Tailoring Polymer Properties from First Principles

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Polymers, commonly known as plastics, are long chain macromolecules having molecular weights in excess of 10,000 g/mol and size of the order of tens of nanometers. Polymers exhibit a host of useful properties such as excellent mechanical strength, low density, thermal and electrical insulation, ease of shaping, low energy consumption per ton of material produced or processed, high production rates, reusability, long service life and the possibility of dialling-in other unique properties such as electrical conductivity, biocompatibility and optical properties. As a result of their versatility polymers have become the materials of choice in many engineering applications. Today the global consumption of polymers exceeds 200 million tons and they are used in diverse sectors such as consumer products, packaging, automotive, appliances, transportation, construction, medical products and strategic and space applications. Indeed it is hard to imagine modern life without plastics!

Plastics can be roughly categorized on the basis of their cost/performance/price into commodity plastics, engineering plastics and high performance plastics as shown in Figure 1. Commodity plastics occupy the bottom of the pyramid because of their low cost and large volumes of consumption; high performance plastics are placed near the apex of the pyramid because of their high cost and low volumes of consumption, and engineering polymers span the region between the two. Demands for lower prices, higher performance and sustainability has spurred new innovations in polymers causing the borders between these three categories to be dynamic. The following examples illustrate this point:

1) Acrylonitrile-butadiene-styrene copolymer (ABS), an engineering polymer, is the material of choice when it comes to manufacturing of large automotive components such as dash boards and fenders because of its ease of thermoformability. On the other hand polypropylene (PP), a commodity polymer, is cheaper and has an end-use property portfolio that is adequate for such applications. Therefore there is a growing demand to substitute ABS with PP, especially in low cost automobiles like the *Nano*. The problem is that PP is not easy to thermoform. Can one tailor PP resin so as to make it thermoformable?

2) Polyethylene (PE) and polystyrene (PS), both commodity plastics, are used in food packaging applications such as films and thermoformed trays and covers. Growing demands on sustainability has spurred the development of degradable plastics such as poly(lactic acid) (PLA), which if used in food packaging applications can significaly reduce the environmental burden of plastics. In this case sustainability issues are forcing the substitution of commodity plastics like PE and PS with an engineering plastic like PLA. However, PLA is not easy to process into films and thermoformed products. Can one tailor PLA to make it easily processible?

3) Polycarbonate (PC) is a transparent and tough engineering polymer that is used in media (CD), displays (LCD screens), sky-lights and windows (construction and

transportation) and many other applications. An increase in the glass transition temperature, UV stability and scratch resistance of PC is desired so as to push it into an application space which is currently occupied by high performance polymers or other engineering polymers. It is however essential for PC to not lose its toughness while improving other properties. Can the toughness of PC or indeed of any other engineering polymer be tailored?

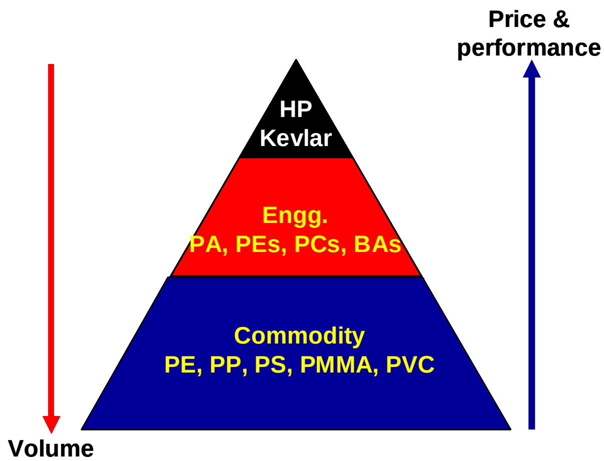

Figure 1: The pyramid of plastics. Consumption volumes increase while price and performance increase as one goes towards the base of the pyramid.

Meeting the challenges described above and indeed many such similar challenges requires a fundamental understanding of how the molecular structure and topology of polymers influences their dynamics, and how the macromolecular dynamics affects the flow and solid-state properties of polymers. While empirical structure-property relations in polymers have been investigated for many decades, it is only in the past three-four decades that a quantitative understanding of macromolecular dynamics has started to emerge. For instance, today we have a better understanding about the mobility of long, flexible and entangled polymer chains which dictates their rheological properties. This knowledge can be used to tailor a PP or a PLA molecule to facilitate the processibility of these polymers. Similarly, today we understand better how the segmental mobility of polymers in their glassy state affects their mechanical response. This understanding can facilitate the modifications of polymers like PC to suit applications that demand toughness under adverse conditions.

Understanding the complex linkages between macromolecular structure and final properties of polymers requires careful translation of knowledge across several orders of length and time scales. In order to develop such fundamental understanding, a sophisticated tool kit comprising experimental, theoretical and numerical techniques is necessary along with a seamless confluence of engineering and science disciplines. In my talk I shall attempt to demonstrate this with the help of a few illustrative examples from research at NCL. I will also present the current unmet scientific and engineering challenges that are required to be overcome in order to complete our understanding in this technologically important area.