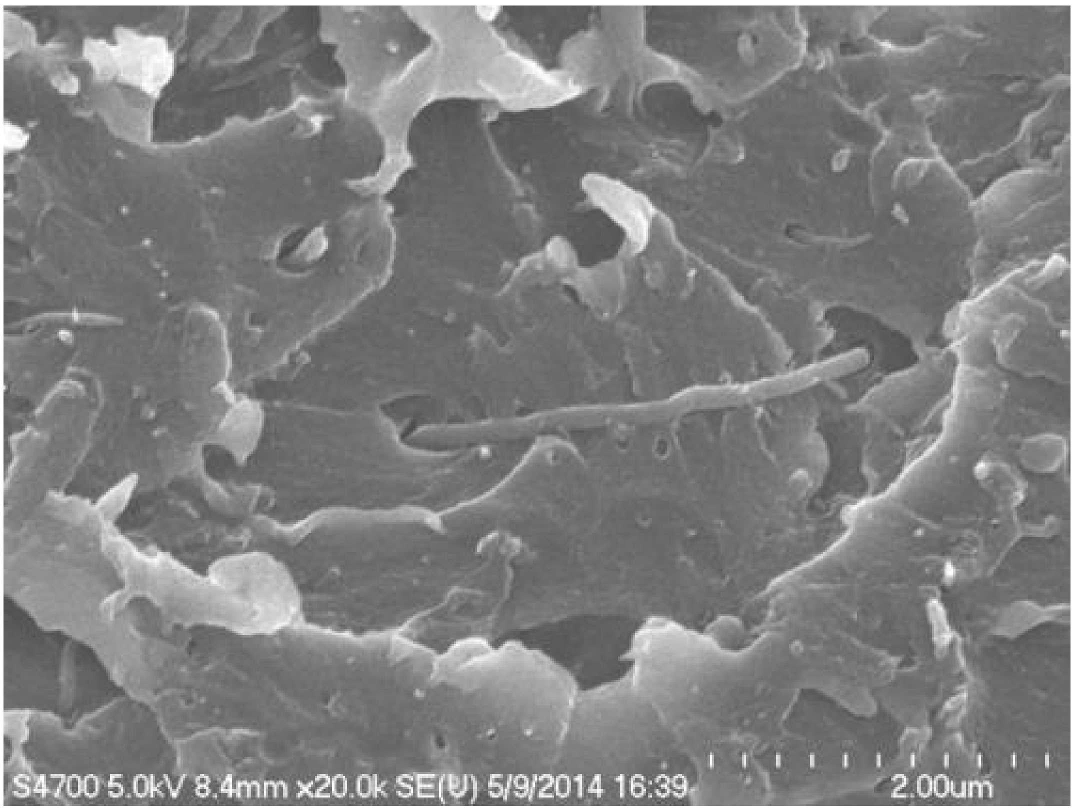
New class of industrial polymers discovered

May 15 2014



A Scanning Electron Microscopy (SEM) image of the new ultra-strong polymer reinforced with carbon nanotubes. Credit: IBM

(Phys.org) —Scientists from IBM Research have successfully discovered a new class of polymer materials that can potentially transform manufacturing and fabrication in the fields of transportation, aerospace, and microelectronics. Through the unique approach of combining high performance computing with synthetic polymer chemistry, these new materials are the first to demonstrate resistance to cracking, strength higher than bone, the ability to reform to their original shape (self-heal), all while being completely recyclable back to their starting material. Also, these materials can be transformed into new polymer structures to further bolster their strength by 50% - making them ultra strong and lightweight. This research was published today in the peer-reviewed journal, *Science*, with collaborators including UC Berkeley, Eindhoven University of Technology and King Abdulaziz City for Science and Technology (KACST.), Saudi Arabia.

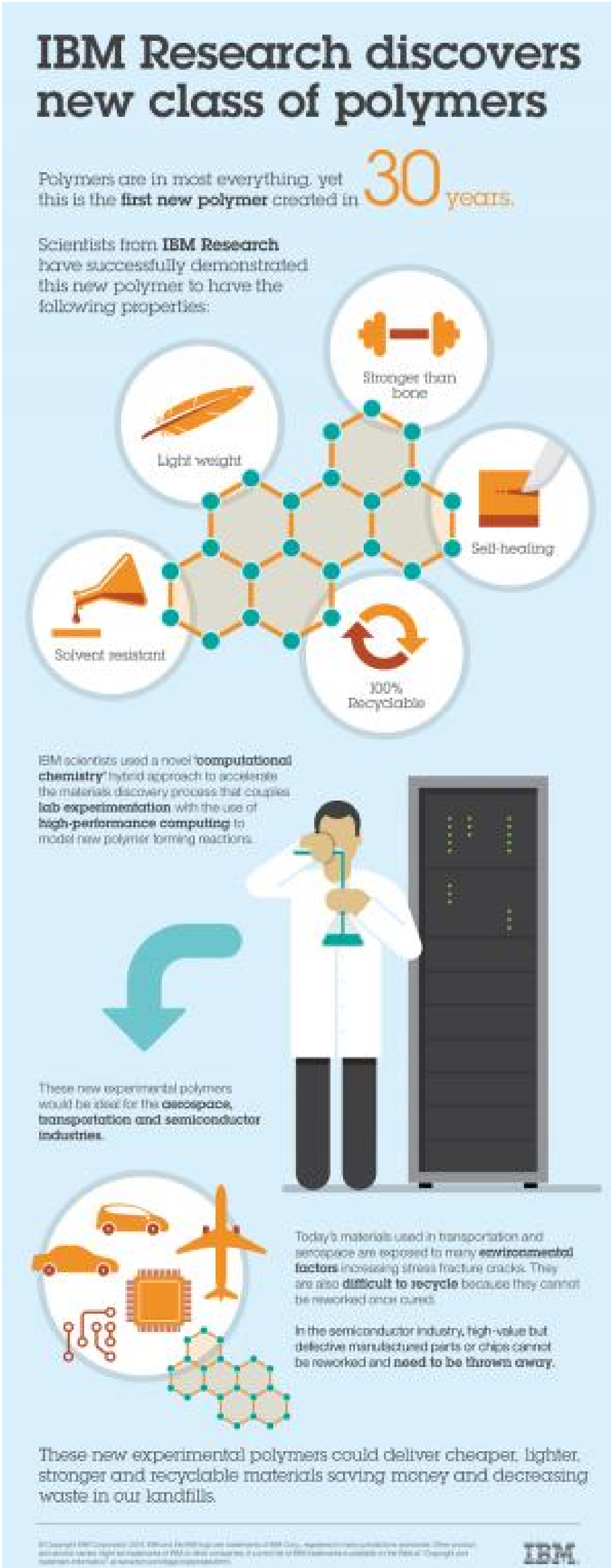
Polymers, a long chain of molecules that are connected through chemical bonds, are an indispensable part of everyday life. They are a core material in common items ranging from clothing and drink bottles (polyesters), paints (polyacrylics), plastic milk bottles (polyethylene), secure food packaging (polyolefins, polystyrene) to major parts of cars and planes (epoxies, polyamides and polyimides). They are also essential components in virtually every emerging advanced technology dating back to the industrial revolution - the steam engine, the space ship, the computer, the mobile phone.

However, today's polymer materials are limited in some ways. In transportation and aerospace, structural components or composites are exposed to many environmental factors (de-icing of planes, exposure to fuels, cleaning products, etc.) and exhibit poor environmental stress crack resistance (i.e., catastrophic failure upon exposure to a solvent). Also, these polymers are difficult to recycle because they cannot be remolded or reworked once cured or thermally decomposed by heating to high temperatures. As a result, these end up in the landfill together with toxins such as plasticizers, fillers, and color additives which are not biodegradable.

IBM's discovery of a new family of materials with a range of tunable and desirable properties provides a new opportunity for exploratory research and applications development to academia, materials manufacturers and end users of high performance materials. Two new related classes of materials have been discovered which possess a very distinctive range of properties that include high stiffness, solvent resistance, the ability to heal themselves once a crack is introduced and to be used as a resin for filled composite materials to further bolster their strength.

Also, the ability to selectively recycle a structural component would have significant impact in the semiconductor industry, advanced manufacturing or advanced composites for transportation, as one would be able to rework high-value but defective manufactured parts or chips instead of throwing them away. This could bolster fabrication yields, save money and significantly decrease microelectronic waste.

"Although there has been significant work in high-performance materials, today's engineered polymers still lack several fundamental attributes. New materials innovation is critical to addressing major global challenges, developing new products and emerging disruptive technologies," said James Hedrick, Advanced Organic Materials Scientist, IBM Research. "We're now able to predict how molecules will respond to chemical reactions and build new polymer structures with significant guidance from computation that facilitates accelerated materials discovery. This is unique to IBM and allows us to address the complex needs of advanced materials for applications in transportation, microelectronic or advanced manufacturing."


IBM Research discovers new class of polymers
Polymers are in most everything, yet this is the first new polymer created in 30 years.
Scientists from IBM Research have successfully demonstrated this new polymer to have the following properties:
Stronger than bone
Light weight
Self-healing
Solvent resistant
100% Recyclable
IBM scientists used a novel "computational chemistry" hybrid approach to accelerate the materials discovery process that couples lab experimentation with the use of high-performance computing to model new polymer forming reactions.
These new experimental polymers would be ideal for the aerospace, transportation and semiconductor industries.
Today's materials used in transportation and aerospace are exposed to many environmental factors increasing stress fracture cracks. They are also difficult to recycle because they cannot be reworked once cured.
In the semiconductor industry, high-value but defective manufactured parts or chips cannot be reworked and need to be thrown away.
These new experimental polymers could deliver cheaper, lighter, stronger and recyclable materials saving money and decreasing waste in our landfills.
IBM

Credit: IBM

Materials Science Innovation

The field of material science is often thought of as a mature field, with the most recent new class of polymer materials being discovered and introduced to the commercial market decades ago. Also, most current polymer research involves studying polymers that are "old" polymers and combining known polymers together or simply adjusting chemical functional groups on known polymers to access desired properties, as opposed to making completely new polymers.

IBM scientists used a novel 'computational chemistry' hybrid approach to accelerate the materials discovery process that couples lab experimentation with the use of high-performance computing to model new polymer forming reactions. The unconventional method is a departure from traditional techniques and led to the identification of several previously undiscovered classes of polymers in what was believed to be an established area of materials science researched extensively since the 1950s.

Ideally, scientists could insert a list of requirements into a computer to design a material that meets those exact conditions. Unfortunately, the reality now is that materials are still primarily discovered only by experimenting in the lab based on the scientist's knowledge, experience and educated guesses. IBM Research's computational chemistry efforts can take out a lot of this guesswork and accelerate a whole new range of potential applications from developing a disease-specific drugs or cheap, light, tough and completely recyclable panels on a car.

"By joining forces with IBM Research and bringing together the minds of KACST and IBM scientists, we have managed to merge the strengths of both sides, making it possible to bring forth novel green materials that exhibit excellent properties while being completely recyclable. We believe that this work can have significant impact to multiple industries and hope to see more great things come from our collaboration," said his highness prince Turki bin Saud, KACST VP of Research Institutes.

How it Works

These polymers, formed from the same inexpensive starting material through a condensation reaction, these molecules join together and lose small molecules as by-products such as water or alcohol and were created in an operationally simple procedure and are incredibly tunable.

At high temperatures (250 degrees Celsius) the polymer becomes incredibly strong due to a rearrangement of covalent bonds and loss of the solvent that is trapped in the polymer (now stronger than bone and fiberboard), but as a consequence is more brittle (similar to how glass shatters).

Remarkably, this polymer remain intact when it is exposed to basic water (high pH), but selectively decomposes when exposed to very acidic water (very low pH). This means that under the right conditions, this polymer can be reverted back to its starting materials, which enables it for reuse for other polymers. The material can also be manufactured to have even higher strength if carbon nanotubes or other reinforcing fillers are mixed into the polymer and are heated to high temperatures. This process enables polymers to have properties similar to metals, which is why these "composite blends" are used for manufacturing in airplane and cars. An advantage to using polymers in this case over metals is that they are more lightweight, which in the transportation industry translates to savings in fuel costs.

At low temperatures (just over room temperature), another type of polymer can be formed into elastic gels that are still stronger than most polymers, but still maintains its flexibility because of solvent that is trapped within the network, stretching like a rubber band.

Probably the most unexpected and remarkable characteristic of these gels is that if they are severed and the pieces are placed back in proximity so they physically touch, the chemical bonds are reformed between the pieces making it a single unit again within seconds. This type of polymer is called a "self healing" polymer because of its ability to do this and is made possible here due to hydrogen-bonding interactions in the hemiaminal polymer network. One could envision using these types of materials as adhesives or mixing in with other polymers to induce self-healing properties in the polymer mixture. Furthermore, these polymers are reversible constructs which means that can be recycled in neutral water, and that they might find use in applications that require reversible assemblies, such as drug cargo delivery.

More information: Recyclable, Strong Thermosets and Organogels via Paraformaldehyde Condensation with Diamines, *Science* 16 May 2014: Vol. 344 no. 6185 pp. 732-735. DOI: 10.1126/science.1251484

Provided by IBM