Multifunctional Materials

EDITORIAL

Multifunctional materials: concepts, function-structure relationships, knowledge-based design, translational materials research

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Abstract

Integrating different functions in one material system is a fundamental challenge, especially if those functions seem to exclude each other. Understanding function-structure relationships and developing a competence in the system approach for multifunctionality enables many modern applications, which can improve quality of life and address important global challenges. The interdisciplinary field recently extends to computational engineering approaches for virtual material design and to advanced fabrication schemes taking advantage of digitalisation. In this way development cycles can be shortened and products based on multifunctional materials can become more and more adaptive and individualised. It is against this backdrop that Multifunctional Materials has been launched, in consultation with the scientific community, to become a selective journal focused on conceptual novelty that will uniquely bring together all aspects of this rapidly developing field.

Introduction

This is the golden age of materials; new material solutions are now being actively developed to cope with the increasing human demand for more efficient mobility; as structural energy storage systems; to promote better lifestyles and improve healthcare by monitoring and remodelling according to our personal wellbeing; to act as intelligent system for active sensing and self-diagnosis; to morph and adapt in response to the local environment; and to improve product sustainability from cradle-to-grave via new assembly and disassembly processes. These materials are designated as multifunctional; they are often inspired by a biological analogue but are designed to perform multiple responsibilities through prudent combinations of different functional capabilities. Typically, each function contributes a distinct physical or chemical process that can deliver system-level improvements beyond the status quo. These materials can be ‘autonomic’, i.e. sense, diagnose and respond to external stimuli with minimal external intervention; ‘adaptive’, i.e. reconfigure or readjust their functionality, shape and structural performance on demand; or ‘self-sustaining’, i.e. integrating power harvesting, storage and/or transmission. This is achieved by designing and understanding the functional requirements of the material building blocks, through a hierarchical structure-property-process relationship, to realise the products of the future.

Multifunctional materials are enabling and accelerating the development and manufacture of the products of the future. This scientific journey is only just commencing with the journal Multifunctional Materials (MFM) providing a forum and repository for the latest advances in our community. Through close collaboration with our colleagues on the editorial team, the scope and characteristics of MFM have been designed to ensure it serves a growing transdisciplinary and dynamic community across academia and industry. The remaining sections of this editorial will: (1) showcase how the multifunctional concepts are now being translated into real life applications; (2) discuss the current and future challenges of multifunctional materials based around key thematic areas; and, (3) discuss the
outlook of this material taxon for the products of the future and highlight how MFM will support and nurture this growing community.

From concepts to translation in real life applications

Multifunctional materials are ‘disruptive’ game-changers and the motivation for designing these systems can come from many foci. It can be driven by the need for modern applications where the system environment defines the material performance. Conversely, it can be curiosity driven research promoting a vibrant entrepreneurial culture for new innovations and applications within universities and research institutions.

The knowledge of individual material functions by itself is not sufficient to predict multifunctional materials’ suitability in an application setting. For gaining system competence, a holistic approach is needed where virtual material design and computer supported material engineering will complement theory and traditional experimental techniques. For example, simulation tools to transfer atomistic material properties to complex functional structures across the length scales are now being developed and applied as a methodology/roadmap for future applications. It is through this philosophy, and the increasing role of informatics and data analytics, which will be critical in the development and upscaling of multifunctional material systems into modern applications. Finally, for multifunctional materials to grow beyond the designers’ imagination and laboratory proof-of-concepts, suitable fabrication schemes for real life applications are also required. Hierarchically separated multifunctionalities either with orthogonal functions at the different levels or a function from the molecular/nano level being applied to the macroscopic level through sequential coupling will require the ability to add, subtract, fuse and grow materials on demand. Whilst the first steps are being taken in this direction, enabling the manufacturing process to be integrated in the discovery, design and development of new multifunctional products, with rapid prototyping and with scale-up capability embedded, is not only challenging but essential to realise the products of the future.

Thematic areas of multifunctional materials research

Multifunctional materials, and their potential for driving technological innovation forward, represents a wonderful future for the materials science community. Key scientific breakthroughs will come not only from the new materials developed but also from more advanced computational simulation techniques targeted at innovative fabrication technologies. Whilst not exhaustive, these challenges can be grouped around a number of thematic motifs which are discussed below and shown schematically in Figure 1.
Designing multifunctional materials

Compared with traditional design approaches, the design of multifunctional architectures will require movement away from ‘merged’ functionalities at the macroscale, towards a design solution which transitions seamlessly between functional and structural materials on both the local level and within the global structure [1]. To achieve this future, it will necessitate the creation of computational simulation and design capabilities which allows the designer to exploit digital manufacturing technologies whilst integrating these into digital workflows to transform the way previously unattainable products are created. The recent application of multi-physics concurrent design methods, of both materials and products, using multi-scale modelling and topology optimisation techniques rather than through ad hoc heuristics approach will accelerate the application of multifunctional products in the near future.

Materials in life sciences and biomaterials

Multifunctional biomaterials which deploy, remodel or release therapeutic functionality are actively being pursued as implant materials for the human body. Multifunctional shape-shifting biomaterials are considered for implants applicable in minimally invasive surgical procedures as well as for health technologies supporting elder people in their housekeeping or other day-to-day routines [2]. In the future, and taking a cue from nature, multifunctional biomaterials will move beyond just remodelling to the surrounding environment but also have the potential to contain sensory capabilities like those of audition (hearing), somatosensation (touch), olfaction (smell) and sensory modalities including thermoception (temperature), nociception (pain) and (equilibrioception) balance, in addition to their structural role. These materials will profoundly expand the possibilities of patient wellbeing and age-appropriate healthcare through new generation multifunctional implant materials.

Self-healing and remodelling materials

The concept of advanced structures exhibiting the functionality of self-healing or remodelling is of high scientific interest [3]. Biologically inspired, self-healing functionality has been shown through the incorporation of material phases that undergo self-generation in response to damage. Healing is achieved through the release of microencapsulated phases and in situ polymerisation. Alternatively, microvascular material architectures in which vascular circulatory systems are integrated in materials to provide a conduit through which functionality can be imparted. Continuous healing and repair of vascular materials is now possible, however, many other functionalities employing the microvascular network are possible including self-cooling/heating, self-diagnosis and assessment and self-morphing structures. The challenge for the future is the ability to self-diagnose and heal at the damage length scale without degrading the structure’s overall performance, i.e. to sense and remodel the strain field prior to attaining a critical stress threshold to initiate and propagate the onset of microcracks. Designing a healing-sensing-structural multifunctional building block is the next challenge.

Materials for sustainability and energy

Available and affordable energy has led to rapid industrialisation and the creation of a plethora of consumer products with ever increasing power requirements. Green energy alternatives are now essential to meet this growing demand. Research in materials science is contributing to progress towards a sustainable future based on clean energy generation, transmission and distribution, the storage of electrical and chemical energy, energy efficiency and improved energy management systems. The challenge for the advanced materials community is not only improvement in sustainable approaches beyond Li-ion batteries, but how these the energy systems can be integrated within mechanical load paths are crucial. Only through this methodology will future products attain efficient material utilisation, minimisation of sub-system mass and volume. Multifunctional materials play a critical role to enable and achieve renewable and sustainable energy pathways of the future.

Actuators, sensors, flexible electronics and wearables

Flexible mechanical and electrical sensing devices have demonstrated great potential in a wide range of applications, such as displays, robotics, in vitro diagnostics, advanced therapies and energy harvesting. Multifunctional materials have been instrumental for e-skins, wearable and implantable devices and advanced sensors with the potential for self-power and self-healing. Such remarkable advances have been achieved through the application of highly flexible, ultrasensitive and transparent multifunctional materials comprised of organic/inorganic matrix arrays, hybrid composites, graphene and nanowires (NWs) or nanotube assemblies. The challenge is the translation of this technology into innovative products (spanning healthcare to robotics) that can revolutionise the way that an individual and society interact.
Materials for robotics
The application of multifunctional materials in soft matter engineering has permitted rapid scientific innovation in robotics and wearable devices which now interface with the human body and adapt to unpredictable environments [4]. Multifunctional materials for soft actuation exploit a wide range of physical mechanisms, including pneumatic inflation, combustion, phase transition, electrostatic force, electro-osmotic flow and biological actuation. Employing these actuators within deterministic structures, fluid–elastomer composites or bio-hybrid systems, with ongoing advances in electronics, has permitted the development of a viable range of technologies ranging from autonomous field robotics to wireless biomedical devices. In the future, advances in new soft multifunctional materials, material integration and robotic intelligence and autonomy, as well as breakthroughs in bio-hybrid engineering and modelling, controls and machine intelligence will lead to the next generation of autonomous soft robots.

Advanced manufacturing of multifunctional materials
In nature, biological taxa are building structures with far more complexity, information capacity and assembly instructions than even the most advanced structures possible with our current manufacturing platforms. The notion of ‘designing for self-assembly’ was identified as the future of material construction [5], i.e. the ability to directly embed assembly information into the raw materials. This proposes an interesting concept for multifunctionality, where the added function is to facilitate complex manufacture rather than add an additional physical functionality or capability. The synthetic growth of a ‘product’ by controlling the hierarchical structure-property-process relationship, to yield the required designed functionalities, is a key challenge for the future. Controlling material evolution at the point of deposition and construction will be critical in the future [6]. It can be envisaged that through the digital fusion of sensing, additive and subtractive processes, as well as new ideas in multi-scale, multi-material fabrication will be the critical in manufacturing the future.

Metamaterials, multi-material systems
The concept of metamaterials was originally defined as novel artificial materials with unusual electromagnetic properties that are not found in naturally occurring materials. This concept has now been extended to a class of materials whose effective properties are generated not just from their bulk behaviour, but also from their internal structuring; offering superior and unusual properties in the aspects of static modulus, density, energy absorption, acoustic and phononic performance, heat transport performance, smart materials and negative Poisson’s ratio [7]. These architected materials continue to redefine the boundaries of materials science, opening up a wealth of new opportunities impacting on health, national security and energy independence. Whilst considerable innovation has occurred, key challenges for the future for the metamaterial community are to develop manufacturing processes for multi-material systems, to upscale current promising manufacturing processes, and developing metrology, simulation, and design tools for multi-scale, three-dimensional and multi-material systems (see, for example, [8]).

Outlook
In the world of multifunctional materials, an interdisciplinary but systematic approach to the complete materials system is required; integrating theoretical, computational and experimental methods in a unifying methodology. The evolution of new manufacturing methods is also a prerequisite, with movement away from traditional processes, which ‘merge’ functionalities at the macroscale, and a transition towards processing platforms, which integrate multiple local building block functionalities into the global architecture on demand. Fabrication schemes will go far beyond shaping of materials as processes engineering is crucial for material functionalisation, having more the characteristics of programming than creating a final setting. Once shaped bodies can program themselves autonomously true adaptivity will reached.

It is these fundamental discoveries, on a conceptual level with high intellectual capital for the materials research community, which can be introduced and applied by designers and product innovators of the future, that are of paramount interest for the journal *Multifunctional Materials* (MFM). As the research area is broad, it requires differentiation according to function categories, which is reflected in the different thematic sections of the journal. MFM will contribute to this research field by fostering the scientific exchange in this highly interdisciplinary community; by educating the next generation of material scientists and engineers; whilst also acting as an advocate to increase public awareness in the possibilities offered by this new generation of advanced materials and processes.
References

[1] Behl M, Razzaq Y M and Lendlein A 2010 Multifunctional shape-memory polymers Adv. Mater. 22 3388–410
[2] Jung F, Wischke C and Lendlein A 2010 Degradable, multifunctional cardiovascular implants: challenges and hurdles MRS Bull. 35 607–13
[3] White S R, Sottos N R, Moore J, Geubelle P, Kessler M, Brown E, Suresh S and Viswanathan S 2001 Autonomic healing of polymer composites Nature 409 794–7
[4] Rich S J, Wood B J and Majidi C 2018 Untethered soft robotics Nat. Electron. 1 1102–12
[5] Tibbits S 2012 Design to self-assembly Archit. Des. 82 68–73
[6] Llewellyn-Jones T M, Drinkwater B W and Trask R S 2016 3D printed components with ultrasonically arranged microscale structure Smart Mater. Struct. 25 1–6
[7] Ren X, Das R, Tran P, Ngo T D and Xie Y M 2018 Auxetic metamaterials and structures: a review Smart Mater. Struct. 27 023001
[8] Chen D and Zheng X 2018 Multi-material additive manufacturing of metamaterials with giant, tailorable negative Poisson’s ratios Sci. Rep. 8 9139