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THE JOURNEY TOWARDS COMPUTATIONAL MATERIALS

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ABSTRACT

This research explores the journey towards computational materials by looking at metals, powder-based materials, composite materials and smart materials. This journey can not be explored without considering the processes used for producing the materials, such as 3D printing along with basic principles of material science. If we wish to push forward the research of computational materials, we have to address critical problems such as energy harvesting, miniaturization of sensors and the ability to create communication between materials (Waghmare, 2020). One of the biggest challenges is to decide upon which type of computational model would be suitable for such an environment. The applications of computational materials are numerous, and they range from wearable materials and furniture to automotive and construction materials.

INTRODUCTION

Early civilizations are often classified as different ages that started by the discovery of a new effective material. After the first age, the stone-age, the bronze-age emerged some 5300 years ago. Bronze is a combination (alloy) of the metals copper and tin and proved to be hard enough defeat stone as the preferred material for weapons and household items (Bahl, 2020). The bronze-age also marks the start of the science of metallurgy (Qader, 2019). The more general field of material science has during the last two centuries focused research into synthesizing new types of materials. These are often divided into four groups: metals, ceramics, polymers and smart materials (Qader, 2019). Material scientists have worked together with engineers to develop materials needed for the advanced products we see today and are important participants in the development of advanced products.

The 20th century is the time when we started talking about smart, or responsive materials (ref), specifically designed for a certain purpose, but at the same time these materials exhibit properties ideal for their specific application. Examples range from photochromic polymers, fiber optics and solar cells to shape memory alloys and piezoelectric materials (Drossel, 2015). However, the 20st century has also brought forward computational science, software engineering and technologies, digital communication and theories and the Internet. They paved the way towards new types of materials: computational materials (Abowd, 2020) . They are viewed differently compared to any other materials, because we assume that they have computational characteristics. However, these computational aspects of modern materials are directly triggered by something else in technology and science. It is the presence of pervasive computing, numerous small and sometimes hand-held devices which can compute, be connected though wireless networks and the creation of the internet of things / internet of everything. They have all been pushing materials science towards computational materials and Internet of Materials (Arora, TBA).

In this paper we look at the pathway towards the reality of creating internet of materials and look at challenges, obstacles and possibilities of making them our instant reality. This journey must include the impact of smart materials on our way of exploiting material science and their characteristics which enable us to talk specifically about computational materials.

SMART MATERIALS

Smart materials are materials that respond to external stimuli such as stresses, humidity, light, temperature fields, electric or magnetic fields (Qader, 2019). When subjected to these fields, one or more material properties changes so that the material can be utilized to perform a specific task. The change is reversible. When the external stimulus ceases, the properties of the materials go back to their original state. However, there is more to smart materials. They may be able to absorb energy from their surroundings and convert it to another form. Examples are pyro-electric materials that create electric energy from heat, and electrostrictive materials that produce mechanical energy if exposed to an electric field. Therefore, smart materials are often divided into two groups: active smart materials (ASM) and passive smart materials (PSM). Those materials that change their properties based on environmental inputs belong to the first group, while those converting energy from one form to another belong to the second group.

There are numerous examples of Smart Materials. Such materials are often used in sensors and actuators, like thermostats or light sensitive detectors. An example known among the public is photochromatic glasses that can change their color when exposed to sunshine (Ferrara, 2020). In the pipeline are smart sleeves on your jacket that will automatically retract when exposed to increased temperature, to keep you cool, and go back to original state when the temperature drops. Also under development are breathable polymer textiles that can expand when subjected to a rise in temperature, increasing the size of small holes in the fabric enabling air to be exchanged and, in this way, cool you down (Qader, 2019).

The difference between ordinary and smart materials can easily be seen by reviewing materials used in temperature sensors. These are often based on the temperature dependence of the electrical resistivity of a conductive material. Often used is platinum which exhibits a resistance that rises constantly with increasing temperature from about 20 K to over 1500 K. This steady increase is advantageous in some applications but in others, the increase in resistance pr Kelvin is not high enough. Replacing platinum with a smart material such as doped barium titanate ceramics can give an increase in resistance six times as high as for pure platinum but over a limited temperature span. This smart material, in contrast to pure platinum, can be used for self-regulating heating purposes (Cao, 1999).

Smart materials have been used especially in transducers and precision mechatronic control systems for a number of years. In the mid-1980s scientists and engineers started integrating smart materials applied in sensors and actuators with large scale structures, thus introducing the concept of smart systems (Tzou, 2004) . By adding the capability to store, process and communicate data, such smart systems can ultimately evolve into intelligent systems.

The field of smart materials is in the crossing point between science and engineering and combines areas such as physics, mathematics, chemistry, and the engineering disciplines of material, electrical and mechanical engineering (Cao, 1999). Of special complexity are sensors combining several types of smart materials, like temperature and humidity driven sensors. Such a web of disciplines creates opportunities, but may also act as inertia, since the development of novel products utilizing smart materials may be hampered by the lack of progress in one of the participating disciplines (Akhras, 2000).

Computational Materials

Computational materials are everyday materials with the ability to behave as connected computational entities (Abovd, 2020). If we can find them or invent them, they might become the building blocks of the internet of materials, IoM.

There are numerous possibilities of inventing or finding computational materials. They can be functional paper, intelligent building materials or intelligent clothing (Dunne, 2021). They can expand the specter of what we today include in the internet of things. We know that IoT devices have for the most part been built using traditional electronics. By contrast, developing computational capabilities through the properties of new materials themselves begins to blur the line between physical and digital products.

Furthermore, the internet of Things has tried to hide computing into everyday objects, such as light bulbs, television sets and speakers, but we are still far from a complete blurring of the physical and digital worlds, as predicted by Weiser (1991). To make something computational still requires "smarts" composed of off-the-shelf integrated circuits housed in modules that are packaged with existing objects. We could lament that computing is too separate from the materials of everyday objects. A different direction, as proposed inn Weiser's vision, suggests starting with the materials of everyday life and creating computation from there. This is at the core of Internet of Materials (Abowd, 2020), where the very materials of objects and surfaces are augmented or manufactured to have computational capabilities.

Applications

Applications are created by designers. These can be roughly separated into two groups. One group is comprised of technical designers, and their background is usually in engineering. The products they design are often technically advanced, and systematic development methods are used during the design. The second group is comprised of product designers. The products are often consumer products, where visual appearance and form is of importance. In contrast to the designers in the first group, these designers often have an eye-minded and intuitive approach. This can be beneficial in some respects, but also comes with the disadvantage that these designers usually do not have a complex technical background in neither smart materials nor computational materials, and hence do not use these during their design process (Drossel, 2015). This problem can be partially overcome by the application of computer aided design tools but will still be an obstacle in the proliferation of new exiting materials.

Electromechanical devices are increasingly miniaturized and may in the future be smart enough to communicate directly with the human brain. This opens up for ears that will enable us to hear sounds beyond normal frequency range, supersensitive noses that will allow us to smell as good as a dog, and eyes that permits us to see what we cannot normally see, such as in the infrared spectrum (Cao, 1999).

One of the most obvious applications of computational materials is in the form of fabric. If used in clothes, the fabric can contain sensors that can relay information of various types to the person wearing the clothing. The sensors can alert if the piece of cloth needs to be washed, or if it is torn. In a military situation a t-shirt can detect a hit by a bullet, analyze the situation and send information about the extent of the injury to a command post.

For civilian use, one can envision fabric that can give a discreet hint that more deodorant is needed in the armpits (Yeric, 2019) or inform of increased body temperature and give advise to remove extra clothing to reduce the body temperature before this increased temperature is noticed by the person wearing the clothes.

Computational materials can find industrial applications which will be of great importance. One example is the idea of embedding sensors into cast metal during the casting process (Carlsson, 2017). With their small sized, distributed microsensors can be incorporated into cast structures without interfering with the normal operation of the component. These sensors can be used to monitor the performance of the product once it has become part of a structure, thus turning metal components into digital components. It can even be possible to use them to monitor the casting process itself, but this electromagnetic noise during casting pose problems for the communication with the sensors which need to be resolved (Kobliska, 2005).

The idea of embedding sensors into a cast product is easily expandable into the areas of additive manufacturing, composite materials and powder-based manufacturing processes. These technologies provide products in an ever-increasing spectrum. One of the most critical areas is the aerospace industry. Recent years have seen a transition from the "silver eagle" era (aluminum-based fuselages) to the "blackbird" area with the fuselage made of composite materials. Composite materials are especially susceptible for hidden damages and the use of embedded sensors may present a revolution in the capability to detect and monitor these damages (Lehmhus, 2013).

Of special interest for most people are applications that affect their daily life. Ordinary products familiar to most people may be equipped with intelligence but may still look the same as before. If you hurt yourself, you put on a band-aid. Future band-aids can be equipped with sensors and processing capability along with ability to communicate with external devices, like a smart phone (Lehmhus, 2013). Such a device needs to be able to harvest energy directly from the phenomenon being sensed. It this case, maybe the pulse of the person will be sufficient. The band-aid can then tell you if you are developing an infection in the wound, or if the wound is still bleeding. It can also tell you when you safely can remove the band-aid. This type of computational material will be short-lived and disposable. For other applications, the material needs to be programmable to be able to adapt to different or improved functionality.

The Impact of Internet of Things

For a decade, the Internet of Things (IoT) has been a buzzword in the communications, computer science, software and general engineering. It started when we mastered wireless and mobile technologies in computing and communications, but it resurged again when pervasiveness became our reality. The field of IoT expanded toward everything we can imagine. CISCO defined Internet of Everything (IoE) almost a decade ago. Today we talk about Internet of Medical Things, Internet of Vehicles, Internet of Trees, and so on.

In the last couple of years, we also witnessed advance in creating infrastructures for making IoT widely operational. These are mostly computational infrastructures, apart from communication technologies which enable connection between physical devices across IoT. Therefore, IoT is now related to cloud computing, but it can also use cloudlets and fog computing (Nadeen, 2020). However, the problems we have experienced with cloud computing (Nadeen, 2020) pushed the research IoT towards the edge of computer network in order to make any implementation of IoT efficient and usable. Edge computing appeared to become the ideal solution for IoT, but this may have consequences in terms of building computational power at the edge. Obviously physical devices which are able to compute have to become more powerful or we have to invent a new generation of devices. Could we invent new materials which will make edge computing more powerful? Could these materials be interwoven into current devices which create IoT and IoE? Will computational materials enhance the experience of internet of things???

OUTLOOK

The multidisciplinary nature of this field is problematic in several ways. One of them is the lack of a common terminology, which can be a source of misunderstandings (Spillman, 1996). It also makes it more difficult for any one participant to maintain an overview of the state of the art in other fields.

There are today still major challenges present in the application of computational materials. Current research focuses on long-term stability, robustness and reliability of both hardware and data processing levels. The challenges are numerous, and it will take a community of professionals to address them, rather than just individual designers.A material/data interface that is developed for mass production allows for continuous data logging during use. This can revolutionize how designers approach a design problem. By having a repository of data from a similar product in use, the designers can move from a "we think" attitude to a "we know" attitude thus enabling data-backed design decisions (Hosny, 2017). Design is, however, not always a purely "scientific" endeavor, or optimization exercise, but often also regarded as an art. The data is giving us mere recommendations and the interpretation of the data is completely up to the designer (Hosny, 2017).

The vast amount of data needs to be handled in an effective way. Machine learning may be a way forward to cope with the shear amount of data (Hosny, 2017).Advances in materials science and manufacturing today signal a time when we will be able to manufacture new everyday materials that have computational capabilities "woven" into them, or wireless sensors that are either so small they are imperceptible or look and feel like the materials into which they are embedded.

In this way, our future world will become increasingly hybrid (Fuchsberger, 2019). The world will move towards a state where the physical and digital are inextricably linked, with all of the potential opportunities and concerns that inspires. The distinction between a physical world and a digital one may even become obsolete. Computation will be (where it is not already) an inherent part of our environment.

It is vital to remember that what drives the adoption of new technologies are key applications that compel consumers to buy and companies to invest in necessary infrastructure.

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