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Guest Editorial

Making the Most of Our Materials

Recent advances in energy technology are driven by the need to mitigate climate change and find sustainable, non-polluting ways to power our communities. However, a large proportion of the impact arises from the materials used to make energy devices (1) and it is therefore important to generate and use materials effectively, while finding ways to minimise waste, energy use and harmful chemicals during device fabrication. This editorial describes the materials science toolbox for making the most of our resources.

The True Value of Materials

Materials have value beyond their price. Raw materials extraction, processing and distribution embody energy and costs which are not reflected in their market value, such as irreversible ecosystem damage, use and contamination of clean drinking water and pollutants produced at every stage. Some materials require scarce or extractively costly minerals (2, 3), for instance cobalt mining involves severe toxins.

Worldwide population growth and rising demand makes sustainability a key consideration. Recycling is one way to achieve this, but it requires considerable resources and often results in low quality products. Therefore, techniques encouraging the best use of virgin materials are needed, for example advanced processing techniques producing highly functional micro- and nanostructures from smaller quantities. Multifunctionality – coupling related functions into a composite material – may increase resource efficiency across the whole supply chain.

A whole systems perspective can ensure that we are focussing on the right aspects and account for costs and impacts over a product's lifecycle. Lightweighting and extending the lifespan of energy products are effective ways to achieve efficiencies across the entire supply chain (3).

Multiscale, Multifunctional Design

Materials should primarily be functional at device level, fulfilling an application's key performance indicators. However, material choice should also consider processing costs, device lifetime, environmental impacts and safety. Device performance is an inherently multiscale challenge, since material properties are strongly linked to atomistic, nanoscale and microscale structures (4), well-structured materials often performing better than their unstructured equivalents (5).

The choice of material for a particular device arises from its constituent elements and atomic structure, defining its electrical, mechanical, chemical and magnetic properties. Databases of structure-property relationships of energy materials are emerging from experimental and theoretical studies, enabling data mining for materials suited to a particular application, termed rational design. Abundant elements forming benign chemistries are indicated, for example sodium-ion batteries replacing lithium (see Titirici's work in Edge *et al*. (6)).

Quantum effects and large surface area to volume ratios at the nanoscale (1–100 nm) enhance or endow new properties. Integration of one-dimensional and two-dimensional nanostructures into composites has led to significant advances, for example carbon-based nanomaterials conferring outstanding electrochemical properties and strong mechanical stability (7). Other important properties, such as porosity and mechanical strength, often rely on microstructures (100 nm to a few cm).

One route to fabricating high precision micro- and nanostructures is additive manufacturing: a range of processes building complex, three-dimensional structures from the bottom up, with minimal waste of both materials and energy and few toxic chemicals. Other advanced, resource-efficient techniques producing complex

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microstructures include electrospinning and graphitising nanostructures from waste biological matter (see Cooper and Titirici's work (6)).

Combining single function devices into systems creates unnecessary complexity in manufacturing and packaging, adding to weight and cost. Functional diversity, where coupled functions are integrated into hybrid materials, creates efficiency opportunities across the supply chain. For example, George's work in Edge *et al*. (6) embeds solar cell structures into battery electrodes.

Modelling Real Materials: The Importance of Defects and Heterogeneity

Advanced simulation capabilities speed up research into new materials and systems and allow technologies to be deployed safely and efficiently (3). Rational design's structure databases consist largely of X-ray diffraction performed on pure crystals, while real materials are heterogeneous, for example through interfaces between components, where critical reactions occur (8) and contain a wide range of defects, such as impurities, vacancies and dislocations. The heterogeneity of materials can define their properties, for example Lucid *et al*. (9) looks at how to simulate grain boundaries: nanoscale interfaces in polycrystalline materials. Defects can diminish performance, but there are many materials, such as semiconductors, whose critical qualities exist because of their impurities. Understanding defects is key to enhancing material properties, for example in battery electrode materials (10). Incorporating both defects and heterogeneity into models will enable more accurate tuning of properties and performance.

Finishing Touches

Given that it is expensive to extract, process and distribute raw materials (1), particularly if they are scarce and particularly for energy devices (1), it is important that energy materials are used as effectively as possible. However, materials are subject to a range of processes throughout the supply chain, including the application of additives or coatings and packaging, all of which may exert mechanical stress, exposure and ageing. The effects of these processes are not well understood and may not have immediately detectable effects, only influencing the long-term performance. Some studies are emerging, examining the effects of processes such as calendering on battery electrodes (11). There is a need for holistic studies and the application of green chemistry principles (12) throughout the supply chain, as well as studies on degradation and its mitigation, to stretch resource usage.

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