

Energy transition:

Measurement needs within
the battery industry



National Physical Laboratory

The National Physical Laboratory (NPL) is the UK's National Measurement Institute. At the heart of our mission is delivering impact by disseminating research and measurement best practice and traceability for the economic and social benefit of the nation.

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Executive summary

Sustainable use of energy is one of the greatest challenges facing the world today. A major transition from fossil fuels to renewables is underway in most developed countries, driven by the need to cut greenhouse gas emissions, mitigate air pollution in urban areas and reduce reliance on fuel imported from politically unstable regions. Due to the intermittent nature of renewable energy sources such as solar and wind, the development of large-scale energy storage solutions is one of the key technological bottlenecks hampering the transition to a sustainable energy landscape.

Batteries provide an efficient means of storing energy in an easily accessible form and have been used for this purpose for over 200 years. The energy density of these devices has increased significantly over the past few decades, with the advent of lithium-ion batteries enabling a revolution in portable electronics (smartphones and laptops) and some limited market penetration of electric vehicles. However, a step change in battery technology will be required to support its use in the widespread electrification of transport and grid-scale energy storage.

The UK is well positioned to develop domestic manufacturing capability in next-generation battery technologies, with a strong research base in this area and a number of innovative SMEs developing potentially disruptive technologies such as lithium-sulphur, lithium-air, sodium-ion and silicon anodes. This has led to the recent announcement of the Faraday Challenge, a £246 million investment over 4 years into battery research, coordinated by the EPSRC, Innovate UK and the Automotive Council. The aim of this initiative is to ensure that the UK leads the world in the design, development and manufacture of batteries for the electrification of vehicles.

In order for high energy density batteries to be competitive with incumbent technologies, there is an urgent need to reduce costs, extend lifetime and improve energy density, while ensuring safety. In many cases, these advances cannot be made without addressing the measurement challenges that underpin them. As the UK's National Measurement Institute, the National Physical Laboratory (NPL) has a responsibility to tackle priority measurement challenges. The UK has internationally prominent measurement capability and established research institutions which could support the development of a world-leading battery industry. This will require both the right expertise and a harmonised effort from funding bodies, industry, research institutes, standardisation bodies and policymakers.

Through detailed consultation with stakeholders from across the battery community, NPL has collated and prioritised the key measurement challenges currently facing the widespread commercialisation of high energy density batteries in the UK. Five challenge areas were ranked by stakeholders as high priority:

1. **Ensuring quality control** throughout the manufacturing process by developing cost-effective screening tools and establishing acceptable tolerance limits to ensure the performance and lifetime of the module or pack is optimised;
2. **Developing diagnostic techniques** to monitor state of health and identify failed or failing cells within a battery module or pack, in order to better understand and mitigate critical degradation mechanisms;
3. **Developing predictive models** for battery performance and lifetime using both data-driven and fundamental approaches, to reduce development costs and facilitate design optimisation;
4. **Identifying end-of-life thresholds** for second life and recycling, including assessment of the commercial viability of processes for re-use and recycling, and;
5. **Establishing standards** for state estimation to generate more reliable and comparable data and ensure safe operation.

The infographic on the following page is a visual summary of the primary measurement challenges identified throughout this report, which are summarised in Section 7.

MANUFACTURING

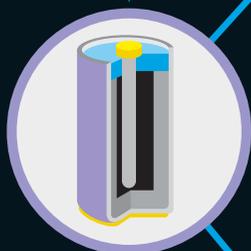
RAW MATERIAL



Identifying critical parameters, such as material properties and formulation methods that influence cell performance

Measuring purity of materials used in manufacture, including materials recovered from recycling, and establishing a definition of 'battery grade'

BATTERY CELL



Standardisation of terminology between cells, modules and packs, including best practice measurement protocols and configurations

Standardisation of test and characterisation methods and validation at the materials and cell level

Determination of state of charge and state of health, including derived parameters that cannot be directly measured

IN SERVICE

BATTERIES FOR TRANSPORT



In situ temperature measurement to support improved thermal management strategies

Identifying failed or failing cells within a battery module or pack and understanding the impact of individual cell failure on overall performance

Coupling of methods for simulation and use of data, including the need for data sharing and benchmarking



Characterisation of degradation mechanisms linked to actual car use to reduce the need for over-sizing

Establishing test protocols to take into account different types of use, for example, fast charging

Non-invasive monitoring of state of health and establishing which parameters are most relevant to industry and the end user

Standardisation of electrochemical test methods, for example impedance spectroscopy for state of health monitoring



END-OF-LIFE

RE-USE AND SECOND LIFE



Life cycle analysis and economics for the design and manufacturing process to better understand scenarios and processes for recycling

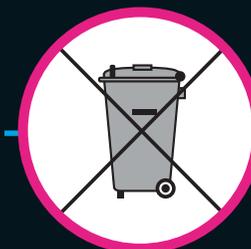
Identifying end-of-life thresholds for first and second use, including economics and safety

RECYCLE



Detection and recovery of recycled metals, including identification and specification of the most critical materials

DISPOSAL



Monitoring environmental effects throughout the life cycle from extraction of raw materials to recycling and disposal of the battery

BATTERIES FOR GRID MANAGEMENT



Accelerated stress tests to establish confidence in lifetime prediction, including external verification and validation

New techniques for post mortem analysis in order to identify failure mechanisms and inform cell design



Understanding propagation of damage as a result of failed cells within a battery module or pack



Measurement of electricity use during the day to inform grid usage for recharging electric vehicles

ENERGY TRANSITION

Measurement needs within the battery industry

1 Introduction

1.1 The use of batteries in the UK

The need for energy to become more affordable, clean and secure requires a shift from fossil fuels to renewable energy sources. This need is becoming increasingly urgent as the UK works towards international and domestic policy commitments such as the Paris Agreement and the Climate Change Act, which demands that the UK reduce its 2050 greenhouse gas emissions by at least 80% compared to 1990 levels ^[1].

While the cost of renewable energy technologies such as wind and solar has fallen significantly in recent years, their intermittent nature means that widespread penetration predominantly depends on the deployment of large-scale energy storage technologies. In recognition of this need, energy storage has been highlighted as a major priority in both the UK Industrial Strategy ^[2] and the UK Measurement Strategy ^[3].

Batteries are electrochemical devices that facilitate the storage and conversion of energy. All of the energy is stored within the electrodes, which are transformed from one chemical form to another during charging and discharging of the battery. The UK Industrial Strategy states that 'battery technology is of huge importance to a range of new technologies, including the automotive sector, smart energy systems and consumer electronics' ^[2].

High energy density batteries have the potential to decarbonise transport and provide grid storage, as well as offer the UK a significant opportunity to develop domestic manufacturing capability in next-generation battery technologies. Lithium-ion (Li-ion) batteries are generally viewed as the most promising technology in the short to medium term ^[4]; however, research into alternative materials and battery chemistries is continually advancing – the challenges around this are explored in Section 2 of this report.

1.2 Purpose of this report

This document – the latest in the 'Energy Transition' report series – identifies and prioritises the measurement challenges that may have the potential to create hurdles and bottlenecks in progress towards the widespread deployment of high energy density battery technologies. It highlights the areas that will require further investigation and investment, with the aim of informing calls for collaborative research activities.

The conclusions presented in this report are based on individual in-depth interviews with battery experts from across the battery supply chain, an industry workshop held at NPL, and several roadmaps and project reports published recently by industry and academia that address overarching issues facing the UK battery industry.

The applications for batteries are multi-scale – from cell (coin, prismatic, pouch and cylindrical), to module, to pack – as well as multi-disciplinary. The purpose of this report is to focus on their potential for large-scale, high energy and power density storage, specifically the role of Li-ion batteries in addressing the challenge of decarbonising the transport sector and balancing the grid through storage.

The measurement challenges faced throughout the lifetime of a battery are explored in this report through the following themes: quality control during the manufacturing process, diagnostics during service operation, modelling and lifetime prediction, end-of-life processing and the need for standards. These are cross-sector challenges that relate to any high energy density battery application, whether that be for stationary power, transport or portable devices.

1.2.1 Transport

In the UK, a rapid area of growth and deployment for batteries is within the transport sector. Electric vehicles (EVs) and plug-in hybrid electric vehicles (PHEVs) are increasing in popularity as people become more aware of the impacts of urban air pollution and greenhouse gas emissions.

- **Around 40,000 premature deaths annually in the UK are attributed to illnesses relating to air quality** according to the Royal College of Physicians ^[5]. On top of health impacts, the transport sector also accounts for over 20% of the UK's greenhouse gas emissions ^[6]. These are critical issues that must be addressed and have influenced the recent announcement by the UK government that the sale of new petrol and diesel vehicles will be banned by 2040 ^[7]. As a result, car manufacturers have begun to shift their research and development (R&D) focus towards low carbon alternatives – the two leading technologies being high energy density batteries for EVs and fuel cells for hydrogen-powered vehicles.
- **EV penetration is currently less than 2% in the UK** ^[8], but the Committee on Climate Change recommends that EVs should comprise up to 60% of new car sales by 2030 (in their Central uptake scenario) ^[9]. UK based car manufacturers such as Jaguar Land Rover and Ford have made commitments to develop EVs, to join the market of existing UK-based EV manufacturers such as Nissan.
- **An investment of £246 million over 4 years in UK battery research** was announced by the Department for Business, Energy and Industrial Strategy (BEIS) in July 2017. The 'Faraday Challenge' aims to ensure that the UK leads the world in the design, development and manufacture of batteries for the electrification of vehicles – co-ordinated by Innovate UK, EPSRC and the Automotive Council ^[10]. In total, the Government plans on providing £841 million of investment towards 'Innovation in the Transport Sector (including electric vehicles and batteries)' according to their Clean Growth Strategy launched in October 2017 ^[11]. The Government are investing a further £200 million into charging infrastructure and £100 million for a Plug-In Car Grant to support the uptake of EVs ^[12].

It is evident that batteries and fuel cells are among the leading candidates to facilitate the transition to a low carbon future for transport. For many they are viewed as competing technologies but in reality, it is likely that given the scale of the challenge, both will have a part to play. NPL has already produced a report detailing the measurement challenges facing hydrogen and fuel cell technologies, which was published in June 2017 and can be accessed via the NPL website.

1.2.2 Grid storage

Within the UK's electricity grid system, there is a growing need for grid-scale storage technologies to mitigate the intermittency of renewables and act as a buffer during peak demand ^[13], as well as to enable the transition away from fossil fuels towards clean and flexible energy systems ^[14].

- **Storage technologies could result in savings of around £2.4 billion per year by 2030** according to a study by the former Department for Energy and Climate Change (DECC) from 2016 ^[15]. Greater flexibility within the system will help deliver reliable power at a lower cost and storage technologies such as high energy density batteries can assist with this, as they are able to absorb and release energy when required ^[16].
- **High energy density batteries are unlikely to be the only energy storage solution;** others include hydrogen, pumped hydro, compressed air, flow batteries, power to gas, liquid air, pumped heat, supercapacitors and flywheels ^[17]. However, batteries do show significant economic potential. Bloomberg has predicted that Li-ion batteries for energy storage will become a \$20 billion per year market by 2040 ^[18].
- **The concept of 'Vehicle-to-Grid'** would allow for EV batteries equipped with bi-directional charging systems to provide a significant storage asset to the grid by offering ancillary power during times of peak demand ^[19].

There is no single optimum mix of integrating flexibility options for balancing the grid due to differences in local weather, demand profile, transmission capacity and existing capacity. However, batteries will likely play a vital role in a future sustainable grid.

Batteries for Heat

Under the Government's Clean Growth Strategy (October 2017), the 'Electricity pathway' towards 2050 envisages a shift from conventional gas boilers to electric heating, which would require an increase of 80% in electricity generation for heating ^[11]. This increased demand will require a grid that is able to cope and reliable energy storage will be fundamental to this.

However, the UK heating network has a structural dependence on gas as an energy source; 84% of homes are heated by gas ^[20] and electrification of the system is predicted to be costly. A report by KPMG estimates that converting the UK gas grid to hydrogen could be £150 billion to £200 billion cheaper than rewiring British homes to use electric heating ^[21]. The focus of this report is therefore primarily on battery applications for vehicles and grid storage.

2 Materials and manufacturing

Advances in battery technologies are of international importance as countries begin to phase out carbon-intensive energy sources such as coal ^[22]. Globally, battery manufacturers plan on increasing their capacity to around 120 GWh from the current 30 GWh by 2020 ^[23], an aim that will need to be supported by improvements in the performance, lifetime and safety of these electrochemical devices.

As is often the case with disruptive technologies, reducing cost is key to their commercialisation, and materials innovation will underpin this. The cost per kW of Li-ion batteries, for example, is currently 2-4 times that of pumped hydro and 8 times that of a gas turbine ^[23], and they also face performance and safety challenges which need to be addressed. Research is ongoing into potentially more cost-effective alternative battery chemistries such as sodium-ion (Na-ion) and metal-air batteries, which bring a host of similar technological challenges, primarily around stability and degradation. These technologies remain largely at the prototype stage of development and as a result, the main focus of this report is on Li-ion batteries.

2.1 Li-ion batteries

Lithium is an attractive element for energy storage due to its low atomic weight and high activity. It is generally accepted that the energy density of conventional Li-ion cells is approaching its theoretical limit. Battery chemistries with higher energy density, such as lithium-sulphur and lithium-air, show great promise for the future, but currently suffer from poor cycling efficiency and high rates of degradation.

For high power applications such as electric vehicles, individual cells are arranged into modules, many of which can be incorporated into a battery pack. Electrical and thermal management of battery packs is a complex process, which is normally handled by a battery management system (BMS), a combination of proprietary hardware and software that regulates the output of the pack and monitors its performance. The measurement challenges for BMS are explored further in Section 3.3 of this report.

While scientific advances in electrode materials and cell design remain a critical aspect of the global research effort, engineering improvements around electrical and thermal management are becoming of equal importance in the drive to minimise efficiency losses when moving from cell to module and pack level.

Lithium-ion battery chemistry

Li-ion batteries are frequently used to power everyday devices as they have high energy density, low standby losses and a tolerance to cycling ^[16].

A secondary (rechargeable) Li-ion cell consists of two electrodes separated by an electrolyte. An electrically insulating porous separator material immersed in electrolyte is inserted between the electrodes to prevent short circuits while maintaining a path for ionic current.

The electrolyte is typically a non-aqueous solution of a lithium salt, such as lithium hexafluorophosphate (LiPF_6), in an organic solvent, for example ethylene carbonate. Aqueous electrolytes cannot be used as lithium reacts violently with water; for this reason, Li-ion cells also need to be tightly sealed to avoid moisture ingress from the atmosphere.

During charging, Li^+ ions move from the positive electrode to the negative electrode, with the reverse process occurring during discharge. It should be noted that the negative electrode acts as a cathode during the charging process and as an anode during discharge (and vice versa for the positive electrode).

A number of positive electrode materials have been commercialised over the past two decades, generally combining lithium with a range of transition metals. Following the discovery of lithium intercalation in graphite, the original lithium metal negative electrode was replaced by a graphite-based electrode for safety reasons.

Silicon is now emerging as a candidate material for the negative electrode due to its higher energy density; however, there are significant issues associated with its volume expansion during intercalation, which is significantly greater than that of graphite.

2.2 Supply chain

Batteries use finite metals, such as lithium and cobalt, which require mining. Reserves of these materials are not as abundant in the UK as they are in other areas of the world such as the Democratic Republic of Congo, Bolivia and Western Australia. While there is significant lithium enrichment underlying Devon and Cornwall, for economic and environmental reasons it remains cheaper and easier to import than extract domestically ^[24]. This means that the supply chain for the manufacturing process usually begins overseas and parts of the cell or the entire battery system then have to be shipped to the UK, adding to the cost of the manufacturing process.

Each country has its own individual regulations with regards to shipping, for example:

- It is a requirement under UK regulations that battery producers (manufacturers and importers) must 'record the tonnage and chemistry of the batteries they place on the market' ^[25].
- Consideration of the chemistry of the cell is also important during shipping, as dependent on the material and cell configuration, calendar ageing can occur which reduces the performance and lifetime of the cell.

Shipping restrictions on certain materials and the reliance on imports could limit the UK's battery manufacturing capabilities.

In addition, given the diverse nature of the battery supply chain, comparison of raw materials between batches received from different suppliers is extremely difficult. Often, manufacturers do not have access to testing facilities to verify that the raw materials match the required standards. Consequently, there is a need for standardisation and traceability. As the UK's National Measurement Institute, NPL is at the pinnacle of the traceability hierarchy in the UK and is ideally positioned to establish the required standardised methods and traceability throughout the battery supply chain should high energy density batteries become rapidly commercialised.

2.3 Quality control

As the energy density of battery cells increase to meet the demanding requirements of emerging markets, including transport and grid storage, battery safety becomes ever more critical. In the design and manufacture stage there is often a trade-off between the performance of the battery and the effectiveness of its in-built safety features.

Thermal runaway of high energy density batteries can occur when manufacturing flaws or abusive use results in a positive feedback loop of over-heating and chemical degradation of cell components, culminating in fire and/or explosion. This is of increasing concern to manufacturers and end users, as highlighted by the recent Samsung mobile phone fires ^[26] and the grounding of the Boeing Dreamliner fleet in 2013 ^[27]. Just one major incident of thermal runaway occurring in an EV due to a battery fault, for example, could severely set back this emerging industry. Stringent quality control is therefore of particular importance given the large number of cells in a typical EV battery pack.

Measurement challenges for battery materials and manufacturing

Identifying critical parameters, such as material properties, formulation methods and key sensitivities within the manufacturing process that influence cell performance is an important step towards establishing metrics for quality control. Establishing acceptable tolerances for these parameters and determining how uncertainty in their measurement is propagated throughout the manufacturing process will also be required.

Standardisation of test and characterisation methods, as well as validation at the materials and cell level, will help to address inconsistencies in battery manufacture and ensure harmonisation between manufacturers.

Extending the range of conditions in which the battery can operate when assessing modules and packs, for example characterisation of parameter space over a greater temperature range, will increase confidence in the safe and effective use of batteries under real-world operating conditions.

Establishing techniques for rapid and cost-effective screening of large numbers of cells, through materials level measurements and continuous in-line monitoring, as well as balancing and matching of cells, will be important for large-scale battery production to become viable.

Performing chemical and structural assessment of cells, including cell chemistry, weld integrity, internal structure and mechanical strength, as this is key to ensuring battery safety.

Measuring the purity of materials used in manufacture, including materials recovered from recycling, and establishing a definition of 'battery grade' to mitigate the influence of impurities on performance and safety.

Identifying techniques for measuring the purity of materials used in manufacture that can be applied in the real-world at low cost.

Undertaking in-line, fast, non-invasive measurement of physical and chemical properties of electrodes and components during manufacture, for example electrochemical properties, particle size, composition, rheology and film thickness.

3 Diagnostics

Understanding and mitigating critical degradation mechanisms is key to the successful commercialisation of next-generation battery technologies. As such, battery diagnostic techniques are fundamental to maintain safe and efficient battery operation. The main challenge is to obtain useful data on cell performance and lifetime using techniques that do not disrupt the operation of the cell. There is also a need to drive the various techniques from cell to module and pack level to generate data that is more representative of real-world applications.

3.1 Pack level diagnostics

Although it is necessary to be able to monitor individual cells within a battery pack to ensure performance and safety, it is also important to perform diagnostics across the entire pack, especially in terms of the environmental conditions of their containment. For example, often a cooling system is required at pack level to prevent overheating and avoid heat-induced failures in the cells leading to thermal runaway. Ensuring uniformity of thermal management across the pack and being able to diagnose and mitigate against any areas where failure could propagate will be essential to the commercialisation of high energy density battery technologies.

3.2 Accelerated testing and ageing

The lifetime of a battery can depend on multiple parameters, such as its manufacturing process, operating environment and frequency of charge and discharge ^[28]. Improvements to battery design and performance require testing of the battery under real-world operating conditions; however to test a battery for its entire lifetime can be very time consuming. Accelerated testing is therefore required to achieve equivalent levels of ageing in a much shorter timescale without activating other degradation mechanisms that could compromise the test result. This is a very challenging goal.

3.3 Battery Management System

A battery management system (BMS) is designed to monitor and regulate battery performance in order to detect and ultimately prevent premature failure in the cells or pack during operation ^[29]. A failure in the BMS can cause significant safety issues when used in a vehicle or in aerospace applications for example, as any damaged or failing batteries could go undetected and lead to thermal runaway. In many cases, the BMS supplied by the battery manufacturer does 'not provide sufficient functionality and robustness to control and manage the pack' ^[30] and therefore improvements to the BMS are essential, especially for applications that require a large number of high energy density cells. According to NASA, the requirements for an optimised BMS are 'a simple and reliable circuit that detects a single bad cell within a battery pack of hundreds of cells and it can monitor and balance the charge of individual cells in series' ^[31].

3.4 State of health

State of health is 'a measure of the battery's ability to store and deliver electrical energy' ^[32] and is generally defined in terms of the capacity of a cell as a percentage of its capacity at beginning of life. Rapid, cost-effective and reliable measurement of state of health is a critical requirement for on-board diagnostics in EVs ^[29]. Conventional methods such as measurement of open circuit voltage and coulomb counting are unreliable and time consuming. There is potential for impedance-based techniques to fill this gap if calibration and modelling issues can be resolved.

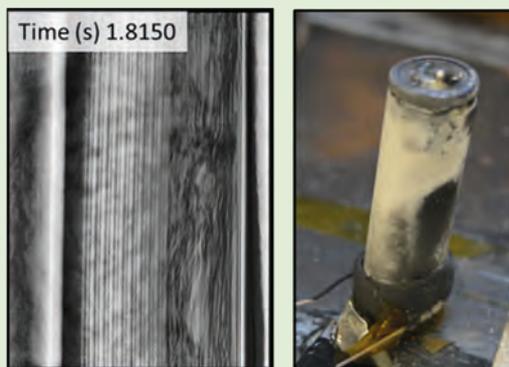
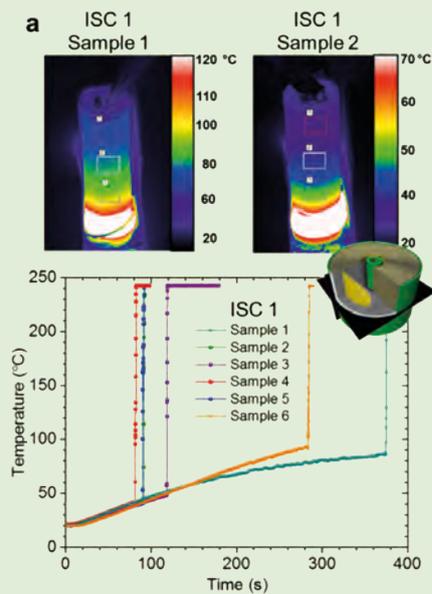
3.5 Post mortem forensics

Understanding what has occurred during and post-failure of a cell or pack can provide valuable information that can be used to improve the design and manufacture of these technologies. This requires investigation of both the physical and chemical parameters that led to the battery failure and a forensic analysis of the conditions and series of events that triggered it.

NPL case study: Thermal runaway in Li-ion batteries

NPL recently took part in a collaborative research project studying failure mechanisms in Li-ion batteries. The project combined an internal short circuit device developed by NASA and the US National Renewable Energy Laboratory with the X-ray synchrotron radiography technique pioneered by University College London, NPL and the European Synchrotron Research Facility.

This allowed, for the first time, 3D imaging of the initiation and propagation of thermal runaway in real-time at a pre-determined location within a commercial cell. This new approach shows great promise in informing the design of improved battery safety mechanisms and recently won The Engineer's 2017 'Collaborate to Innovate Award' in the Safety and Security category.



Measurement challenges for battery diagnostics

Identifying failed or failing cells within a battery module or pack and understanding the impact of individual cell failure on overall performance.

Developing *in situ* temperature measurement techniques at both cell and pack level, such as differential temperature measurements and thermal imaging, to support improved thermal management strategies.

Understanding propagation of damage as a result of failed cells within a battery module or pack to be able to mitigate against thermal runaway.

Establishing key performance indicators which combine parameters to give a consistent measure of health similar to 'MOT' testing regimes.

Designing accelerated stress tests to establish confidence in lifetime prediction and other parameters. These accelerated test methods will require external verification and validation.

Performing diagnostics and modelling around the behaviour of alternative battery materials with different degradation mechanisms to inform materials selection, component design and the development of operating strategies.

Standardisation of BMS at system or pack level, including the challenge of scaling-up from academic research to industry use, for example application of impedance-based techniques in noisy, hot, vibrating environments.

Establishing new techniques for post mortem analysis in order to identify failure mechanisms and inform cell design, for example tomography at module scale to understand failure propagation.

Determining state of charge and state of health, including derived parameters that cannot be directly measured, to provide assurance to car manufacturers and end users that the system will perform as required.

Identifying and mitigating degradation mechanisms to improve performance and safety. This will require indicator measurements for potential failure to be established.

4 Modelling and lifetime prediction

Modelling has been widely applied to the study of battery performance and lifetime, including fundamental electrochemical and thermal models, data driven techniques, battery management algorithms, lifetime prediction models and equivalent circuit modelling for impedance spectroscopy. Fundamental electrochemical and thermal models are potentially more powerful than empirical models, but their development is extremely challenging due to the complex interplay between material microstructure, electrochemical reaction, mass transport, heat transfer and side reactions.

Modelling of thermal management at cell, module and pack level is becoming increasingly important due to the increasing risk of thermal runaway with higher energy density systems. Modelling of next-generation cell chemistries such as lithium-sulphur and lithium-air will also be critical, particularly to support a fundamental understanding of critical degradation mechanisms that are hampering their commercial viability.

4.1 Real-time scenario prediction and data

Due to the relatively recent introduction of some energy storage technologies – for example Li-ion batteries – in systems such as vehicles or grid storage, there are limited data available for modelling and analysis^[33]. The proprietary nature of on board diagnostic data is limiting progress in this respect. Major advances could be achieved if agreement can be reached on data sharing mechanisms across the industry. Data for modelling and lifetime prediction could be used when monitoring real-time user habits, allowing scenario predictions and suggested usage profiles for optimum performance to be fed back to the user. This would allow for modifications to be made to user habits that may extend the lifetime of the battery system.

4.2 Degradation modelling

When in use, each battery system will experience differing operational conditions dependent on the user. For example, some individuals who are used to putting their mobile devices on charge overnight may plug-in their EV in a similar manner to ensure it is fully charged in the morning, whilst others may choose to charge it for short periods of time as and when required throughout the day. This makes degradation modelling and lifetime prediction challenging.

Measurement challenges for battery modelling and lifetime prediction

Undertaking non-invasive monitoring of state of health and establishing which parameters are most relevant to industry and the end user.

Using data for scenario prediction where information is monitored and fed back to the user, offering a suggested usage profile for optimum performance.

Developing self-diagnostics for real-time scenario prediction to create a link between monitoring technique and performance.

Modelling of degradation mechanisms linked to actual car use, such as the effect of calendar life versus operation and electrochemical properties at particle and pore size length scale during operation.

Coupling of methods for simulation and use of data, including the need for data sharing and benchmarking.

Addressing the data capacity issue, for example the inability to record continuous temperature data for thousands of cells. Evidence will be required to prove that the benefit of having this information outweighs the cost of collecting and storing it.

Ensuring the security, reliability, validation, standards and interoperability of the data used for modelling and lifetime prediction.

Designing techniques to optimise uniformity, for example for pressure in modules and coolant flow in packs.

5 End-of-life

It is evident that at the point of use, battery technologies are 'greener' than fossil fuels as they emit no greenhouse gas emissions. However, it is important that the entire life cycle of these technologies is considered when promoting them as sustainable alternatives to carbon-intensive energy sources. Batteries have a limited in-service lifetime and depend upon specific chemistries and finite materials to function. This means that consideration of how these technologies could be re-used in 'second life' applications, recycled, or appropriately disposed of is fundamental to their effectiveness as a sustainable, decarbonised technology in the UK's energy transition.

5.1 Re-use and second life

After use in EVs, many batteries could become a second life stationary storage option in domestic and commercial settings^[34]. This is a rapidly growing sector that could contribute to reducing the upfront cost of EVs by creating a market for batteries that no longer have the capacity for transport applications. There is also potential for batteries to be shipped to developing countries for second life use where the energy demand on the battery system is less intensive.

5.2 Recycling

Recycling batteries is often expensive and produces waste that itself cannot be recycled or reused^[34]. As little as 5% of all Li-ion batteries used in the EU are currently recycled^[35], predominantly due to the fact that there have not yet been any significant constraints on the supply of raw materials and therefore little financial incentive to recycle or find replacement materials^[24]. However, as the demand for applications such as EVs and grid storage (the preferred type of battery being Li-ion) continues to grow, the economic case for recycling battery materials will become more evident, particularly in the UK. The ability to extract useable material from domestic used batteries for recycling would reduce the UK's dependency on the raw material being extracted and imported from dwindling sources overseas^[36].

EU regulation states that it is the duty of the car manufacturers to collect and recycle Li-ion batteries at end-of-life^[37]. However, what is done with the batteries once collected can depend on the quality of the battery at that stage; whether it can be repurposed for its original use, or whether an alternative market for second life is required^[36].

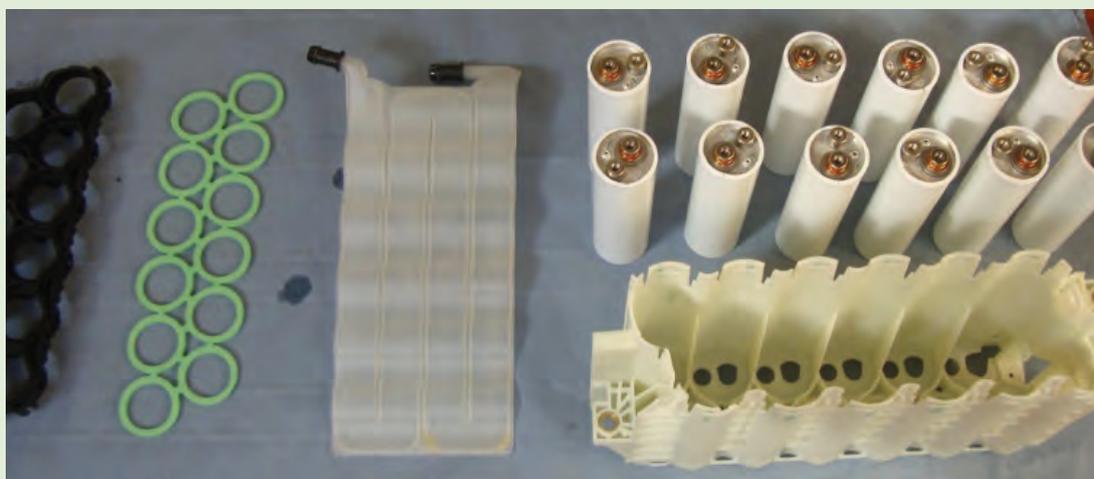
5.3 Disposal

The UK Government's Regulatory Delivery department states that the manufacturer or importer that first places batteries on the UK market is ultimately responsible for compliance with the regulations for battery disposal. This requires the batteries to be 'properly treated and recycled, rather than being sent for incineration or to landfill, both of which are illegal'^[25]. It is also law in the UK that batteries placed on the UK market 'must contain less than the maximum prescribed levels of mercury, cadmium and lead'^[25], as per The Batteries and Accumulators Regulations (2015)^[38], as these are extremely harmful to the environment.

NPL case study: End-of-life testing for EV batteries

Recycling and re-use of batteries is a major issue that is often overlooked. Batteries require the use of finite materials, as discussed in Section 2, and therefore it is important these resources are used as efficiently as possible.

NPL is developing rapid and non-invasive standard test methods for automotive batteries at end-of-life to make it easier to use them in second life applications, such as for grid storage. This will not only reduce the upfront cost of EVs, but ensure that the useful life of the battery is maximised.



Measurement challenges for batteries at end-of-life

Identifying end-of-life thresholds for first and second use, including economics and safety. Considering life cycle analysis and economics for the design and manufacturing process to better understand scenarios and processes for recycling.

Standardisation of key parameters for second life use prediction are fundamental measurements that will be required to test the feasibility of re-use. This will include recording first life history and assessing how it can be fed into second life use.

Establishing an information database of operational history if the battery is to be re-warranted for second life use.

Monitoring environmental effects throughout the life cycle from extraction of raw materials to recycling and disposal of the battery, to reduce the environmental impact and ensure materials such as cobalt are properly treated.

Detecting and recovering recycled metals, including identification and specification of the most critical materials.

Detecting and disposing of hazardous materials to maximise the sustainability of the battery industry.

6 Standards

Sir Mark Walport – the then Government Chief Scientific Adviser – stated in response to the Industrial Strategy and the Faraday Challenge that ‘there are a number of areas where technical standards may ultimately drive competitiveness and BEIS should work with the National Physical Laboratory, the science community, and the Automotive Council to consider what part the development of standards might play in the overall programme for the purposes of maximising UK competitiveness’^[39].

Establishing standards across the battery supply chain and throughout its lifetime for any application is fundamental to ensuring traceability, comparability and performance in these systems. It is also clear that training will play a major role in the dissemination of standards and best practice to industry, including courses on measurement, assembly and appropriate test protocols.

6.1 Grid application standards

Homes and small to medium-sized enterprises are expected to become actively involved in modifying their energy use patterns by monitoring their actual consumption in real time^[40]. Coupled with the increase in the use of solar panels and wind turbines, ‘Vehicle-to-Grid’ and other ancillary energy storage systems will require measurement of complex flows of electricity in both directions between consumer and grid, for which standards will play a critical role.

6.2 Vehicle application standards

Whilst there has been some activity around standards for electric vehicles, for example IEC 61851-1:2017 ‘Electric vehicle conductive charging system’^[41], many gaps still remain, particularly around reliable accelerated testing of battery performance and lifetime.

Measurement challenges for battery standards

Establishing test protocols to take into account different types of use, for example, fast charging. This includes assessment and characterisation of unsafe operation modes, as well as state of health measurements which need to be standardised and benchmarked. These standards must be internationally recognised.

Standardising electrochemical test methods, for example impedance spectroscopy for state of health monitoring, to ensure comparability of measurements and consistent interpretation of impedance spectra.

Establishing a standard definition of state of health. This includes determination of measurement uncertainties and accuracy, which is key for warranty and legal purposes.

Establishing regulations on the identification and labelling of battery cells, modules and packs to ensure traceability.

Standardising terminology between cells, modules and packs, including best practice measurement protocols and configurations.

Measuring impurity levels in recycled materials and establishing acceptable standards for what can be recycled or reused.

Measuring electricity use during the day to inform grid usage for recharging vehicles. This will require billing tools, management of the charging process and establishing how the charging infrastructure will feed into the grid.

Establishing standards for communication between BMS, charger and grid, including fast charging, to facilitate multiple products in the market.

7 Summary of measurement challenges

The measurement challenges listed in the above sections, which are summarised in the following table, were identified through desk based research, in-depth interviews with key stakeholders within the battery industry and through a dedicated workshop on this topic held at NPL in September 2017. A list of the contributors can be found at the end of this report.

The table combines the challenges identified within each sector and technological application as explored throughout this report and prioritises these within the key themes of quality control, diagnostics, modelling and lifetime prediction, end-of-life and standards.

NPL battery related capabilities

NPL has a broad range of world-leading measurement, modelling and testing capability that is well suited to battery research. Multi-disciplinary collaboration between NPL technical areas has the potential to make a significant contribution to advances in diagnostic techniques at cell, module and pack level through innovation in measurement.

Examples of relevant NPL capability include:

Electrochemistry

- Standardisation of Electrochemical Impedance Spectroscopy (EIS) as a diagnostic tool to monitor state of health
- Combined *in situ* electrochemical and spectroscopic (Raman and infrared spectroscopy) imaging of electrodes to correlate performance with chemical changes

Temperature

- Advanced techniques for *in situ* temperature measurement in cells, modules and packs
- Thermal imaging of exterior surfaces to inform cooling strategies

Dimensional

- *In situ* measurement of cell swelling due to electrolyte decomposition to monitor performance degradation and risk of thermal runaway
- Measurement of dimensional tolerances for quality control

Surface Chemistry

- Measurement of lithiation and delithiation during battery cycling
- Characterisation of solid electrolyte interphase (SEI) layer

Electromagnetics

- Time domain reflectometry to pinpoint local impedance hotspots
- Detection of local cell currents using magnetometry

Modelling and Data Science

- 3D modelling of battery performance using continuum thermodynamics
- Reliability and traceability of large datasets

Theme	Measurement challenge	Description	Priority
Quality control for manufacturing	Parameterisation and technique identification	Identifying critical parameters, such as material properties and formulation methods that influence cell performance. Establishing acceptable tolerances for these parameters and determining how uncertainty in their measurement is propagated throughout the manufacturing process.	High
		Standardisation of test and characterisation methods and validation at the materials and cell level.	Medium
		Extending the range of conditions in which the battery can operate when assessing modules and packs, for example characterisation of parameter space over a greater temperature range.	Low
	Fault identification	Techniques for rapid and cost-effective screening of large numbers of cells. Balancing and matching cells, materials level measurements and continuous in-line monitoring.	High
		Structural assessment of cells, including weld integrity, internal structure and mechanical strength.	Low
	Material quality and purity	Measuring purity of materials used in manufacture, including materials recovered from recycling and establishing a definition of 'battery grade'. Understanding the influence of these impurities on performance and safety.	Medium
		Identification of techniques that can be applied in the real-world at low cost.	Low
		Non-destructive diagnosis of cell chemistry.	Low
	In-line monitoring	In-line, fast, non-invasive measurement of physical and chemical properties of electrodes and components during manufacture, for example electrochemical properties, particle size, composition, rheology and film thickness.	Medium
		Avoiding rejection of serviceable batteries through in-line measurement processes. Measurement of coating thickness, porosity and wet versus dry electrode materials.	Low

Diagnostics	Pack level diagnostics	Identifying failed or failing cells within a battery module or pack and understanding the impact of individual cell failure on overall performance.	High
		<i>In situ</i> temperature measurement techniques at both cell and pack level, such as differential temperature measurements and thermal imaging, to support improved thermal management strategies.	Medium
		Understanding propagation of damage as a result of failed cells within a battery module or pack.	Medium
		Establishing key performance indicators which combine parameters to give a consistent measure of health similar to 'MOT' testing regimes.	Medium
	Accelerated testing	Accelerated stress tests to establish confidence in lifetime prediction, including external verification and validation.	High
		More representative test methods, for example measurements on thermal runaway.	Medium
		Diagnostics and modelling around behaviour of alternative battery materials with different degradation mechanisms.	Low
	Battery Management Systems	Standardisation of BMS at system or pack level, including the challenge of scaling-up from academic research to industry use, for example impedance-based techniques in noisy, hot, vibrating environments.	Medium
	Post mortem forensics	New techniques for post mortem analysis in order to identify failure mechanisms and inform cell design.	Medium
	State of health	Determination of state of charge and state of health, including derived parameters that cannot be directly measured.	Medium
Identifying and mitigating degradation mechanisms to improve performance and safety. This will require indicator measurements for potential failure to be established.		Medium	
Modelling and lifetime prediction	Real-time scenario prediction	Non-invasive monitoring of state of health and establishing which parameters are most important to industry and user. Using data for scenario prediction where monitoring information is fed back to user, offering a suggested usage profile for optimum performance.	High
		Self-diagnostics to create a link between monitoring and performance.	Low
	Degradation modelling	Modelling of degradation mechanisms linked to actual car use to reduce the need for over-sizing.	Medium
	Data	Coupling of methods for simulation and use of data, including the need for data sharing and benchmarking.	Medium
		Addressing the data capacity issue, for example the inability to record continuous temperature data for thousands of cells. Determination of optimum trade-off between monitoring capacity and cost.	Low
		Security, reliability, validation, standards and interoperability of data for modelling and lifetime prediction.	Low
	Design optimisation	Techniques to optimise uniformity, for example of pressure in modules and coolant flow in packs.	Low

End-of-life	Recycling, re-use and Second life	Identifying end-of-life thresholds for first and second use, including economics and safety. Considering life cycle analysis and economics for the design and manufacturing process to better understand scenarios and processes for recycling.	High
		Standardisation of key parameters for second life use prediction, including recording first life history and assessing how it can be fed into second life use.	Low
	Re-warranty for second life	Establishment of information database of operational history.	High
	Environmental monitoring	Monitoring environmental effects throughout the life cycle from extraction of raw materials to recycling and disposal.	Medium
	Identification of waste components	Detection and recovery of recycled metals, including identification and specification of the most critical materials.	Medium
	Disposal	Detection and disposal of hazardous materials.	Low
Standards	State estimation	Establishing test protocols to take into account different modes of use, for example fast charging. Assessment and characterisation of unsafe modes of operation.	High
		Standardisation of electrochemical test methods, for example impedance spectroscopy for state of health monitoring.	Medium
	Traceability	Standard definition of state of health with uncertainties and accuracy as this is important for warranty and legal purposes.	Medium
		Regulations on identification and labelling of battery cells, modules and packs.	Low
	Test methods	Standardisation of terminology between cells, modules and packs, including best practice measurement protocols and configurations.	Medium
		Measurement of impurity levels in recycled materials and establishing acceptable standards for what can be recycled or reused.	Low
	Charging infrastructure	Measurement of electricity use during the day to inform grid usage for recharging electric vehicles.	Medium
		Standards for communication between BMS, charger and grid, including fast charging.	Low

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