Digitalisation of Material Science – Improving Product Design in the Context of Industry 4.0

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Abstract.

The pace of transition from rapid prototyping to rapid manufacturing within the framework of Industry 4.0 has increased in recent years. Metal-based additive manufacturing is now quite widely deployed in the aerospace industry and in the tooling industry due to the significant weight savings which can be made using additive manufacturing and through topology optimization as well as the freedom in design. Plastic parts manufactured using 3D printing are now becoming more common place with the capability to produce large sized plastic parts from a range of high-performance materials. There are now growing applications in dentistry and medicine. This increased rate of use of direct digital manufacturing to produce commercial products takes place within the backdrop of the major societal challenge of climate change. There is now an increased realization of the need to make wider use of sustainable materials in the manufacturing of products with a much -reduced carbon foot print.

It is very challenging to develop a universal approach to the digitalization of Material Science given the broad range of materials in use and the realization during the 20th Century, that the properties and performance of a material not only critically depend on its chemical composition but also on the distribution of those atomic elements in the microstructure of the material and the texture of the microstructure. Over recent years, there has been major developments in the field of material simulation which has been acting as a trigger to the discovery process of pharmaceuticals and the selection of promising compounds to take forward to the synthesis, characterization and testing phases of this discovery program. Although there are promising developments with simulations of metal alloys and polymers, there is no method which is available for such material optimization to be incorporated and automated in the work stream of direct digital manufacturing.

This paper is focused on the development of a structure which enables the integration of the processes of material synthesis, characterization, material optimization, product design and fabrication into a single automated work flow. We will identify the areas where considerable development is required and how existing methodologies can be adapted. We introduce the concept of morphology or property optimization .We explore how we can use this approach to optimize the complete manufacturing process from synthesis to fabrication to yield high value products with new designs closely linked to the spatially resolved digital specification of the material. This structure will clearly enable the effective development of digital twins for the whole manufacturing cycle from raw materials

selection, synthesis, characterization, product design and fabrication which we believe in the future will extend to the future life cycle and end of life processes of reuse and recycle.

Introduction

Industry 4.0 is an umbrella concept to describe what is usually seen as the 4th Industrial Revolution [1]. The first industrial revolution, which took place in the 18th Century and introduced the mechanization of industrial production using machines powered by water and steam. The second industrial revolution which occurred in the 19th Century centered on mass production based on the assembly line. It took place as a consequence of electrification which enable the provision of localized power. The third industrial revolution took place in the mid 20th Century and arose due to automation based on electronics and computers. The fourth industrial revolution is taking place now in the early 21st Century and arises from Digitization and the introduction of digital technologies. Now of course this is a broad topic, but essentially involves real-time control and decision making, the introduction of smart processes, the optimization of processes and integration of computer networks.

To give a particular example, with which many will be familiar. The process of selecting the "best" route to travel from A to B, pre 1980s involved working with maps and distance tables. Now the widespread user of satellite navigation not only provides a quick method for establishing the "best" route but also a choice of criteria for the best route such as avoiding tolls or motorways [2]. However, the system provides much more than that by taking advantage of the many sensors (in other words the users) in the system, it is able to locate slow moving traffic and stationary traffic and so as to identify dynamically the fastest route, The latter aspects arise from what is sometime referred to as the Internet of Things (IoT) [3].

In manufacturing much of the system is digitized as the products are now designed using computer aided design which can integrate the optimization of the design through techniques which included topological optimization. Recently, the rapid development of direct digital manufacturing has taken place using technologies such as 3D printing, stereolithography, directed energy deposition, selective laser melting and other powder bed techniques [4]. Now in the research laboratory, techniques are being developed which provide for the automatic correction of products being fabricated by direct digital manufacturing, using computer vision and dynamic decision making [5]. There are thoughts of Digital Factories of the Future which can be digitally reconfigured to align the factory with the product required in a particular period of the year [6]. Some of this has arisen from the repurposing of factories during the COVID 19 pandemic.

Within this rapidly changing manufacturing environment, there appears to be a critical area which is not receiving a great deal of attention which is the area of the materials. We need to incorporate materials in to the digital flow of manufacturing. Production, manufacturing and operations can be greatly improved if all the relevant processes are linked through digital processes. This requires the digitilisation of the material space [7]. This is the focus of the remainder of this paper.

Digitalisation of Materials

The digitizing of materials space is critical if materials are to be fully incorporated in to the digital manufacturing value chain. Materials occupy a more complex space than that of manufacturing, as clearly the material is defined by its composition, thermal and processing cycles. We might conclude that a largely elemental material such as a metal can be defined by its atomic composition [8]. To a certain extent this is correct, but the size and orientation of the metal grains also has an impact on the properties as does the distribution of the atomic composition with space. The development of precipitates whether in the matrix or at grain boundaries will have a significant effect on properties. If we explore the coordinates for polymeric materials, the connection between atomic composition and the polymer is even more disconnected. We could use monomer composition and this will work well for a set of similar polymers, but the distribution of the monomers along the chain length are equally critical and in the solid state the morphology of that polymer will be most important. If consider more complex polymer systems, such as thermosets, the work of Stukhlyake et al underlines the importance of a multiscale approach to the characterization and property relationships [9]. If we consider the full range of materials including ceramics and glasses, we can see that similar consideration apply.

We conclude from this consideration of materials that the material space will need to involve composition, structure and processing.

Design

Design in the digital space of manufacturing is usually performed using computer aided design, in which a material or a component is selected from a pull-down list. The consideration of multi-materials is usually considered within the scope of a multi-part assembly. Systems for incorporating areas of different properties, such as color, have been discussed but no agreed system has been developed.

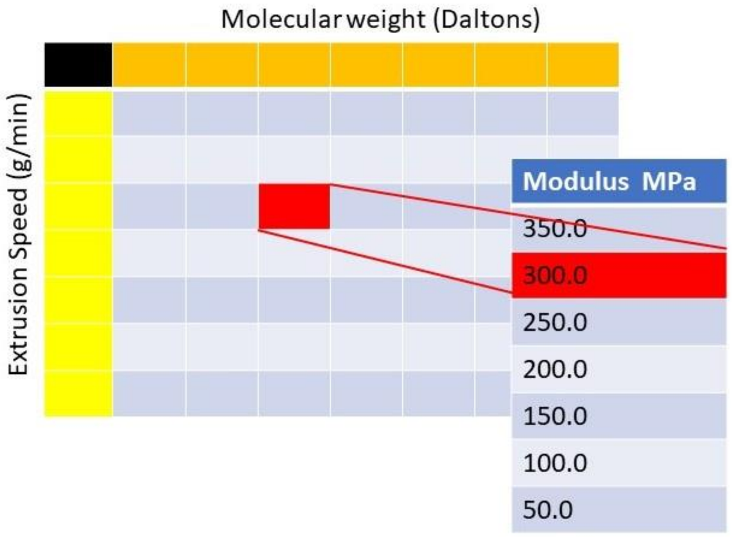

Figure 1 An illustrative example of the mapping of properties to a multidimensional look up table of processing parameters and material characteristics. Here we show only a 2D mapping for simplicity but in practice there will be a much more complex mapping. Note that we have include both a material characteristic and a processing parameter.

When developing the design of a product, it is the properties of the material which are important. We see the materials space as being multi-stage in which the design provides the definition of the limits to each region which has constant properties and the properties are defined in a multidimension look up table which contains information on the base material, the thermal and processing cycle as relevant to that material. The multi-dimensional lookup table will be specific to the manufacturing process and only contain information relevant to that process.

The design process will involve a set P which contains the properties $P=\{p_1, p_2, p_3 ......\}$ which are available and each property maps on to a set of conditions $C = \{ c_1, c_2, c_3, ...\}$ which contain the processes and conditions necessary to produce material with that property. The schematic example shown in Figure 1 includes both a material characteristic and a processing parameter.

We can envisage that this multi-dimensional look-up table will be generated automatically by the process equipment with a digital flow to the measurement of properties. This will ensure consistency with the processing equipment used. Such an approach can be seen as an auto-calibration of the processing equipment. Some 3D printers will need to be redesigned to accommodate switching between different feedstock materials, for example, pneumatic feed lines as used with injection moulding [10]. The possibility of continuously adjustable extrusion dies [11] would be most beneficial to the development of digital work flow and we anticipate the inclusion of multitemperature zones of the extruder will be required for processing biopolymers [12].

Mapping of Properties

We have shown in previous work that the process parameters of extrusion-based 3D printing, such as extrusion rate, print speed and temperature can be exploited to deposit material in different parts of the printed object, with a different structure and morphology [12,13] and hence difference properties. This concept has been demonstrated with semi-crystalline polymers such as Poly(ε-caprolactone) [12] and low-density polyethylene [13]. This work was carried out by 3D printing *in-situ* on the ALBA NCD-SWEET beamline as shown in Figure 2 and evaluating the structure and morphology of the polymer using time-resolving small-angle X-Ray scattering techniques (SAXS) [14,15]. SAXS patterns are shown in Figure 3 which illustrate the different orientational distributions of the chain folded lamellar crystals which can be obtained by adjusting the print parameters in the case the print speed (A Slow, B Fast). The difference in morphology arises due to the difference in cooling rate of the extrudate and its impact on the possibility of the formation of row nuclei [16]. In the work with PCL the difference in the highly anisotropic morphology and the isotropic morphology principally manifests itself in the stiffness or modulus of the solid polymer. Tests show that the modulus of these differing morphologies may differ by a factor of 3 or more. As the control parameters, such as extrusion rate, print speed and temperature, can be adjusted on the fly during the printing process,

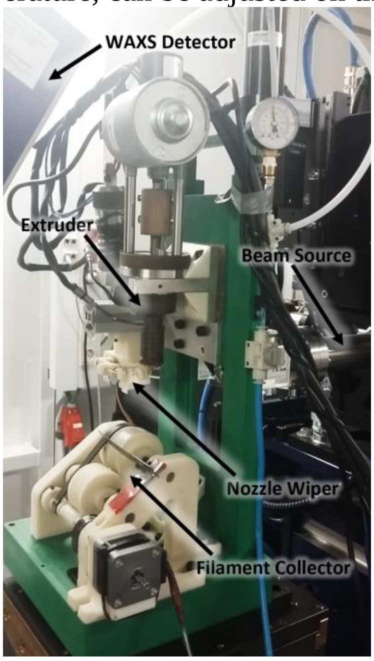

Figure 2 The 3D printer mounted on the NCD-SWEET Beamline at the ALBA Synchrotron Light Source in Barcelona. Reproduced from [15] with permission

albeit with differing time responses and hence the properties may be varied through the print area in a defined manner. A possible limitation of this new approach, is that the symmetry axis of the anisotropy introduced during printing will lie along a direction parallel to the extruder head path as shown schematically in Figure 4.

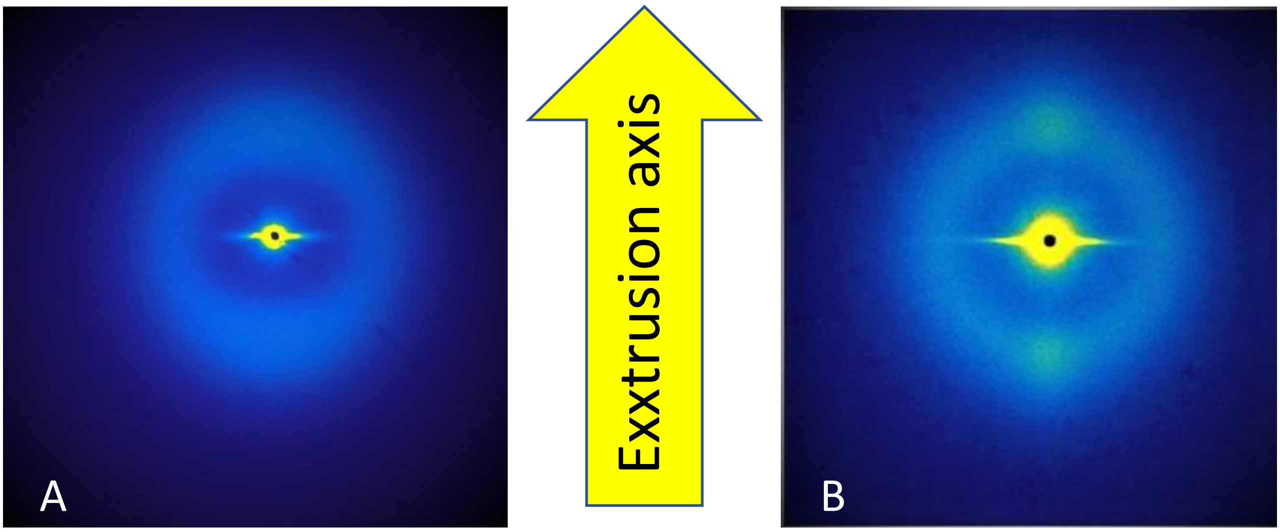

Figure 3. Small-angle X-ray Scattering Patterns of the extrudate from the 3D printer shown in Figure 2 mounted on the ALBA Synchrotron Light Source NCD-SWEET Beamline. The arrow shows the extrusion axis. Figure 3A shows an almost isotropic pattern of the scattering arising from the chain folded lamellar crystals which form on cooling whereas Figure 3B shows a similar pattern but which contains a highly anisotropic distribution of some of the chain folded lamellar crystals indicated by the two intense spots at the top and bottom of the diffraction ring in the figure.

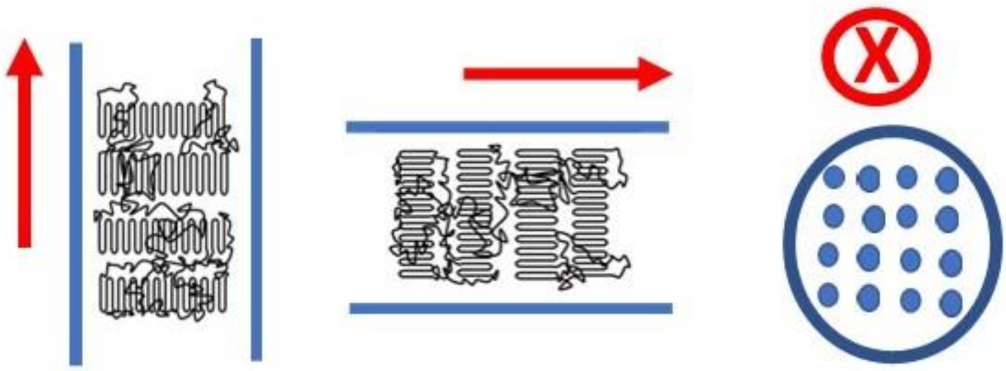

Figure 4 A schematic of the relationships between morphology in the extruded strand and the extrusion direction. The red symbols show the write direction, the blue lines are the boundaries of the extrudate. Updated from [15]

This method of property mapping is particular to extrusion-based 3D printing with semi-crystalline polymers, but we anticipate other methods will become available in time for the differing additive manufacturing technologies.

Digital Twins

The availability of a 3D printer equipped with feedback on the properties of the printed material moves the prospect of a multi-scale digital twin closer to reality. A digital twin is a virtual model designed to accurately reflect a physical object [17]. The object being studied is fitted with various sensors related to vital areas of functionality. These sensors produce data about different aspects of the physical object's performance. This data is then relayed to a processing system and applied to the digital copy. Once informed with such data, the virtual model can be used to run simulations, study performance issues and generate possible improvements, all with the goal of generating valuable insights — which can then be applied back to the original physical object. We can envisage a scenario where optimisation of the design of a product can be performed using morphology or property optimisation. Currently in connection with digital manufacturing, topological optimization is commonplace [18]. This is a mathematical approach or method which performs the optimization of the distribution of material within a defined region or domain, by applying specific constraints and minimizing a predefined cost function which is commonly related to the mass and the mechanical performance. This mathematical tool is just a first order approach to morphology or property optimization as it focuses on the presence or absence of material, where morphology optimization focuses on the morphology and hence properties of the material present, in otherwords, topology optimization develops binary patterns, whereas morphology optimization provides grey scale if not colour. Topology optimisation has developed idto a very powerful tool which has itself been optimized to take less time as possible. Many of the mathematical and computational procedures currently deployed in topology optimisation will not translate through to morphology optimisation, as the areas within the part intrinsically exhibit anisotropic properties and the purpose is more involved than simply calculating the structural compliance.

The most ambitious digital twin under development is "DefinE" whose objective is "to monitor and simulate natural and human activities and to develop and test scenarios that will enable more sustainable development and support European environment policies" [19].

Of course, models and simulations have been in use for a long time [20]. Although simulations and digital twins both utilize digital models to replicate the various processes in a system, a digital twin is effectively a virtual environment, which makes it considerably more useful [21]. The difference between digital twin and simulation can be thought of as largely a matter of scale. While a simulation typically studies one particular process, for example melt flow and extrusion, a digital twin can itself run any number of useful simulations in order to study multiple processes. Simulations are usually stand-alone and do not benefit from having real-time data. But digital twins are designed around a two-way flow of information that first occurs when object sensors provide relevant data to the system processor and then happens again when insights created by the processor are shared back with the original source object [22]. One of the key challenges in the development of a digital twin system for a complex manufacturing process is the availability of data related to all scales relevant to the process and materials.

Multiscale Digital Twin for 3D Printing

Extrusion based 3D printing is the most rapidly technology for the fabrication plastic parts, but it is usually sparsely instrumented. This has led some to the thought that molecular level simulations could be used to provide data streams for digital twin systems. The properties of the final plastic product depend critically on the processes involving temperature and flow which determine the morphology of the plastic which develops as the polymer melt cools to room temperature. There are some simulations methods which attempt to predict the development of morphology as a function of time during processing [23]. We propose an experimental methodology using time/resolved x-ray scattering using the intense x-ray beams available at a synchrotron based beamline. We are able to follow in real time the structural evolution of the polymer during the 3d printing cycle and subsequent cooling processes. We have developed a software system which is able to process the large quantities of data involved in a largely automatic manner [24] and to convert these data to meta data to be utilized in the digital twin system. One of the major approaches to the optimization of plastic products is through the formulation of the material which is injected. Such optimization requires a multiscale understanding of the interplay between the material components and the flow and temperature profile during processing. These scales are critical if the digital twin system is to enable new design approaches or materials design. It is crucial to understand in detail the impact of each parameter in order to iteratively create a digital twin model that mimics its physical counterpart.

Discussion

We have detailed a specific approach to the digitialisation of materials and in particular polymer-based materials. We have emphasized the complex nature of achieving this and we propose that the materials digital space must focus on properties so that this space is immediately accessible at the design and optimization stages. We propose that the digital space of properties is linked to a multidimensional space which describes how those properties may be achieved using a specific processing equipment. In the case considered here, that of extrusion-based 3D printing, the coordinates of the processing space will be based on the operational parameters of the 3D printer which include extrusion temperature, extrusion rate, geometry of the extrusion die, the print speed (relative speed of print head and build platform), the build platform temperature, and the environmental temperature. The most natural way in which the mapping between the material property space and the processing conditions can be established is through the automation of the printer to produce a systematic series of samples with the different processing parameters and the properties to be evaluated automatically using a digital work-flow. Indeed one of the advantages of materials digitalization is the development and use of such digital work flow in to the manufacturing process.

The availability of digital material space as described above opens up opportunities for developing new work flows which may lead to new product designs and new products. We have outlined how the process of topological optimisation can be enhanced to morphology or property optimization. This may lead to lighter products, better end of life options and new properties or options for the end user. Since the morphology will directly affect the degradation of the polymer, the use of morphology optimization may be particularly relevant to personalized medical products, such as scaffolds for tissue engineering intended for absorption after implanting in the body.

Clearly the concepts introduced in this paper are critical for the complete digitilisation of manufacturing by ensuring that there is a methodology to optimize the complete manufacturing process from synthesis to fabrication to yield premium value products with novel designs closely linked to the spatially resolved digital specification of the material. However, this is but the first step and there is much more to achieve. One area which is critical is the automated characterization techniques for properties, which are still based in the main on isolated equipment operated by skilled personnel rather than intergrated into a digital work-flow. This involves much more than the introduction of robots into a materials science laboratory. The preparation of samples, the mounting of samples and the intelligent processing of data all need to be incorporated into the digital work-flow.

Conclusions

The digitilisation of materials is vital is we are to realize the full benefits of digital manufacturing allowing optimization of the complete process from synthesis through to end of life treatment. Materials are a critical component of manufacturing which are challenging to digitalize and there appears no convenient generalised solution. We have propose such a generalised approach in which the materials digital space is focused on properties in the widest sense and that each property element needs to be mapped to a multi-dimensional space which identifies the processing parameters required to achieve that property. We envisage that one of the first opportunities which arises from materials digitalization will be the implementation of morphology mapping using extruder based 3D printing to enhance all aspects of product design. We have emphasized the value of multiscale evaluation of any processing technique and we highlight this approach and the facile connection with multiscale digital twins. We recognize that there is much to be achieved to realise this situation and the importance of introducing digital work flows into the characterization of the properties of materials. Moreover, we stress the close coupling needed between the fabrication equipment/process and the characterisation processes in order to achieve the required digital work flow

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