addition, carbohydrates are good resources to make oxygenated feed-stocks, not olefins and aromatics. The only material that makes sense to make from biomass derived resources is aliphatic polyesters. Although important, this class of material alone can hardly replace the vast majority of polymers that we consume now. However, for most of the large volume

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materials that we consume today or will need tomorrow, hydrocarbons are still the most efficient raw materials.

There is a buzz in the press about Bio PE, Bio PP, Bio PET, Bio PVC, Bio Butyl, Bio butadiene etc. All these products are based on sugar or starch and involve complex chemistries for conversion. The conversion of starch to ethylene has an overall atom efficiency of 65 per cent compared to > 90 per cent for the conversion of hydrocarbons to ethylene. To produce sufficient ethylene from ethanol to build one 350,000 TPA of polyethylene, we will need 400 square miles of land planted with sugarcane! To put things in perspective, the current global capacity of polyethylene exceeds 100 million tonnes. Renewable resources derived polymers will offer some unique solutions in specific cases. Functional monomers and polymers which are difficult to access using synthetic chemistry should be the most sought-after targets. Just as fossil fuel derived polymers, bio-derived polymers will be valued for the properties they bring to applications. The fact that they are derived from a renewable resource may just be incidental.

The other issue is the sustainability in use of polymers. Polymers are the subject of onslaught of negative public perception on account of the fact that they are non-biodegradable and also, in select cases, some of the chemicals or additives used in the manufacture of polymers may cause health hazards. We as a society abhor seeing plastic litter without any qualms of causing it in the first place. There is evidence that significant quantity of plastic waste ends up in water bodies and oceans causing long term damage to marine ecosystems and finding its way into the human food chain. Many solutions are available for mitigation, but compliance is complicated by poor human habits and the question of who bears the cost of waste management infrastructure. Evidence based science must contribute better to understanding the life cycles of plastics in different environments. More innovation is needed in the design of packaging materials that incentivise recovery. Single use plastics must be voluntarily phased out and more sustainable materials must be found to replace them. Capabilities for recycling must be built-in at the initial stages of product design and deployment.

Precision Polymer Synthesis

Polymers are products of chemistry, that is, the ability to create new compositions of matter using principles of chemistry. Over the years, a large number of tool boxes have emerged which enable chemists to assemble molecular structures at will. However, challenges still remain. For example, we still cannot adequately control polymerisation catalysed by metals or those prepared by step growth reactions. Synthesis of polymers which precisely defines the sequence of co-monomers or control of both, topology and molecular geometry over large length scales still poses several challenges.

From Structures to Functions

Materials found in nature are mostly functional, whereas, man-made materials are mostly devoid of functions. An intriguing and complex question is - can man make materials with functions that mimic natural materials? This is one of the most sought-after areas of contemporary research where polymer science has made only small progress. The reason is because polymer science is only just beginning to understand the concept of 'emergent properties', when the whole becomes larger than the sum of the parts. The key to success in this area will be the ability to assemble complex hierarchical structures using controlled kinetic and thermodynamic pathways.

Design of New Materials

Polymers are organic materials with defined molecular structures and physical properties. They are shaped into useful objects predominantly by melt processing techniques. Exploiting the molecular structure-properties-processing-performance relationships is the key goal of polymer material science. With the availability of large data, it is possible to reasonably define molecular structures, super-molecular structures and solid state properties which will lead to desired product performance. Similarly, it is possible to predict processing performance from knowledge of polymer melt properties. What was once a linear, intuitive and largely trial and error experimentation process is now moving into a more structured integrated design continuum, called Materials Genomics. Material genomics will blend computational modelling with physical experiments, integrate computing and information technologies with advances in material characterisation and replace empirical studies with mathematical modelling and simulations. Progress in this area will require ability to create accurate material performance models and their validation using theory and experiments and a shared open source platform for data exchange that will enable scientists to index, search and compare data. Such tools and approach based on large data repositories and increased data transparency will allow concurrent design, systems engineering and manufacturing, reducing the time to market of new product technologies.

In Conclusion

The science of polymer materials is now entering a second wave. This wave is equally exciting and challenging. There are still many unmet property gaps in polymer materials for defined end applications. So the story is far from over. One of the hallmarks of this wave will be increasing importance of 'convergence research', which is the unification of two or more disciplines of science to address a research problem. This wave will also demand greater collaboration between academia and industry as partners in development.