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Materials for Energy

An Energy Futures Lab Briefing Paper

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Acknowledgments

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Executive Summary

The transition to Net Zero will require substantial quantities of critical materials in order to build and maintain new technologies, from renewable generation to batteries for electric vehicles. Materials such as lithium will be required in much larger quantities than before, while novel materials may need to be developed to replace expensive or scarce conventional materials. This Briefing Paper considers the current availability and development of materials for the energy sector, investigating both current availability and forecasted production of several critical materials and looking at the state of development of novel materials in the energy sector.

Four materials considered critical to new energy technologies and the low-carbon transition were investigated for availability based on known reserves and projected future demand: lithium, cobalt, tellurium and copper. These materials were selected to illustrate the key themes that relate to concerns over the demand and supply of those metals and other materials that will be required for the transition to a global low-carbon energy system.

- There are a wide range of long-term demand forecasts for the four metals studied;
- The fundamental level of resource availability for these four materials is not currently a primary source for concern;
- The supply chain – extraction, recycling and production – is the source of greater concerns, due to the long lead times typically required for scale-up of facilities and to develop new extraction and production projects, especially compared to the rapid action required to deliver on carbon emissions targets;
- The extraction and production of specific materials tends to be geographically concentrated, which presents stability risks, and other factors, such as materials produced as by-products, complicates forecasts further. It is also important not to assume ease of substitution of specific materials.

Countries wishing to mitigate impacts of potential material constraints should focus on several key areas:

- First, it is important to ensure that resource extraction, production and recycling activity is able to respond to increasing demand in a timely fashion, either by reforming planning regulations or by providing financial incentives;
- Second, where practicable, the issue of geographical concentration of critical materials should be addressed, either by developing new reserves and production facilities or by increased stockpiling;
- Finally, demand forecasts should be periodically reviewed and updated to ensure that they remain relevant and in line with current technological trends to transition towards Net Zero. Those (outlying) forecasts predicting shortages or exhaustion of key materials should be analysed for their reliability and to understand under what circumstances their predictions may eventuate.

As important as the availability of existing materials is the search for novel materials to substitute or augment existing materials with more effective, available or economically viable alternatives. Three technology areas were examined for the current state of novel materials development, due to their importance in the low carbon transition: photovoltaics, batteries and hydrogen and other energy carriers.

Silicon PV has fuelled the rapid growth in solar PV installations over the last decade, due to rapid cost reductions in silicon and silver supply and production chains. Most current studies forecast the continued dominance of silicon PV into the 2040s, with continuing reduction of silicon and silver usage intensities. Large-scale deployment of cadmium-telluride solar cells could face production shortfalls of tellurium by 2040, which would need to be met by increased production and more aggressive recycling efforts. There are also significant areas for improvement in materials solutions to module heating and dirty panels, even to established technologies such as silicon PV. Many emerging PV materials technologies such as dye-sensitised solar cells and perovskites have the potential to transform the market in the longer-term, being light-weight, easier to manufacture and suitable for a wide range of use cases. However, significant challenges to large-scale commercialisation remain, including degradation, materials availability and scaling-up of manufacturing processes.

Battery technologies are an essential component of the transition to clean energy. Materials R&D in this area could lead to improved energy and power densities, as well as better longevity, lighter weight and enhanced safety. The preeminent battery technology used today is lithium-ion (Li-ion), used in applications from mobile phones to electric vehicles. There are increasing demands for higher energy densities than current lithium-ion batteries can supply, especially from the electric vehicle and electronics sectors. Several technologies in development which could improve on these characteristics are lithium sulphur (LI-S), lithium-oxygen (Li-O) and solid-state batteries. There are, however, key science challenges that need to be addressed, including the composition of the electrodes and electrolytes and the challenge of ensuring the cell reaction is fully reversible. Scale-up and commercialisation challenges will also need to be addressed, as several technologies will require the development of new manufacturing methods and supply chains and will face price competition from the more established Li-ion ecosystem. However, there are significant efforts to commercialise these new technologies, and several technologies may see substantial rollouts in the latter part of this decade.

Hydrogen has long been seen as an important part of the drive to a low-carbon economy, as it can be used as an energy carrier where electrification is difficult or expensive. Electrolysis of hydrogen from water using low-carbon electricity is currently the most promising low-carbon hydrogen generation technology to deploy in the near-medium term. There are several materials challenges in making hydrogen electrolysis more efficient and reducing the intensity of critical materials.

- Low-temperature electrolysis will benefit from research to replace platinum-group catalysts with lower-cost substitutes, as well as improving the lifetime and stability of catalysts and cell modules;
- High-temperature electrolysis is currently at demonstration stage, with research challenges in durability and performance of electrodes and interfaces over long periods of time;
- Ammonia has potential as an energy carrier due to substantially cheaper transport and storage costs – though conversion efficiency losses are greater. Research is currently at a more basic level and substantial advances will need to be made to make this a commercially viable energy vector.

As part of this project, a workshop was held with representatives from the UK academic and industrial sectors to explore the UK materials R&D space. The purpose of the workshop was to understand the strengths of the UK's novel materials for energy R&D capability, the challenges currently facing this field, and the policy decisions which need to be made to support researchers and technology developers. The workshop found a dynamic, impactful and internationally recognised UK novel materials research community, producing significant, high quality basic R&D. However, leveraging this research was often inefficient, with a lack of platforms for characterisation and testing, difficulties in navigating technology transfer and partnerships with private industry, and access to support for demonstration and commercialisation. Five recommendations were elicited from the workshop to improve shortfalls in the sector:

- A dedicated UK resource for testing including degradation testing, benchmarking, standardisation, and certification should be funded;
- It should be made easier for companies and academia to work together to transfer R&D up the technology readiness chain;
- More commercialisation incentives are required - greater access to venture capital and support, easy access to test-beds and demonstration platforms, and further tax incentives for innovation and applied R&D;
- Speculative research should be funded with fewer concerns about immediate results to ensure that the UK has a steady supply of future discoveries and disruptive impact;
- To ensure greater consideration of research continuity, people with well-developed and relevant skillsets should be incentivised to stay in their roles and institutions, along with expanded training for the next generation of researchers.

Introduction

The transition to net-zero carbon emissions is a massive global effort, requiring significant and ongoing investment and buildout in new technologies, processes and products. Large quantities of raw materials will be needed to build low-carbon generation, transportation and end-use technologies, in addition to materials for any substances used in synthetic and bio-fuels.

Materials challenges will often be different, both in the kinds of materials required and the scale that they will be required in, from previous fossil fuel-based technologies. Low-carbon technologies often require more materials during construction than the conventional technologies they are replacing, with the IEA stating that a typical electric car requires six times the mineral input of a petrol-fuelled car, and an onshore wind plant requires nine times the mineral input of that for an equivalent gas-fired plant (International Energy Agency, 2021), ignoring well-plant factors. The materials required differ as well, with greater needs for rare-earth metals, copper for electricity networks, nickel for alloys and lithium and cobalt for battery technology. Some of these materials are difficult and expensive to extract and produce at scale, fuelling the need for discoveries of novel materials to replace or augment them and technology designs to minimise the usage of expensive, environmentally damaging and difficult to source materials.

This Briefing Paper considers the current availability and development of materials for the energy sector. Using four illustrative case studies, it first assesses the issues relating to the availability and production chain of materials which are critical to the production of low-carbon energy technologies. Utilising a technology-based approach, it then investigates the state of development of novel materials in the sector, presenting policy recommendations to improve the R&D chain and accelerate the development of novel materials and more efficient utilisation.

Section 1 investigates the resource availability of selected critical materials and compares them to projected demand as low-carbon technologies continue to be deployed. It focuses on four materials (lithium, cobalt, tellurium, and copper) to highlight key themes of concern – resource availability, production and refining constraints, uncertain future levels of demand and the contribution of recycling. This section also summarises key developments in the past half-decade in the availability of these materials and present a summary of key challenges.

Section 2 looks at the development of novel materials in the UK, centring on four low-carbon technology areas (photovoltaics, batteries, hydrogen and thermodynamic energy storage) which have significant materials challenges, either through scarcity or environmental impact. Utilising in part roadmapping work from the UK's Royce Institute, this section examines these technology areas, identifies key materials challenges and potential solutions, and showcases UK capabilities in these areas.

Section 3 builds on the capabilities and challenges identified in Section 2 by presenting the findings from a workshop of senior academics and industry professionals on the UK's strengths and weaknesses in the development of novel materials. This section summarises key insights from the workshop into recommendations for policy interventions to provide support to grow this important sector.

1. Resource availability and Demand Forecasts: Case Studies

1.1 Background

The availability of materials for energy technologies has become an area of increasing concern in the broader resource availability debate due to needs for new materials with additional functionalities, the relatively undeveloped supply chains for many critical metals, and the rapidly rising demand for low carbon energy technologies that use them. Several existing studies have attempted to investigate the availability of a range of different technology metals or other resources, using different selection criteria, different definition of availability and different methods of examining past and future supply and demand trends (U.S DoE, 2011; Zepf *et al.*, 2011)

These studies often address a number of the same key materials, including lithium and cobalt, used in modern lithium-ion batteries, metals used in solar PV technologies like tellurium, and copper, interesting for its ubiquitous role in electrical technologies and electricity transmission and distribution. The ongoing interest in availability of these materials is captured in a 2021 IEA study, which is one of the most recent comprehensive assessments (International Energy Agency, 2021). This study highlights the rapidly rising demand for many critical metals, and the mismatch to current levels of supply.

A 2014 report published by the UK Energy Research Centre (UKERC) also highlighted the wide range of resource and reserve estimates for materials that were considered likely to be critical to the low-carbon energy transition (Speirs, Gross, *et al.*, 2014a) The UKERC research team also noted how those estimates change over time in response to actual and forecast demand, the prevailing wider economic conditions, and continuing efforts in resource exploration. The report also discussed different approaches to assessing the degree of material scarcity (or otherwise). Whilst acknowledging its widespread use in fossil fuel extraction industries in particular, the report observed that the reserve to production ratio (R/P) 'gives little indication of the likely trend in metal availability in the future' and discussed an alternative approach that has also been widely used, that is to compare current production or known resources to projected future demand (either on an annual or cumulative basis). Although this method does address the issue of future demand, it is important to recognise that predicting future demand is still highly uncertain since that in turn depends on a host of factors including price, regulation, technology, recycling rates, and economic and behavioural trends.

The 2014 UKERC report identified three categories of demand estimates in the literature: (1) expert elicitation, which involve asking an identified set of experts in the field for their opinions; (2) bottom-up analyses, which typically calculate future demand based on fundamentals such as the amount of material required for a given unit of technology and estimates of the future deployment of that technology: (3) third-party estimates, which in turn may ultimately have used either one of the first two methods or some combination of the two. As the UKERC report also noted, there are issues and complexities around the definition of terms such as 'reserves' and 'resources' and full details of how the USGS defines these terms are available in (USGS, 2021b). Briefly though, reserves are 'that part of the reserve base which could be economically extracted or produced at the time of determination' and 'resources' are 'a concentration of naturally occurring solid, liquid, or gaseous material in or on the Earth's crust in such form and amount that economic extraction of a commodity from the concentration is currently or potentially feasible'.

Definitions of what constitutes a critical material are not exact, and in any event such materials are not a homogenous family of metals and minerals. Further, these reports do not or cannot account for innovations yet to be manifest. However, the respective sets of characteristics of those materials that are considered critical to the low carbon energy transition can, and frequently do, overlap. The approach adopted for this briefing paper therefore is to select for discussion a sample of materials (lithium, cobalt, tellurium, and copper) which between them illustrate key themes that are of concern. These themes include the level of fundamental resource availability, the role of assumptions of technology development trends, the effects of production capacity constraints and by-production, the effects of market dynamics on supply over differing time scales, and the contribution that recycling can make to meeting future demands.

1.2 Lithium

Lithium is a metallic element, whose future demand forecasts are driven largely by its use in batteries for electric vehicles and stationary energy storage. The 2014 UKERC report (Speirs, Gross, *et al.*, 2014a) identified a wide range of future demand estimates for lithium, suggesting that estimates for the percentage demand growth between 2012 and 2030 were between a little under 200% to just over 700%. A paper accompanying the UKERC report calculated that in absolute terms, the future demand for lithium for electric vehicle batteries (by far the most important source of future demand) was approximately 60,000-280,000 tonnes by 2030 and 180,000 to 1 million tonnes by 2050 (Speirs, Contestabile, *et al.*, 2014). For comparison, the 2014 report gave current (at the time) primary production and reserves values for lithium of 35,000 and 13,000,000 tonnes, respectively.

For this briefing paper, the authors have collated the most recent US Geological Survey data available from (USGS, 2021a), and present in Figure 1 below the evolution of lithium production, reserves and resources during the decade to date, and the resultant reserves to production ratio (measured in years) in Figure 2. Production volumes for the most recent year (2021) are designated as estimates by the USGS, and also the whole production data series does not include production figures for the US 'to avoid disclosing company proprietary data' since the only current US production is from a single operation. That notwithstanding, (Sanderson, 2016) observed that 'Almost all of the world's lithium comes from just four countries — Chile, Australia, Argentina and China' so this exclusion of US production data is not considered hugely significant.

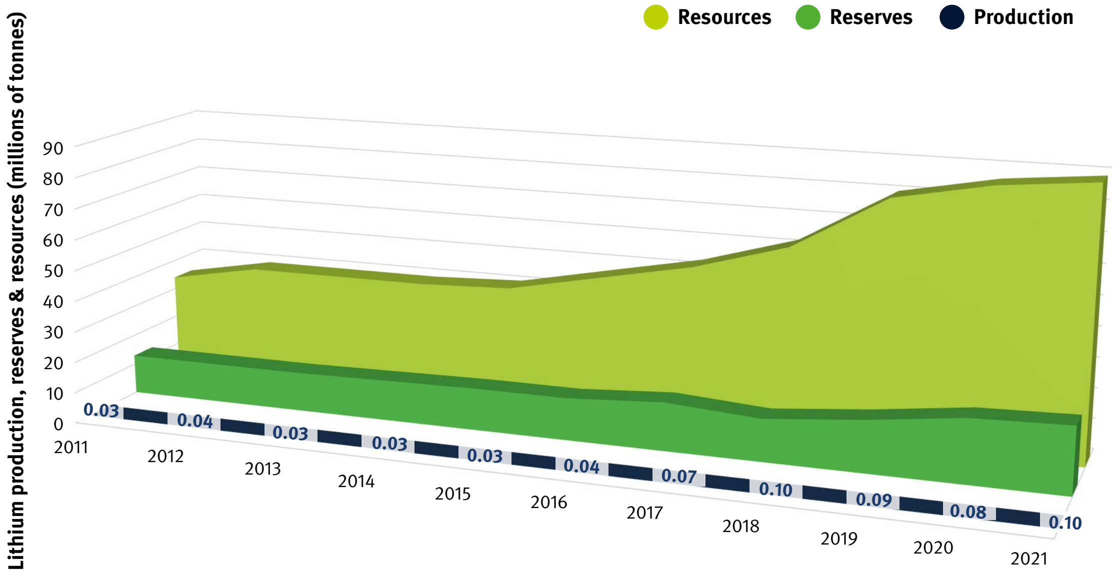

Figure 1 Global lithium production, reserves and resources

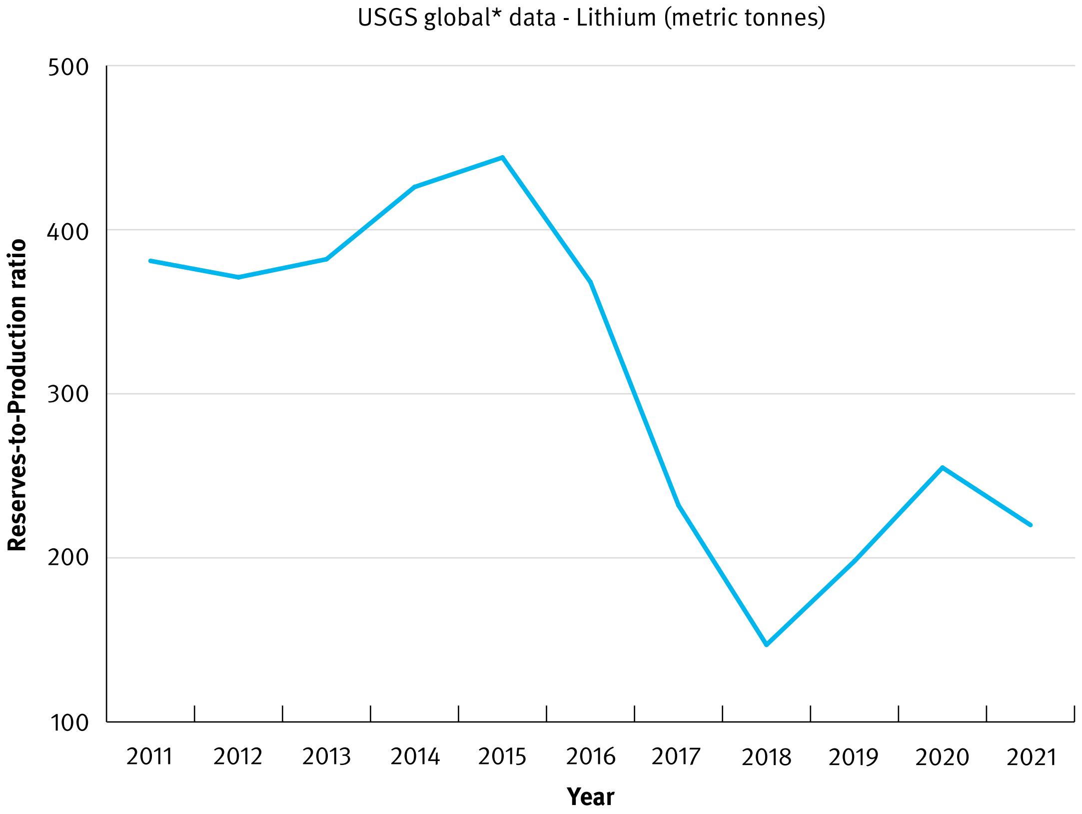

Figure 2 Global lithium reserve to production ratio

* Note that US Production data is excluded from the USGS dataset

Two points are readily apparent from Figure 1. The first is that annual production volumes for lithium are a very small fraction of reserves as identified by the USGS. Even though annual production has increased by 240% in the period from 2011 to 2020, reserves have also increased considerably. This means that the reserve to production ratio has changed from 381 years in 2011 to 256 years in 2020, with considerable variation throughout the decade, as show in Figure 2. The second point that Figure 1 makes clear is that global lithium resources are several times greater than currently estimated reserves, and very large indeed when compared to current production levels, with the most recent estimates suggesting that resource levels are over a thousand times greater than 2020 production, and that identified lithium resources have increased substantiality, by over 250% in the last decade. This is consistent with many commentators acknowledging the relative abundance of global lithium resources (Lex, 2021).

However, lithium demand is projected to grow very considerably over the next few decades, combined with rapid near-term demand growth forecast. Whilst there is broad agreement on the overall direction of this future demand for lithium, discerning the most likely out-turn is fraught with unknowns and uncertainties, depending for example on prospects for use of hydrogen and associated chemicals for energy storage, and these are reflected in the extraordinarily wide range of demand projections found in the literature.

A recent paper focused on lithium demand from low-carbon technology use (J. Lee, Bazilian, Sovacool, & Greene, 2020) suggested that this would grow by 965% up to 2050, based on the actual production figure of 43,000 tonnes in 2017 rising to 415,000 tonnes by 2050. This compares with a projected figure for 2030 of 147,000 tonnes in (Jones *et al*., 2020) although note that this related to the annual lithium demand associated only with electric vehicles. A recent report from the International Energy Agency (IEA, 2021b) which focused on the mineral and metals requirement for the low carbon transition, forecast annual lithium demand of between 160,000 and 378,000 tonnes by 2030, rising to between 276,000 and 904,000 tonnes by 2040. The Lee *et al* 2020 paper used data from the World Bank, who also published their own analysis of the key mineral and metal requirements for a transition to low carbon energy system (Hund *et al.*, 2020) In that analysis, the authors calculated that by 2050 the annual demand for lithium attributable to energy technologies would be 490% of the 2018 production total.

The 2020 World Bank report also found that for the cumulative total lithium requirement through to 2050, there is a very wide range, between a low of approximately 4 million tonnes and a higher value of approximately 10 million tonnes. The range is largely driven by which of the carbon reduction scenarios is being modelled and assumptions over efficiency improvements in the use of the lithium in batteries. The authors of the World Bank study also estimate that if recycling rates were increased considerably from the current (very low) base then cumulative demand for lithium up to 2050 could be reduced by around a quarter. These estimates can be compared with the summary presented in (Junne *et al.*, 2020) which drew on estimates of cumulative demand to 2050 from nine other studies, and included demand from all sectors, not just transport and stationary energy storage. Estimates ranged from 3 million to 27 million tonnes, with a median value of 12 million tonnes, and an average of 15 million tonnes. However, in that paper the authors presented their own estimates and they represent an outlier, with a cumulative demand for lithium by 2050 of between 16 million and 108 million tonnes.

This theme of very wide ranges for future demand is continued in (Deetman *et al.*, 2018) who estimate annual demand for lithium for transport, energy and appliance technologies at between 55,000 and 810,000 tonnes by

2050, with the majority of this coming from demand in the transport sector, followed by the stationary battery storage sector. This is consistent with (Tsiropoulos *et al.*, 2018) who conclude that rapid and sustained growth in electric vehicle sales and stationary electricity storage will drive future lithium demand, and the European Raw Materials Alliance who suggest that European lithium demand will increase by a factor more than 50 by 2050 (ERMA, 2020).

Lithium summary

The overall message in relation to projected lithium demand and identified reserves and resources is that all but the very highest projections can be met from the current global reserves of 21 million tonnes and represent only a fraction of currently estimated global resources. Whilst this may be a reason to be sanguine, this would be to ignore the very significant challenge implied by the projected annual demand figures described above. This is the scaling up of the current lithium production supply chain required to meet very large, anticipated demand increases that are a feature of even the lowest of the demand forecasts (excluding those which model a 'business as usual' baseline where no further concerted efforts are made to electrify transport or increase stationary battery storage provision). Shorter-term production bottlenecks also pose a challenge (EC, 2018; Tabelin *et al.*, 2021). Added to this are concerns over the degree of resilience in the supply chain and the reliance on a single (or very small number) of suppliers (ERMA, 2020). In addition, the market dynamics and cyclical nature of investment in extractive industries typically means that there will be lags between rising demand and expanding supply capacity. This may lead to periods of rising prices, which in turn would be expected to lead to increased investment in extraction projects. This is borne out by the current situation in the lithium market of high, and volatile (Dizard, 2022), prices where production is highly profitable for most current projects (Lex, 2021), and where producers are actively seeking opportunities to develop new projects (Sanderson, 2021; Smyth, 2021).

Current lithium reserves and resources far exceed existing demand and are sufficient to cover even the highest projected cumulative demand over the next three decades. Current production capacity is constrained, and this is reflected in rising prices and signs of increased activity in the development of extraction projects. Nevertheless, near-term supply seems likely to remain tight, and this will contribute to price volatility. There are concerns of over-reliance on a relatively small number of supplying countries and producing companies, and the implications this has for the resilience of the supply chain. Very little recycling or reuse takes currently place but this could make a significant contribution to reducing long-term demand.

1.3 Cobalt

Cobalt is used mostly in rechargeable battery electrodes, a growing use that largely dictates changes in future demand. An increasing proportion of this end use demand comes from electric vehicle batteries, which has recently overtaken mobile phone and laptop lithium demand for the first time. 65% of demand is driven by the rechargeable battery market, indicating potential for demand growth as battery demand increases (Financial Times, 2022). Another major use is in superalloys, which are used to make parts for gas turbine engines. Academic estimates of future demand suggest over 200,000 tonnes per year of Cobalt may be needed by 2050, while the Cobalt Institute estimates cobalt demand at over 300,000 tonnes by 2026 (Tisserant & Pauliuk, 2016). Figure 3 collates the annual reported reserve and production data from the USGS (U.S. Geological Survey, 2022). Figure 4 presents the cobalt reserve to production ratio from 2011 to 2020. The USGS do not report resource data for cobalt.

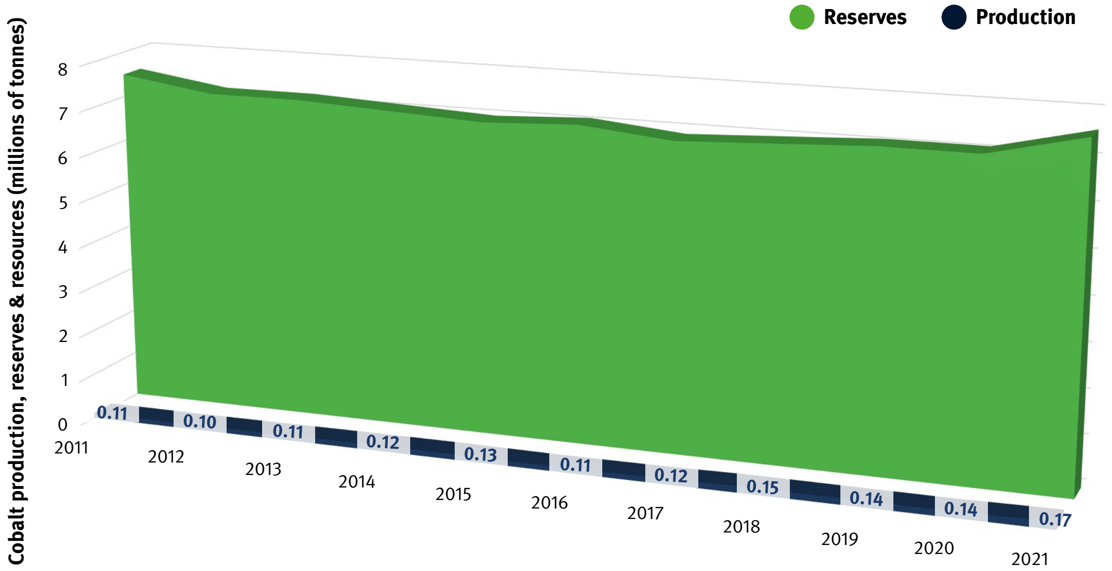

Figure 3 Global cobalt production and reserves

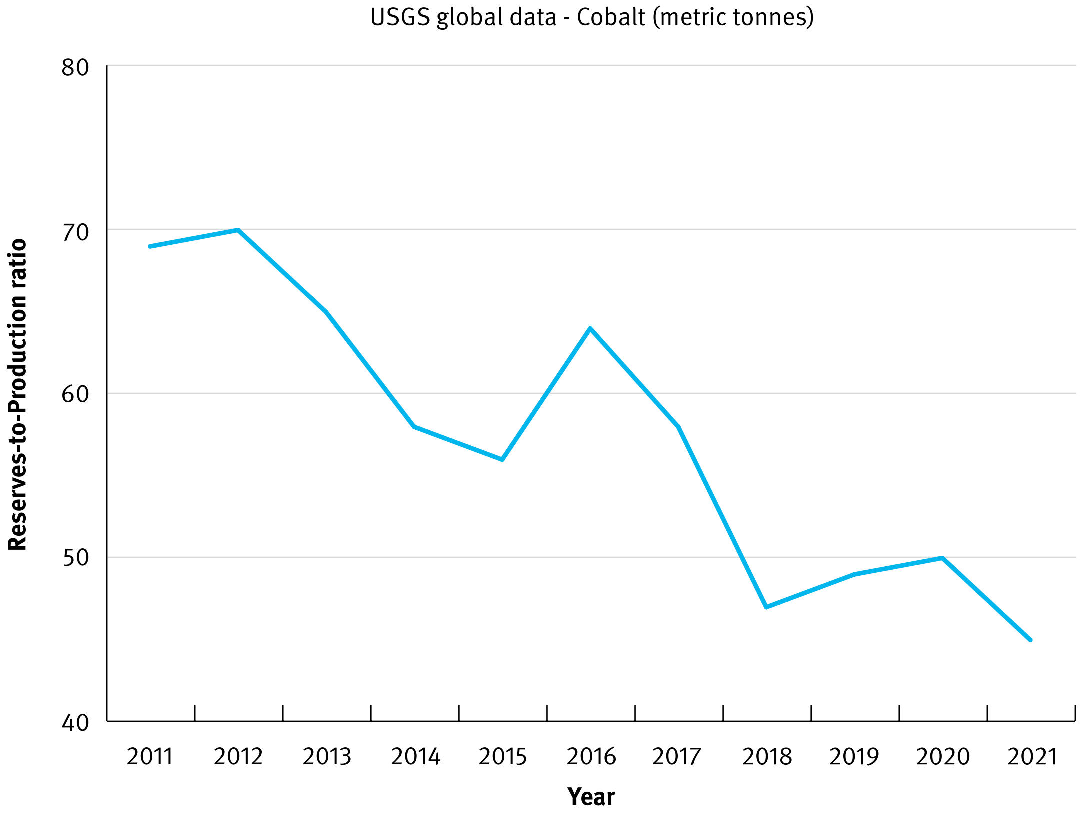

Figure 4 Global cobalt reserve to production ratio

Cobalt annual production is a small fraction of reserves, with estimated reserves in 2021 of 7.6 million tonnes and increasing, while production was 170,000 tonnes. Production grew by over 20% between 2011 and 2020, driven by increasing demand (U.S. Geological Survey, 2022) Reserves, however, decreased over the same period by over 5%, though reserve estimates grew to slightly over the 2011 estimate at 7.6 million tonnes in 2021. This is reflected in the apparently declining reserves to production ratio in Figure 4. With a reserves to production ratio of around 45, there is clearly sufficient resources to meet current demand for some time, subject to significant changes in future demand. However, a large proportion of cobalt production is as a by-product of nickel and copper mining [USGS MCS 2022]. This may impact the price elasticity of cobalt, requiring significant price increases to elicit increases in supply above that currently supported by the copper and nickel mining industry.

Cobalt supply may provide the best historical example of a constrained metal supply chain. It meets several of the key criteria that define a metal sensitive to supply constraints, namely:

- Significant resource and production concentration in one country;
- Geopolitical instability in the producing country; and
- Relatively few opportunities for substitution in key metal uses.

During the 1970s the Democratic Republic of Congo (formerly Zaire) was responsible for approximately half of global cobalt production (Figure 5). Typical uses of cobalt in the 1980s included cobalt containing alloys for high strength magnets, as an alloy component in heat resistant applications and to produce blue pigments for paints (Gross & Speirs, 2014). In the late 1970s conflict in Zaire and neighbouring countries interrupted cobalt supply routes and ultimately affected cobalt mine production, reducing international cobalt supply and causing concern in international cobalt markets (Westing *et al.*, 1986). Supply disruptions precipitated several responses, including a significant price increase (Figure 6), strategic stockpiling (Guttman *et al.*, 1983), and concerted effort towards developing substitute materials (Sichel, 2008). An interesting outcome of cobalt substitution research is the development of neodymium alloy magnets, which were developed to reduce reliance on cobalt supply in the high strength magnet market (Speirs, Gross, *et al.*, 2014b). These new neodymium magnet alloys possessed even greater magnetic properties than cobalt alloys and have subsequently superseded them in many high strength magnet applications.[1] This has, however, raised material constraints concerns of its own given the resource availability of rare earth element neodymium (Speirs, Gross, *et al.*, 2014b).

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[1] Neodymium Iron Boron (NdFeB) magnets have stronger magnetic fields and are cheaper than Samarium Cobalt (SmCo) magnets. However, SmCo magnets perform better at high temperature and in corrosive environments.

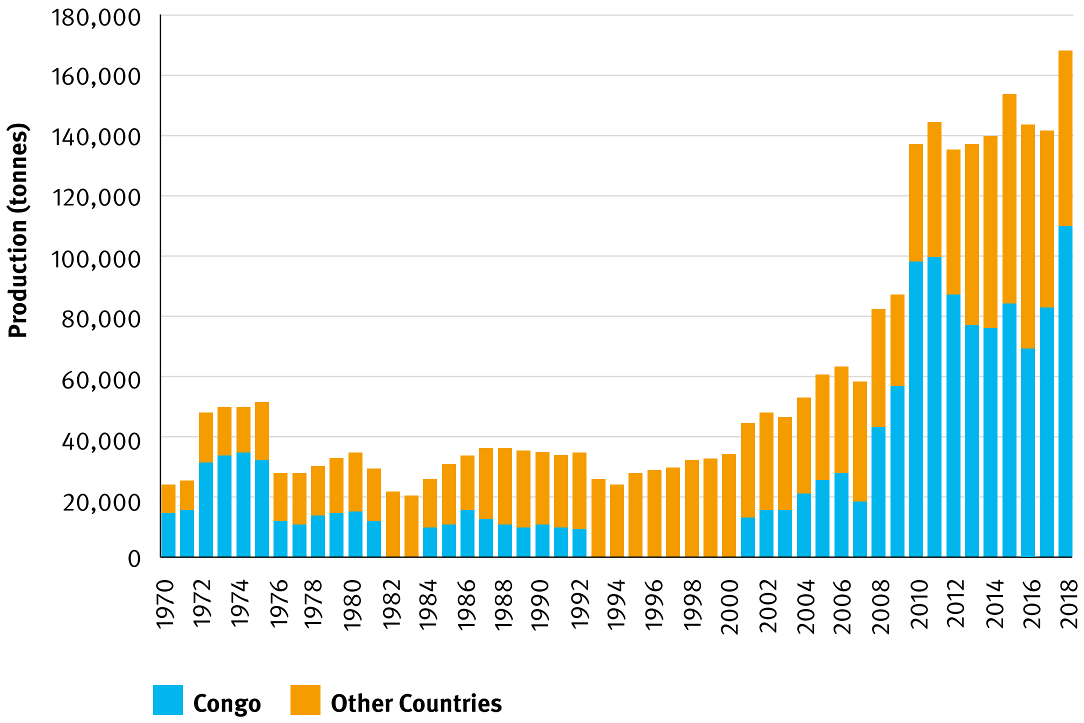

Figure 5 Global cobalt production 1970 - 2018
Source: https://faraday.ac.uk/wp-content/uploads/2020/05/Insight-cobalt-supply-chain1.pdf

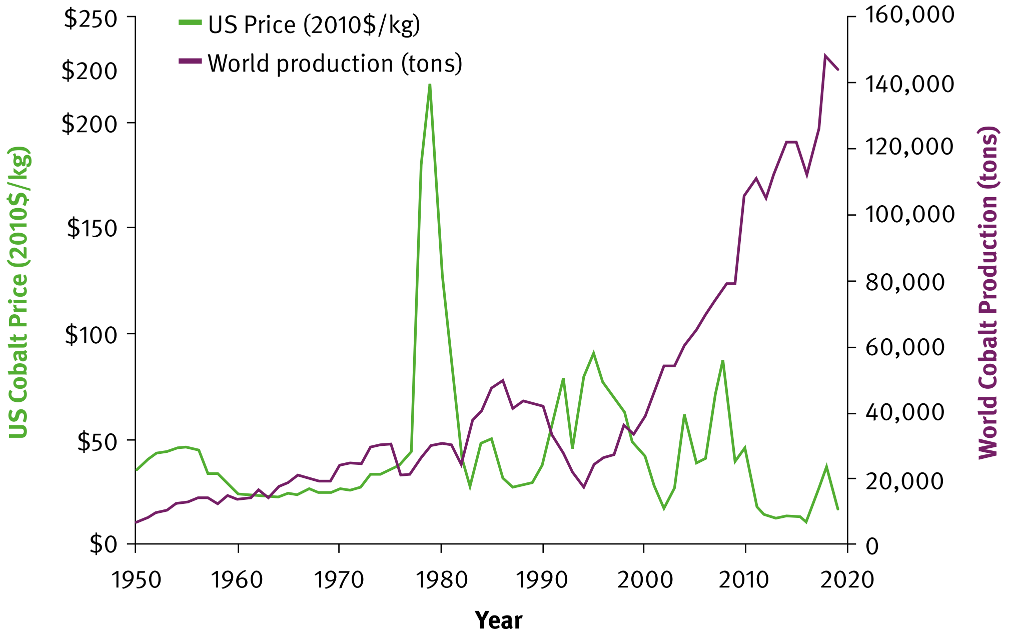

Figure 6 US cobalt price and world production showing significant price spike between 1978 and 1980 and more recent increase in production
Source: U.S Geological Survey Minerals Yearbook (2019)

In recent times cobalt has become a key material in the production of lithium-ion batteries. The significant growth in the lithium-ion battery market has led to significant increases in global cobalt demand and therefore production (Figure 5). However, the Democratic Republic of Congo (DRC) is still the dominant producer of cobalt globally (Figure 7). This is a risk factor in the potential for future supply constraints in the global cobalt market.

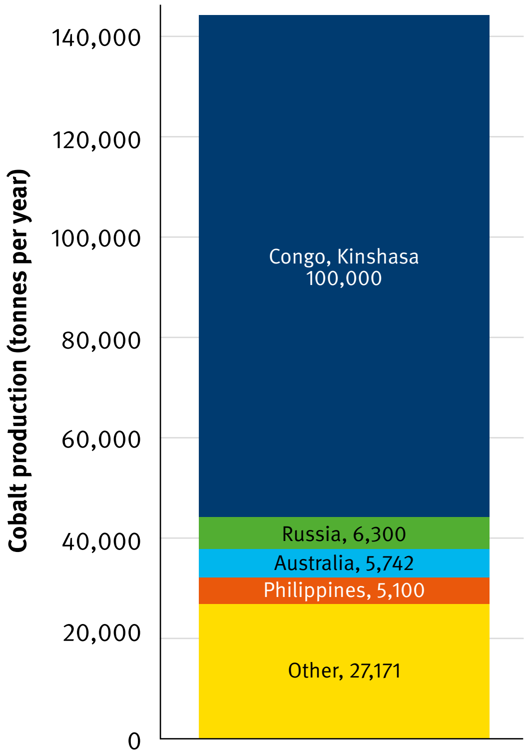

Figure 7 Cobalt: world mine production, by country or locality

Cobalt summary

Current cobalt reserves and resources far exceed existing demand, though the RP ratio was declining between 2011 and 2020, suggesting that discoveries of economically recoverable cobalt were not keeping pace with production. However, this trend was reversed in 2021, with reserves of 7.6 ,million tonnes estimated by the USGS in that year, slightly above reserve estimates in 2011.

Current production capacity is constrained, and this is reflected in rising prices and signs of increased activity in the development of extraction projects. Nevertheless, near-term supply seems likely to remain tight. The reliance on a small number of countries for cobalt production, particularly the DRC, is acute. This reliance has existed for many years and leaves the cobalt market exposed to supply constraints if the DRC experiences any supply disruption. Very little recycling or reuse currently takes place but this could make a significant contribution to reducing long-term demand. A number of practical measures are needed in order to improve recycling rates, including the development of new recycling processes, recycling regulations and optimised collection systems (Gaines, 2019; S&P Global Market Intelligence, 2021a). The historical dynamics in the cobalt market provide one of the clearest examples of material availability constraint. This constraint was ultimately short term, and responses included significant price increases, stockpiling of resources and efforts to develop novel substitute materials, particularly successful in high powered magnets.

1.4 Tellurium

Tellurium is a rare metalloid element most typically found in copper ores, but at very low concentrations, and the vast majority of global production to date has therefore been a by-product of copper refining (Houari *et al.*, 2014).The primary use of tellurium in the context of energy systems decarbonisation is in the production of cadmium telluride (CdTe) 'thin-film' PV cells. A decade ago, the energy conversion efficiency advantages then offered by CdTe cells led many commentators to suggest that this technology could play a major role in future global PV deployment. This led to concerns that future production of CdTe cells may be constrained by the availability of tellurium, with Candelise, Spiers and Gross (2011) identifying several studies that raised this issue, and reporting that some industry estimates suggested that thin-film PV could take 30% of the global PV market by 2020. However, in their paper, they went on to conclude that their own analysis of the available evidence did not support the view that future CdTe PV production was likely be constrained by tellurium availability.

When the UKERC produced its 2014 materials availability report (Speirs, Gross, *et al.*, 2014), there was a prevailing view that CdTe PV was likely to become very competitive with crystalline silicon PV in terms of overall costs, and this was anticipated to lead to CdTe PV taking a significant share of the overall PV market. Houari *et al*. (2014) reported that thin-film technologies were estimated to take up to 40% of the PV market by 2030, but also observed that crystalline silicon PV costs were falling rapidly by that point, and that if this trend were to continue then that would have a significant negative impact on the likely demand for CdTe PV (and therefore on tellurium demand). The current PV market share of crystalline silicone technologies is ~90%, with CdTe approximately half of the rest of the market at 5% share (McNulty & Jowitt, 2022). This is currently significantly short of the 2030 market share estimated in previous studies (Speirs, Gross, *et al*., 2014b). As predicted, this market share has been driven, in part, by the cost reductions in crystalline silicone technologies (Allouhi *et al*., 2022). The CdTe cell share of the global PV market may increase in the future in response to improving cell characteristics. For example, contemporary studies estimate current material intensity for CdTe cells in line with long term future estimates of previous studies (McNulty & Jowitt, 2022). However, future tellurium demand is unlikely to reach the levels estimated in the worst case examples in previous studies, largely due to the changes in long term market share estimates. For example, McNaulty and Jowitt (2022) estimate future demand for Te for CdTe manufacture in the order of 800 tonnes per year in 2050, compared to highest case estimates by Houari *et al* (2014) of 3,500 tonnes per year in 2050.

The 2014 UKERC report estimated annual primary tellurium production of 500 tonnes and reported reserves of 24,000 tonnes. The UKERC team found a wide range of future demand projections, with 2030 demand estimates being between approximately 100% and 350%, relative to 2012 production (which was assumed to be the previously estimated 500 tonnes). Looking further out to 2050, the range of projections for annual demand was found to be between approximately 500 tonnes and approaching 3,000 tonnes.

Figure 8 presents USGS data on tellurium production and reserves from 2016 onwards (USGS, 2021a). Note that global figures are not available from the USGS for earlier years and that refinery production data from the US is also withheld by the USGS to preserve company confidentiality. The data for reserves include only tellurium that is contained in copper reserves and is based on an assumed ›50% tellurium recovery rate during the copper refining process. Data on global resources are not available, although estimates of crustal abundance are similar to gold and platinum.

The USGS identify several countries that produce tellurium but that the 'available information was inadequate to make reliable production estimates', which suggests the possibility that the production data used in Figures 8 and 9 is lower than actual global production. Although not plotted on the chart, reserves data is available for years prior to 2016. In 2011, global reserves were estimated at 24,000 tonnes and this had increased slightly to 25,000 tonnes by 2015. Given the most recent estimates, this means that reserve levels have grown by the 25% in the decade to date. It is immediately clear from Figure 8 that current tellurium production levels are a small fraction of reserves, and this message is reinforced by the reserve to production ratios shown in Figure 9, which have varied between a low of 60 years and a high of 67 years during the period from 2016 onwards.

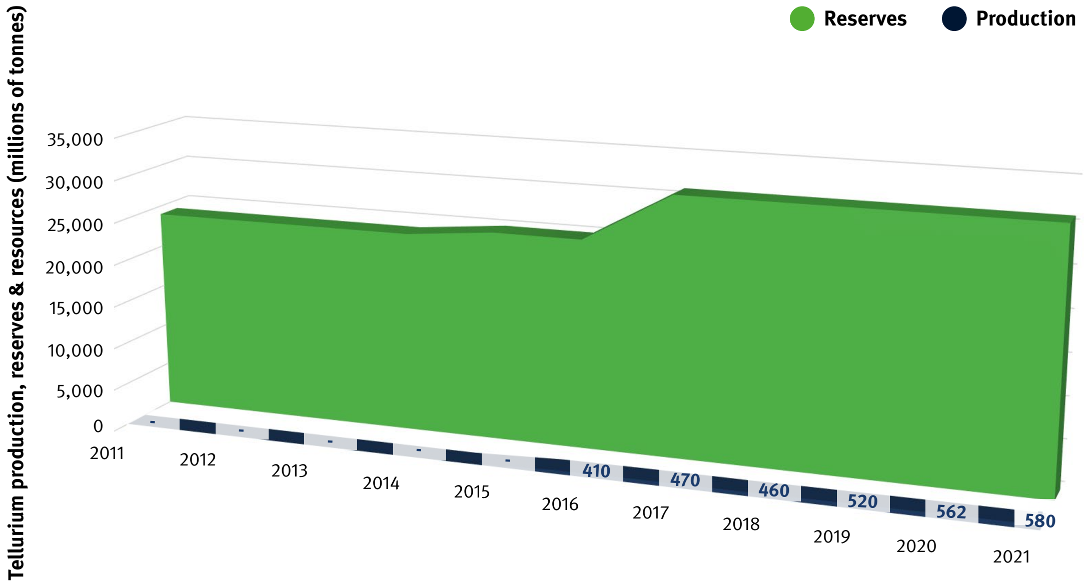

Figure 8 Global tellurium production and reserves

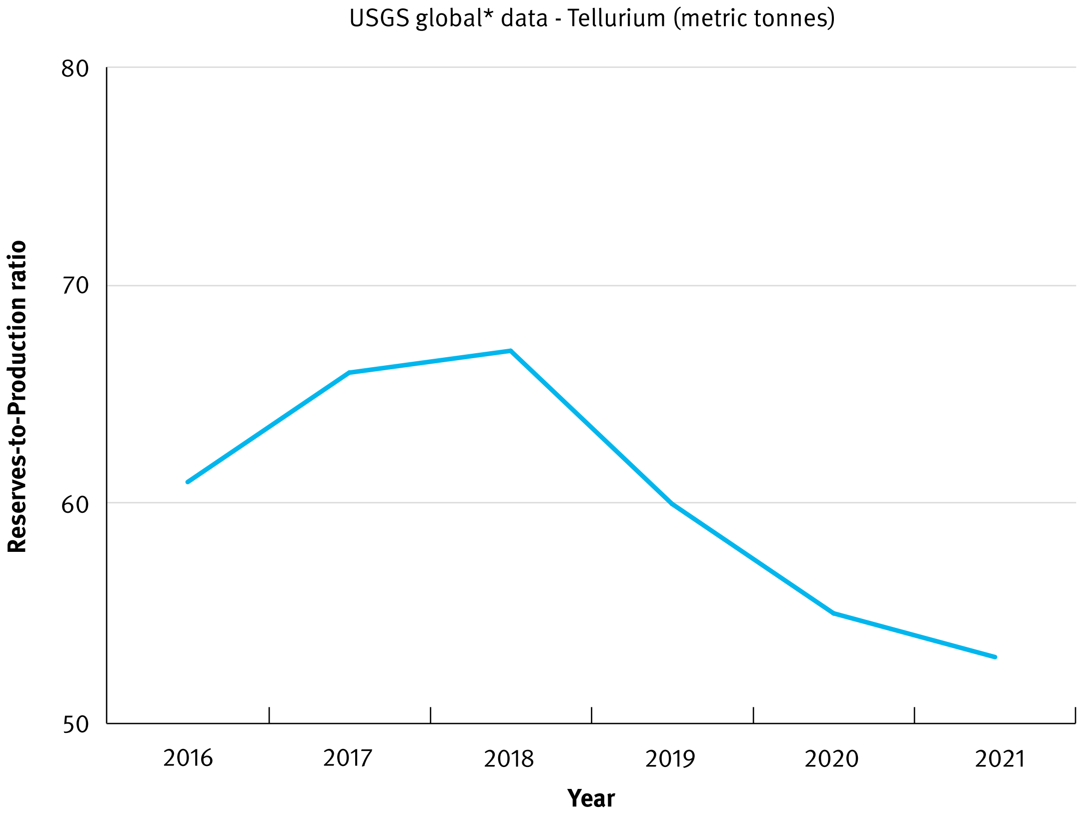

Figure 9 Global tellurium reserve to production ratio

* Note that US Production data is excluded from the USGS dataset

Current production and reserve levels suggest that the availability of tellurium for use in the low carbon energy transition is not an issue of immediate concern. However, this does not mean that this situation will necessarily sustain, and there have been concerns from some analysts that tellurium supply could tighten considerably in the future. Watari *et al.* (2019) for example, highlight several recent studies that suggest tellurium supply (along with other materials) has the potential to be a bottleneck, a concern also raised by Wang *et al.* (2019). These concerns were reinforced by a subsequent review of material outlook studies (Watari *et al.*, 2020), which found a very wide range of projected tellurium demand out to 2030 and 2050, with the highest at around 25,000 tonnes per year, although most estimates were in a range up to 5,000 tonnes per year. This is broadly consistent with the 2050 annual demand values projected by Calvo and Valero (2021) and Bustamante and Gaustad (2014) of 1,500 tonnes and 4,500 tonnes, respectively. The recent report from the International Energy Agency (IEA, 2021b) suggested considerably lower figures in their central scenarios, of up to 300 tonnes annually by 2040 although this figure increases to 1,400 tonnes per year in their alternative 'High CdTe scenario'.

As would be expected, estimates of cumulative demand up to 2050 follow this pattern of having a wide range, with Valero *et al.* (2018) projecting a figure of 39,000 tonnes, and further noting that they anticipated a supply bottleneck around 2035 and beyond, albeit with an acknowledgement of the considerable uncertainties involved. That message of uncertainties is highlighted by an outlier study, Davidsson and Höök (2017) who modelled scenarios with very high take up of CdTe PV out to 2050 and calculated a projected cumulative tellurium demand of between 120,000 and 725,000 tonnes (corresponding to annual demand rates of between 2,900 tonnes and 24,000 tonnes). Grandell *et al.* (2016) project cumulative demand to exceed global tellurium reserves by more than 250% by 2050, although this drops to a little under 150% when the impact of improved recycling rates is considered. This study took the then current USGS reserve estimates as a starting point but implicitly assumed that tellurium refining rates would increase to approaching 100%.

The very wide range of projected tellurium demand result from a combination of the differing assumptions over the deployment of solar PV relative to other low carbon technologies, CdTe PV deployment rates relative to other PV technologies, changes in the tellurium intensity of the cells, and projected material recycling rates. Added to these uncertainties are the risks of demand/supply imbalance that results from the by-product nature of tellurium production, since production rates may not be able to respond as might be expected to tightening demand (and higher prices) since it is so closely bound to copper production. Having said that, it has been suggested that if the price incentives were right then tellurium yields from the copper refining process could be improved substantially, perhaps up to around 80% (Bustamante & Gaustad, 2014), and higher copper prices, (they are currently at a 10-year high (Hume, 2021), would be expected to lead eventually to increased availability. Some studies have suggested that this reliance on the complex dynamics of a by-product supply chain poses a significant risk to a substantial increase in production (Ren, Tang and Höök, 2021;Lee, Bazilian, Sovacool, Hund, *et al.*, 2020; Bustamante and Gaustad, 2014), and that concerns over future supply create significant uncertainty for the future of CdTe PV (Hund *et al.*, 2020).

Two key characteristics of tellurium – that its current production is linked directly to production of another metal, and that future demand is linked to projections of the technological direction and scale of the PV market – creates considerable uncertainty and complexity in determining whether future supply is likely to be constrained relative to demand. In this regard, the evolution of CdTe within the overall PV market is important.

As identified above, in the early 2010s there was considerable optimism regarding the likely competitiveness of CdTe cells when compared to the dominant incumbent crystalline silicon technology, with projections suggesting that CdTe would take a major market share in the future. In reality, this has not happened to anything like the extent that was widely anticipated, with crystalline silicon currently having a 95% share of the global PV market, and CdTe making up around 4%, from a peak of around 13% in 2011. This continued (and increased) dominance of crystalline silicon PV technology has been driven largely by rapidly falling production costs, in turn driven by technological improvements and economies of scale resulting from the dramatic PV market expansion during the last decade (Fraunhofer, 2020). Looking again at the range of projected demand for tellurium that is related to PV cell manufacture, there does seem to be something of a mismatch (or perhaps a lag) between those studies which model very high CdTe PV deployment and the current direction of this technology. Of course, these studies are not necessarily predictions, and such analyses are often intended to explore the consequences of a range of possible rather than probable futures.

Tellurium summary

A decade or more ago, many analysts suggested that CdTe PV technologies would form a very significant share of global PV deployment. Multi-decadal projections of tellurium demand reflected this, and many formed the view that this could lead to demand exceeding both production capacities and total reserves in the medium and long terms. These concerns were exacerbated by the by-product nature of tellurium production, tied as it is to the production and refining of copper. Against earlier predictions, crystalline silicon PV increased its already dominant position in the global PV market, with CdTe PV currently representing a small, and recently declining, market share. Unless this changes substantially, the evidence suggests that it is unlikely that tellurium supply will significantly constrain CdTe deployment in the short and medium term.

1.5 Copper

Copper is a very widely and intensively used metal, and in relative terms abundant, with iron and aluminium being the only metals which are used in greater quantities. Around two thirds to three quarters of global copper production is used in electrical applications, including generation and transmission, wiring, telecommunications and electrical products. (ICSG, 2020; USGS, 2021a). The most recent USGS estimate is that a total of 25 million tonnes of copper were produced worldwide in 2020, slightly more than the 24.5 million tonnes produced in 2019. Figure 10 below shows copper primary production, reserves and resources data for the last ten years, with the reserves to primary production ratio for the same period shown in Figure 11.

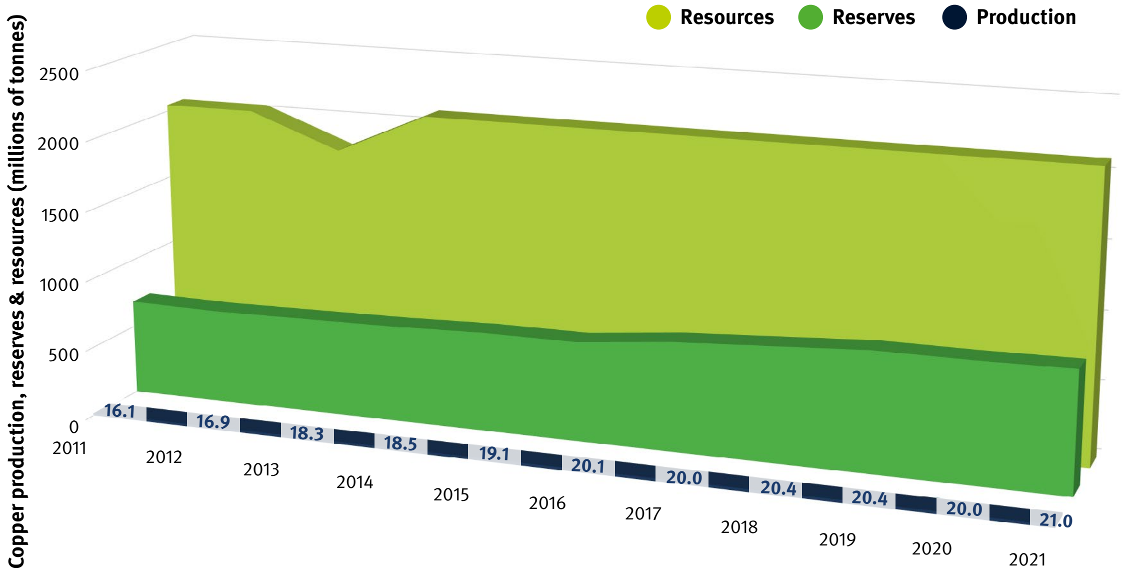

Figure 10 Global copper production, reserves and resources

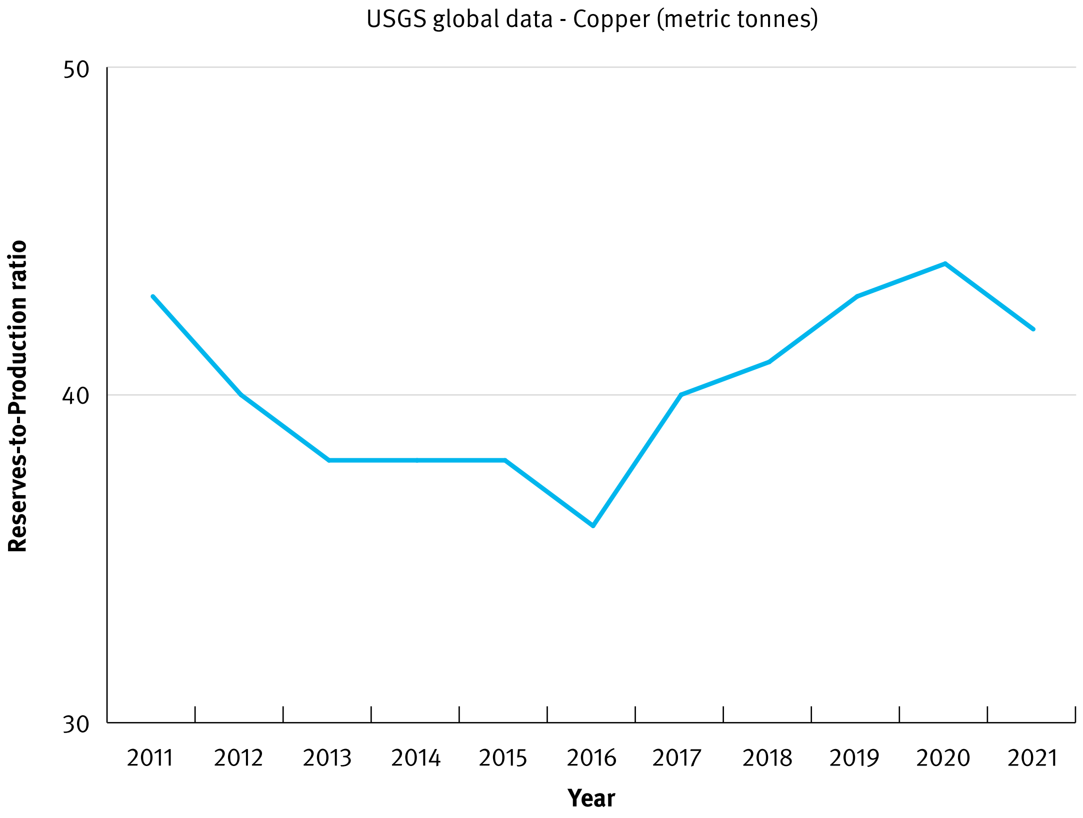

Figure 11 Global copper reserve to production ratio

Primary copper production has risen by approximately 24% to 20 million tonnes per year in the last decade, with estimated reserve levels rising by 26% to 870 million tonnes over the same period. During this time, the reserve to production ratio has been relatively stable, varying between a low of 36 years and a high of 44 years (see Figure 11). Estimated global resources have also remained relatively flat during the last decade, at around 2.05 billion tonnes in 2011, rising slightly to 2.1 billion tonnes by the end of 2020. Note that the dip in the resources data for 2013 did not reflect a downward revision of estimates, but is due to a change in the inclusion criteria of resource data, a change that was only applied in that year. The considerable difference between the most recent primary and total production data (20 million tonnes and 25 million tonnes respectively) largely reflects the drawing down of inventories.

Despite the very large amounts of copper used annually, this must be seen in the context of two key attributes. The first of these is its relative abundance (see above), and the second is the ease with which it can be recycled, with production from copper recycling currently estimated to contribute around a third of global use (ICSG, 2020). It was for these reasons that this metal was not included in the 2014 UKERC analysis (Speirs, Gross, *et al*., 2014). However, ambitions for the scale and speed of the global low carbon energy transition have increased dramatically since then, and the key role that copper has in many of the technologies that will be required to meet these aspirations (Hund *et al*., 2020) has led to revised projections of future demand for this metal. In common with many other materials, these projections have a wide range, reflecting the significant uncertainties in the future technology mix, resource intensity, and assumptions of the level of global economic development. By way of illustration, a recent paper (Watari *et al*., 2021) which reviewed 70 studies of the long term outlook for six major metals found a range of projected annual copper demand of approximately 25 million to 75 million tonnes for 2030, 30 million to 125 million tonnes for 2050, and 30 million to 200 million tonnes for 2100. Median values across the studies reviewed were found to be approximately 40 million, 50 million and 100 million tonnes for 2030, 2050 and 2100, respectively. The authors cautioned that the methodological approach adopted by some of the studies they examined may significantly overestimate future demand over long time horizons.

An analysis by Schipper *et al.* (2018), using five scenarios and two different methodological approaches, calculated a range of annual copper demand between approximately 45 million tonnes and 115 million tonnes for 2050, with the majority of their results being below 70 million tonnes. The corresponding figures for 2100 show an even wider range, between approximately 70 million tonnes and 450 million tonnes, with the majority of results being below 130 million tonnes. The majority results for 2050 are broadly consistent with the 40 million to 70 million tonne range found in Kuipers *et al.* (2018), a study which focussed on the overall environmental impacts of copper production using a life cycle sustainability analysis methodology, finding that these impacts are likely to more than double by 2050. An interesting finding from (Schipper *et al*., 2018) was that under most of the scenarios modelled, primary copper demand levels off from the middle of the century onwards once the effect of increased recycling is considered. This message of the increasingly important role for recycling for the level of primary copper production required is supported by other analyses including Dong *et al.* (2020), Ciacci *et al.* (2020),and Zhang *et al.* (2015).

The recent report from the International Energy Agency (IEA, 2021b) which focused on the mineral and metals requirement for the low carbon transition, forecast increased copper demand but somewhat lower than these other analyses. The IEA projects annual copper demand across low carbon generation, electric vehicle and battery storage, electricity networks, and hydrogen production of between 8 million and 11 million tonnes by 2030, and between 10 million and 15 million tonnes by 2040. For comparison, the same report gives a current figure of 6 million tonnes of annual copper demand across these sectors. Between two thirds and three quarters of the totals are attributable to electricity networks. In their 2020 report, the World Bank forecast that the annual global copper demand related to energy technologies (but excluding electricity transmission infrastructure) could be 1.4 million tonnes by 2050, with a cumulative demand up to that point of 29 million tonnes (Hund *et al*., 2020).

A paper by (Seck *et al*., 2020) projected cumulative primary copper demand up to 2050 (assuming a 45% recycling rate) of between 1.6 billion and 1.9 billion tonnes, which they compared to the corresponding figures from (Schipper *et al*., 2018) and (Elshkaki *et al*., 2016) of 0.8 billion to 1 billion tonnes, and 1.5 billion to 1.9 billion tonnes, respectively. The authors caution that this would mean cumulative primary demand would considerably exceed currently estimated reserves and consume the majority of currently estimated global copper resources. This is consistent with (Elshkaki *et al*., 2016) who also noted that projected primary demand exceeds the reserve base, but not the estimated ultimately recoverable resource, in most of the scenarios they modelled. Whilst these cumulative demand projections are broadly consistent with many of the annual projections summarised above, there does seem to be a large gap between these and the forecasts from the IEA and the World Bank, even when accounting for the fact that those two analyses focus only on demand from the energy sector.

Although by no means unique to copper, this metal does make an interesting case study in respect of the impact of market dynamics on future supply. Despite current prices being close to their all-time high and with some commentators expecting further price rises (Hume, 2021), there are concerns that this will be insufficient to encourage the required investment in new mine projects that will be needed to meet projected future demand levels, and that even if investment is made the lead time to develop a new mine is of the order of a decade (Hume, 2021) (Hume & Terazono, 2021). Some industry leaders have suggested that copper prices would need to rise by another 50% to incentivise the new investment required (Hume & Sanderson, 2021). These two key points of the need for higher prices, and the relatively long time it takes to develop new mine projects are supported by the analysis in (Jones *et al*., 2020) who advise that ‘significantly higher long-term prices could be required to support the required investment in meeting the need for increased conductivity’. This situation is exacerbated by the cyclical nature of copper price dynamics (a characteristic that is not unique to copper or materials generally), and the history of copper markets which have experienced considerably volatility in recent decades, with (Su *et al*., 2020) observing four episodes of very significant market bubbles (and subsequent collapse) within the last 35 years. Whilst it might be expected that higher prices may encourage the use of substitute metals, this does not appear to have happened to a significant degree during previous episodes of high copper prices. Substitution rates have remained consistently at very low levels, reflecting the enduring advantages that copper has over potential substitutes in terms of conductivity and resistance to corrosion (ICA, 2021)(MIR, 2019).

Copper Summary

Copper is relatively abundant, and readily recycled. Although recycling rates are higher than for many materials, it seems likely that further increases in recycling rates will play an important role in the future, particularly over multi-decadal timescales. Copper is likely to have a key role in the energy systems transition, and it is resistant to substitution by other metals or materials, despite very significant historic price volatility. Future demand is projected to increase substantially, but there is a wide range of estimates, even when the high outliers are discounted. At the higher end of the projected demand range, currently estimated reserves may be exhausted. There are concerns that market dynamics will constrain the investment in future production capacity that will be required to meet projected future demand.

1.6 Materials case studies conclusion

The materials discussed above were selected to illustrate the key themes that relate to concerns over the demand and supply of those metals and other materials that will be required for the transition to a global low-carbon energy system. The main points that emerge from these case studies can be summarised as follows:

- There are a very wide range of demand forecasts over multi-decadal timescales due to differing assumptions over the degree of policy ambition, technology development, the level of global economic development, and improvements in production and recycling processes.
- The fundamental level of resource availability is not the primary source of concern, although there are a small number of outlier findings from some studies which suggest that there is a possibility (rather than likelihood) of resource constraints in the long term under some scenarios.
- A much more pressing concern is the extent to which extraction, production and recycling capacity can be scaled up from current levels to the dramatically higher levels envisaged for some materials.
- Linked to this concern is the issue of the very long lead times typically required to develop new extraction and production projects, especially when set against the very rapid transition required to deliver on global CO_2 emissions reduction targets. This is exacerbated by the observed lags between increased demand (and the resultant higher prices) leading to the development of new projects to satisfy increased demand.
- Although there is evidence that the material extraction and production industries have been able to respond to rising demand in the past (albeit often with lags described above), the medium to long-term forecasts of the increased requirement for some materials will represent a step change in the required speed and scale of that response.
- Increasing the supply of those materials whose production is a by-product of another material is a particular challenge because supply does not necessarily respond conventionally to price signals because it is tied to the demand for the ‘primary’ material.
- The generally high degree of geographical concentration in the extraction and production of many critical materials presents a risk to the stability of global supply chains.
- The evolution of dominant technologies in some sectors has led to dramatically revised demand forecasts for some materials, and there is no fundamental reason why this might not happen again.
- Assumptions over the ease or likelihood of material substitution require careful examination since there is evidence that substitution is difficult for some materials.
- A small number of studies have produced long-term forecasts which suggest very high demand for some materials under some circumstances. Whilst these are generally outliers, they do perhaps warrant attention so that the underlying reasons are fully understood.

Given the global nature of materials industry, policy measures to influence metal production are limited. However, countries wishing to mitigate impacts of potential material constraints should focus on several key areas.

The first of these is to ensure that resource extraction, production and recycling activity is able to respond in a timely fashion to increasing demand. This may take the form of expediting permitting and planning applications, and/or financial incentives to reduce some of the barriers to timely development of new projects.

The second area of policy focus is to address, as far as is practical, the issue of geographical concentration, not just of the extraction process but also production, refining and recycling. Clearly, if known reserves for a particular material are very strongly concentrated geographically then options may be limited, but even in these cases there may be opportunities to ameliorate some of the most acute affects through for example increased inventory or stockpiling requirements (a policy measure adopted by many countries in respect of fossil fuels).

Thirdly, the rate of change in respect of low carbon technology developments, and the implications that these may have for material requirements forecasts, suggest that these forecasts should be kept under periodic review to ensure that they are revised as required to ensure that they remain in line with current technological trends. Finally, in respect of current forecasts, those (admittedly small number) which predict that current known resources for some materials may be exhausted in the coming decades need further analysis to understand how reliable an indicator they may bet.

2. Novel Functional Materials

2.1 Introduction

As decarbonisation efforts gather pace globally, the demand for materials to allow new energy generation, storage and utilisation likewise increases greatly. Section 1 has explored materials availability, focusing on demand projections for four materials that could be critical to the low-carbon energy transition. As important, however, is the search for novel materials to substitute or augment existing materials with more effective, more available or more economically practical alternatives. The search for novel functional materials to power the energy transition has two key drivers: developing materials which can improve the characteristics of energy technologies, either by increasing conversion/storage efficiencies or by delivering lower cost and higher availabilities than current materials, and secondly developing novel materials which can act as replacements to existing materials which may be facing scarcity issues, high costs or associated environmental damage.

Novel functional materials in the energy sector spread over a wide range of categories. This report will consider the following three, due to their importance in current decarbonisation pathways. These categories correspond to the Henry Royce Institute's Materials for the Energy Transition roadmaps (Henry Royce Institute, 2021)

Photovoltaics
These consist of materials to capture and convert solar radiation into electrical energy through the photovoltaic effect.

Batteries
This category consists of materials to store electricity, including both evolutions of current battery chemistries and novel battery materials.

Materials for hydrogen and other energy carriers
This category consists of materials to produce, store, transport and consume hydrogen, as well as other energy carriers such as ammonia.

» BOX 1: What is a functional material?

Functional materials are often described as 'those materials which possess particular native properties and functions of their own' (Imperial College London, 2021). These could include properties such as magnetism, piezoelectricity, ferroelectricity, thermoelectricity or the ability to store energy, and are thus used at the heart of devices to impart properties or functions. These differ from structural materials (steel, concrete, aluminium, etc.) which provide rigidity and support to a device, system or building but do not provide inherent functionality by themselves.

This report considers only functional materials.

2.2 Photovoltaic Materials

2.2.1 Introduction

Photovoltaic cells convert solar radiation to electricity using a mechanism known as the photovoltaic effect, discovered in 1839 by Becquerel. In order to create a photovoltaic cell capable of generating electricity from this effect, two sections of semiconductors are needed, one with an excess of positive charges, and one with an excess of negative charges. (Luceño-Sánchez *et al.*, 2019).

These are typically layered in a 'sandwich' configuration in a photovoltaic cell, with the region at which they contact being known as the *p-n junction*. When excited by photons and connected to an electrical circuit, there will be a flow of charge carriers across the p-n junction, causing a potential difference across the cell and an electrical current to flow. Solar cells can either be single-junction or multi-junction, with layers of semiconductors providing multiple p-n junctions which can be tuned to different wavelengths of photons.

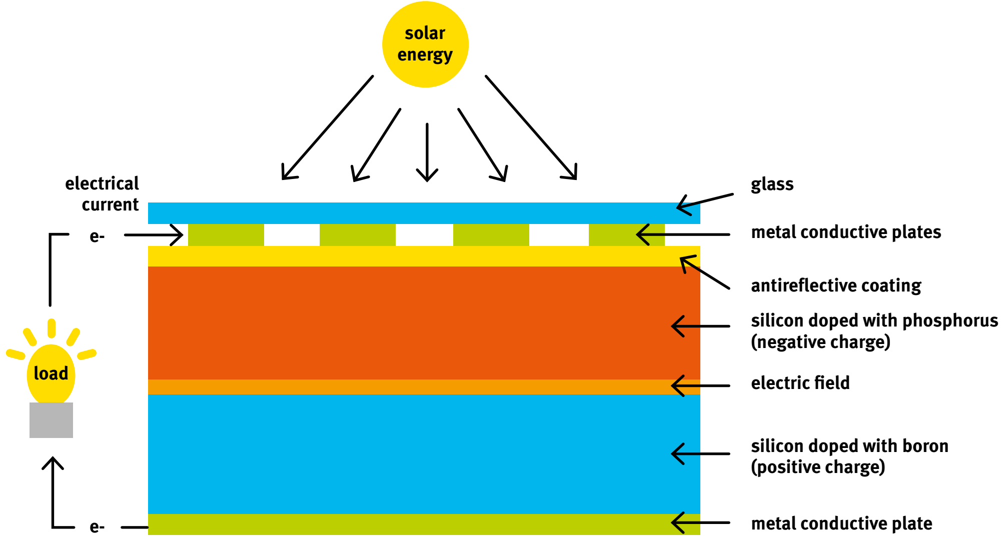

Figure 12 Indicative diagram of a solar cell (Lexology, 2019)

These solar cells are wired together into modules, or single PV panels. Modules wired together form arrays.

PV panels have been developed for nearly eighty years, with the first monocrystalline solar cell being constructed in 1941 and the first germanium cells arriving in 1951. Bell Labs demonstrated the first practical solar cell, with an efficiency of roughly 6%, in 1954 (APS, 2009). PV panels were initially very expensive and utilised for specific cases such as satellites, space exploration and power for remote areas, before low-powered solar cells became popular for portable devices such as calculators in the 1980s (Lexology, 2019). The growth of manufacturing of solar PV panels has grown exponentially over the last fifty years. In 1977, the global production of PV panels exceeded 500 kW for the first time. In 2020, the global manufacturing capacity of PV panels was 165 GW, with 90 GW of installations occurring (IEA, 2021a).

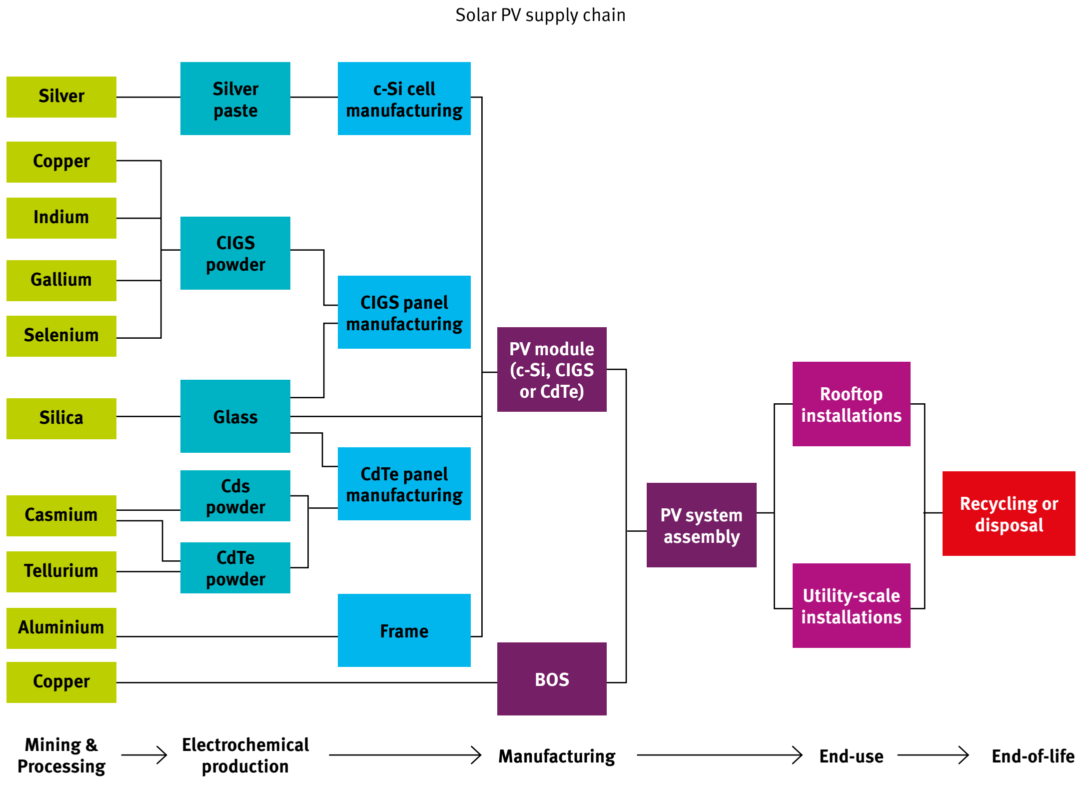

Figure 13 An overview of the supply chain for PV panels (Giurco *et al.*, 2019)

» BOX 2: Generations of PV Technology

There are commonly held to be three major generations of photovoltaic technologies (Luceño-Sánchez *et al.*, 2019). These are:

1st Generation: First-generation solar cells utilise wafer-based technologies, such as crystalline silicon.

2nd Generation: Second-generation cells utilise thin-film deposition methods. Cell materials include cadmium telluride (CdTe), copper indium gallium selenide (CIGS) and amorphous silicon.

3rd Generation: This incorporates a range of emerging materials and technologies potentially capable of improving efficiencies, including perovskites, organic cells, quantum dot cells and dye-sensitised cells.

2.2.2 Solar cell material technologies

There are several types of solar cell technology, some well-established and some novel challenger materials. In terms of structure, solar PV cells are classified as either *wafer* (formed by cut slices of semiconducting ingots) or *thin-film* (where layers of semiconducting materials are deposited on insulating substrates) (Ibn-Mohammed *et al.*, 2017). Two types of solar cell technology are in mass commercialisation: crystalline silicon, which accounts for about 95% of the market, with two thin-film technologies, cadmium telluride (CdTe) and copper-indium-gallium-selenide (CIGS) accounting for the remainder (Giurco *et al.*, 2019). Several novel materials, often grouped as third-generation photovoltaics, are at the research stage including dye-sensitised solar cells, perovskites, and organic cells. This section provides a brief overview of the major material technologies.

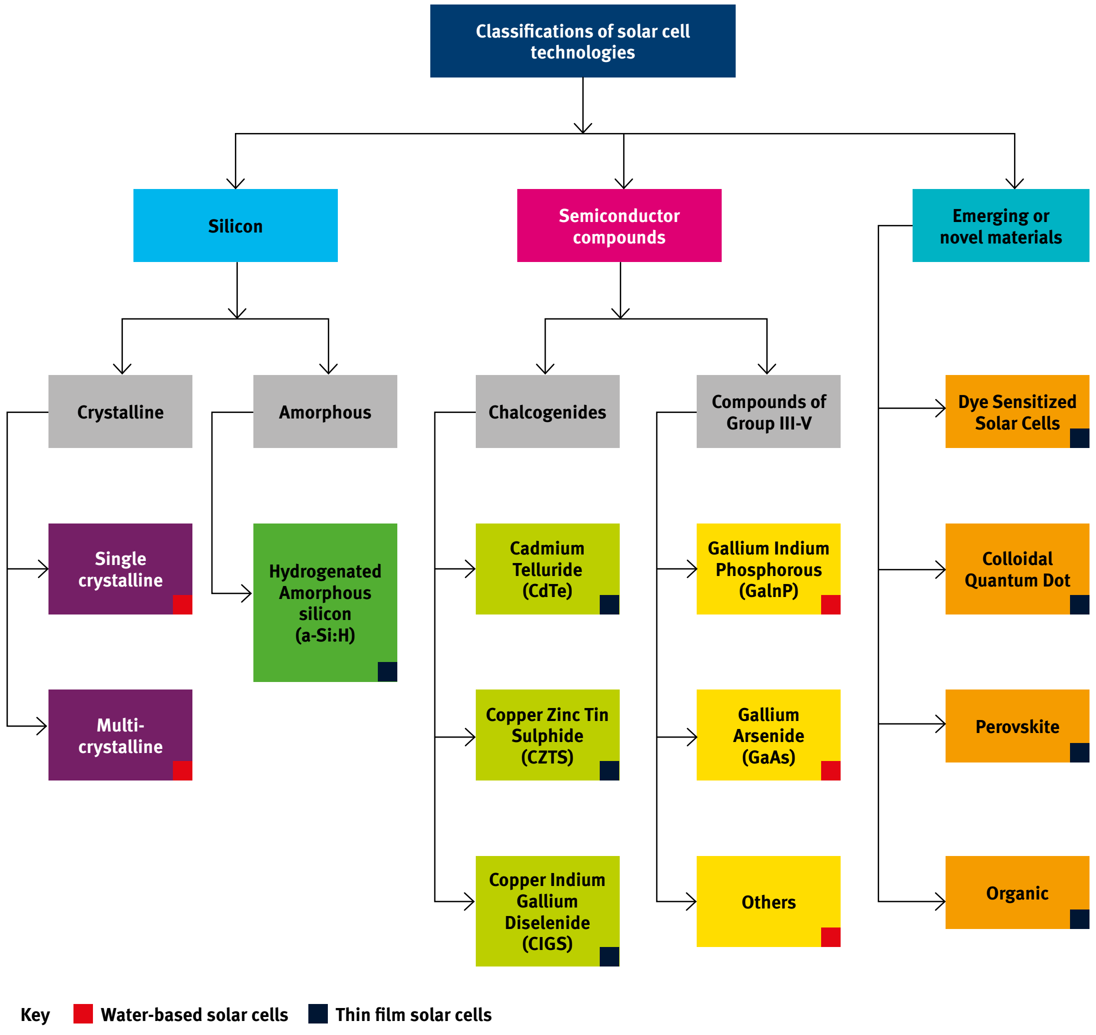

Figure 14 Types of solar cell technologies (Ibn-Mohammed *et al.*, 2017)

2.2.2.1 Silicon Solar Cells

Crystalline silicon-based cells are the predominant solar technology, with about 95% of current global production being wafer-based silicon technology (EC JRC, 2019). Although one of the oldest solar technologies and exhibiting efficiencies of only 18-22% in commercial use (DoE, 2018), crystalline silicon has achieved market dominance due to the maturity of the manufacturing processes, high levels of reliability of the solar panels, an abundance of crystalline silicon following an oversupply in the early 2010s, and the low costs of manufacturing and maintenance that these three factors imply (Luceño-Sánchez *et al*., 2019). There are two major types: single-crystalline, which is formed from cut wafers from a single silicon ingot, and multi-crystalline, which is formed from many silicon crystals melted together and formed into an ingot. Multi-crystalline panels are less efficient, as the conducting electrons cannot travel through crystal boundaries, but they are cheaper to manufacture (EnergySage, 2020).

Silicon is an abundant material, comprising about 28% of the earth's crust by mass in the form of various silicate minerals, however the refining and purification process requires large facilities and significant energy use. China manufactures more than half the world's supply of silicon as of 2019 (USGS, 2020). The vast majority of silicon solar cells are manufactured in China, which boasts seven out of the top ten largest manufacturers of solar cells (GlobalData, 2020). Cost reductions achieved by scaling-up of manufacturing coupled with an oversupply of silicon has led to China's dominant market position. This has led to geopolitical tension, with the US and EU imposing anti-dumping tariffs on Chinese solar panels several times over the last decade (Forbes, 2018). The UK currently has no manufacturing capacity for these panels.

Research challenges for silicon-based PV differ from more emerging solar materials, as it is an established technology. Improvements in both manufacturing and conversion efficiency, as well as improving operational lifetimes (from 25 years to 30-40) by preventing degradation, are areas in which even small improvements could have significant impacts due to the size of the market (Royce Institute, 2020c).

2.2.2.2 Gallium arsenide (GaAs) cells

Gallium arsenide (GaAs) is an excellent semiconductor material for solar PV use, with GaAs multi-junction cells recording extremely high conversion efficiencies, approaching 50% in some cases (NREL, 2021). Due to this, it is used in high-value applications such as space exploration. However, the cost of producing GaAs wafers is extremely high – up to 50 times more expensive than silicon – and this currently makes the technology cost prohibitive for all but specialist use (International Energy Agency, 2021). However, recent advances in deposition and fabrication methods could make scale-up and cost reduction possible within the next decade (International Energy Agency, 2021; NREL, 2019).

2.2.2.3 Thin-film solar cells

A thin-film solar cell is constructed by the deposition of thin layers of photovoltaic material on a glass, plastic or metal substrate. The film layers are typically in the nano- to micrometre range, and originally were cheaper to manufacture but less efficient than silicon PV panels. The tumbling cost of silicon PV in recent years, however, combined with advances in thin-film PV efficiency, have made the two technologies less distinctive.

There are two major thin-film technologies commercialised for building- and grid-scale PV, cadmium telluride (CdTe) and copper-indium-gallium-selenide (CIGS). CdTe cells consist of a semiconducting compound of cadmium, which is a toxic heavy metal obtained as a by-product of zinc refining, and tellurium, a rare metalloid obtained as a by-product of copper refining, with an abundance in the Earth's crust similar to platinum. Tellurium availability is explored in Section 1.4 of this report. CdTe panels make up approximately 5% of the global market due to the competitiveness at scale of silicon panels but have the potential to become both cheaper and less-carbon intensive than silicon panels, with approximately half the production carbon footprint (De Wild-Scholten, 2013). There are significant concerns over the toxicity of cadmium both during manufacturing and at the panels' end-of-life. These concerns plus the rarity of tellurium suggest recycling of CdTe panels will be increasingly important (Ravikumar *et al*., 2020). CdTe panels are manufactured mostly in the US and China, with some manufacturing in Europe. US company First Solar is the market leader, producing 6GW annually with an ambition to grow to 8GW in the near future.

The UK has significant R&D experience in CdTe technology, especially in the glass substrate and cover layers (Pilkington, 2021). Research challenges include improving the capture efficiencies of CdTe panels, preventing degradation of the panels by improving their hydrophobic and dirt-repelling qualities, and providing low-reflectance and IR-blocking glass covers to improve efficiencies. To improve the UK's standing in this technology, access to testing facilities for stability and degradation testing, industrial scale-up capabilities, and partnerships with major international players should be pursued (Royce Institute, 2020c).

2.2.3 Challenges in Materials for Established PV

The rapid growth in solar PV installations over the last decade has mostly been fuelled by the rapid cost reductions seen in silicon PV. In part, these have come from a reduction in silicon and silver, the most expensive materials used in the panels, due to the utilisation of thinner silicon wafers and less silver-intensive conduction pastes (ITRFP, 2019). Most current studies forecast the continued dominance of silicon PV into the 2040s, with continuing reduction of silicon and silver usage intensities such that demand for these materials are lower in 2040 than 2030 even in scenarios which forecast quick deployment to meet Net Zero goals (International Energy Agency, 2021). An alternative model forecasting large-scale development and deployment of CdTe cells to a capacity addition share of approximately 20% per annum by 2040 suggests shortfalls of tellurium, with global production needing to be increased to 1400 tonnes from 500 tonnes today (International Energy Agency, 2021). This shortfall could be met in part by a more aggressive recycling programme for CdTe cells, but more production capacity will still be required.

There are also significant areas for improvement, even to established technologies such as silicon PV. New materials solutions are needed to address issues such as module heating (the effect of sunlight hitting the panel causes it to heat up, making it less efficient and accelerating its degradation) and panel soiling (where dust, dirt and bird droppings accrete on the panel, lowering its efficiency). Module heating could be addressed by either developing an inverted-temperature coefficient solar panel, where current flows are greater at high temperatures, or by developing materials to efficiently conduct heat away from the panels (Royce Institute, 2020c).

2.2.4 Third Generation: Novel and Emerging Materials

This section looks at new materials and technologies emerging for photovoltaic cells. There are a wide variety of these materials, including organic PV cells, quantum dots, perovskites, dye-sensitised cells, multi-junction cells and others. This section will concentrate on two major promising technologies, dye-sensitised solar cells and perovskite cells.

2.2.4.1 Dye-sensitised solar cells

Dye-sensitised solar cells (DSSC) are a design of thin-film solar cell which utilise a photosensitive dye, usually formed from a complex of ruthenium. Similar to the photosynthesis process, this dye absorbs a large amount of the sunlight hitting the solar cell, exciting electrons which flow into an electrolyte layer and then into a transparent top electrode, where they provide electrical power. Electrons then flow back into the cell via a backing counter electrode, where they re-join the electrolyte. The thin-film in the liquid electrolyte is typically made up of titanium dioxide nanoparticles which, as well as providing the semiconducting substrate, acts as a scaffold to hold up the nanometre-sized dye particles (Sharma *et al*., 2018). These cells are simple to manufacture, flexible, robust, can be patterned on many surfaces, are lightweight due to a lack of cover glass and are able to operate from artificial indoor light, making them ideal for mobile devices and low-density power applications such as building-integrated PV (AltEnergyMag, 2019).

Dye-sensitised solar cells have found limited initial commercialisation in small mobile applications, such as electronics, chargers, backpacks and other small integrated devices, where their flexibility is an advantage. There is a large potential market for building-integrated PV, which dye-sensitised cells are well-positioned to capture. This is due to their flexibility and potentially low cost of fabrication, which can offset their presently low conversion efficiency values (currently around 11-14%) (C. P. Lee *et al*., 2017). However, they currently suffer from degradation issues with the electrolyte and counter electrode under standard light, humidity and temperature conditions, making them unable to maintain performance for the 20-25 years that building integrated applications would expect (C. P. Lee *et al*., 2017). Disadvantages also include the liquid electrolyte potentially freezing at low temperatures and expanding at high ones, as well as the hazardous volatile organic solvents utilised in the electrolyte, which need to be sealed carefully to prevent escape (Boldrini *et al*., 2018). Research on solid electrolytes is ongoing, but these currently suffer from a lack of flexibility and a high rate of degradation (Rong *et al*., 2013). Current research challenges are to improve the operational lifetime and conversion efficiencies of both liquid and solid DSSC panels, as well as identifying lower-cost alternatives to the dye and electrode materials (Mozaffari *et al*., 2017).

2.2.4.2 Perovskites

Perovskite molecular structures are crystalline structures wherein a central cation is surrounded by a lattice of rhombic structures, named after the naturally occurring mineral of the same structure (ScienceDirect, 2021). Perovskites can exhibit many properties depending on which ions are present in the structure (Ossila, 2021), including superconductivity, catalytic properties and magnetoresistance. Their usage in solar PV cells was first demonstrated in 2012 (M. M. Lee *et al*., 2012), with dramatic and rapid increases in conversion efficiency seen in the years since to a point where they match or exceed other thin-film materials (NREL, 2021). Perovskites for PV applications are commonly lead or tin halide compounds. These compounds are relatively low-cost and simple to manufacture, making them ideal candidates for a new generation of cheap, flexible and efficient PV cells (Luceño-Sánchez *et al*., 2019). As well as providing efficient single-junction solar cells, perovskites can also be used in tandem multi-junction cells with silicon and other materials, where the perovskites absorb a different wavelength of light to the base cell in order to improve efficiencies. Tandem perovskite-silicon solar cells have been observed to have conversion efficiencies of over 29% (Al-Ashouri *et al*., 2020), and are at a relatively high stage of development, with the UK company Oxford PV preparing for volume production by early 2021 (Royce Institute, 2020c).

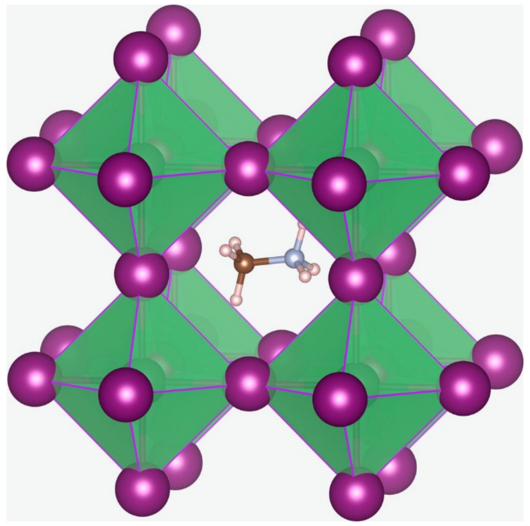

Figure 15 Crystal structure of CH3NH3PbX3 perovskites (X=I, Br and/or Cl). The methylammonium cation (CH3NH3+) is surrounded by PbX6 octahedra (Eames *et al*., 2015).

Single-junction perovskite cells are still at a precommercialisation phase with research challenges focusing on improving operational lifetimes, as the stability of perovskite cells can be affected by several factors including oxygen, temperature, light and humidity (Bryant *et al*., 2016). These cause the cells to degrade quicker than other technologies. Research on improving this stability as well as developing manufacturing, testing and characterisation processes at scale and utilising cheap, non-toxic components will be needed to progress single-junction perovskite PV cells to a commercialisable state (Royce Institute, 2020c).

2.2.5 Challenges in Materials for Emerging PV

Novel materials have the potential to transform the PV market. Many emerging technologies are lightweight, easier to manufacture with the potential for lower costs through scaling up manufacturing and are suitable for a wide range of use cases, from building-integrated PV to indoor and mobile uses. The development of multi-junction cells could provide far greater conversion efficiencies per area than conventional silicon PV. However, there are several significant challenges to overcome. Chief among these is degradation – the slow loss of functionality as the solar cell ages, caused by the active materials degrading, both intrinsically and under external environmental conditions such as heat, humidity, light, or oxygen. While a standard silicon solar cell typically has a working lifetime of 25-30 years (Jordan & Kurtz, 2012), the maximum lifetime for perovskite cells has been observed to only be about a year at present (Meng *et al*., 2018). Dye-sensitised cells face degradation when exposed to ultraviolet light, as well as issues with liquid electrolytes at high and low temperatures and the possible escape of volatile organic solvents (Mozaffari *et al*., 2017). Given that many of the use cases for these cells involve external, exposed placements, these issues will need to be mitigated before mass rollout. Degradation testing facilities are essential in this process to provide standardised assaying of panel candidates.

Materials availability and toxicity are also important considerations. Perovskite cells have a potential issue in this area - the perovskites used for solar cells are typically lead-halide compounds, which are highly effective but contain quantities of lead, associated with major adverse health effects. Substitution of lead in the perovskite structure is being explored but is a complex problem (Qiu *et al*., 2018). The sustainability and recycling potential of materials and the panels themselves should be developed into the manufacturing process to ensure that lifecycle emissions are reduced as far as possible (Royce Institute, 2020c).

Developing and scaling up manufacturing processes is crucial to the commercialisation effort, and this is typically where novel technologies run into problems, as capital and infrastructure requirements drastically increase. New solar PV materials also face stiff competition from silicon PV, with its established manufacturing chains and downward price pressures, making it difficult for new entrants to effectively compete.

2.3 Batteries

Batteries are an essential component of the clean energy transition, being required to store electrical charge for times when it is needed, replacing in many cases stores of fossil fuels. Batteries work by converting electrical energy to chemical energy, storing this in an electrolyte located between two electrodes. When discharging, the electrolyte undergoes two reactions simultaneously at the anode and cathode, equilibrating the chemical potential and allowing electrons to flow through a connected circuit (MIT, 2021).

2.3.1 Lithium-ion

The preeminent battery technology used today is lithium-ion (Li-ion), first commercialised by Sony in 1991 and now used extensively in applications ranging from mobile phones and portable electronics to electric vehicles and grid-scale storage. Lithium-ion batteries, compared to other commercial technologies, offer affordability coupled with high densities of both energy and power, as well as comparably lengthy lifetimes and high cycling efficiencies (Blomgren, 2017). Economies of scale have dramatically reduced the cost of Li-ion batteries, with one study estimating a 97% fall in cost since their introduction in 1991 (Ziegler & Trancik, 2020). This, however, makes the costs of raw materials as a percentage of total battery costs greater, now accounting for 50-70% of total costs, up from 40-50% five years ago and making costs more dependent on raw material supply (International Energy Agency, 2021). Global reserves and production of lithium and cobalt are investigated in Section 1 above.

In order to underpin the energy transition to Net Zero, the demand for batteries is expected to rise by over an order of magnitude, mostly for use in electric vehicles. (Greim *et al.*, 2020). While lithium reserves are ample to satisfy this demand, the production capacity is currently constrained and concentrated in a relatively small number of countries and companies, with little recycling taking place. Most Li-ion batteries being manufactured today also require cobalt, which, while abundant, is supply-dependant on only a few countries (see section 1.3). Expanding this capacity and ensuring a safe, sustainable battery value chain, including responsible sourcing of the other raw materials involved in battery production, is essential to ensure that the move to electric vehicles and other large-scale uses of lithium batteries does not cause significant environmental impact. Current lithium-ion battery technologies are covered in greater depth in the Energy Futures Lab White Paper on Safe and Sustainable Lithium-ion Batteries (Kallitsis *et al.*, 2022).

2.3.2 Novel Battery Technologies – beyond Lithium-ion

There are increasing demands for higher energy densities than current lithium-ion batteries can supply, especially from the electric vehicle and electronics sectors. New battery chemistries and technologies have been the subject of intense research over the last decade, but with only limited commercial success. The energy density of a rechargeable battery is determined mainly by the specific capacities and operating voltages of the anode and the cathode, with most of the other cell components offering only limited room for improvements. To dramatically increase energy density in a battery, therefore, new chemistries between charge-carrying ions and electrode materials offering mechanisms for greater reaction densities than Li-ion will be needed (Choi & Aurbach, 2016).

Lithium-ion batteries operate using an intercalation mechanism, where lithium ions insert themselves into gaps in the electrodes' crystalline structures during charging and discharging. Battery chemistries that rely on solid-state or gas-phase reactions theoretically have greater energy densities than the intercalation mechanism seen in Li-ion batteries. However, short battery lifetimes caused by low reversibility of the reactions are hindering further progress towards commercialisation. These low reversibilities are caused by uncontrolled reactions and degradation at the electrode interface as well as the slow degradation of non-aqueous electrolytes (ibid). Future commercialised batteries, at least in the near-term, are likely to include lithium as a charge carrier, due to difficulties in developing and commercialising redox chemistries with other possible carriers at high energy density levels (Grey & Hall, 2020). As such, this section only considers lithium chemistries, though sodium, magnesium and zinc chemistries show promise for high-density batteries. There are several promising next-generation battery technologies on the horizon, including the use of organic materials, lithium-oxygen (otherwise known as lithium-air), lithium-sulphur and solid-state battery technology.

Of interest is that many challenges facing next-generation batteries are currently in the realm of fundamental science, including the investigation of new battery chemistries, the perception of reaction dynamics at electrode surfaces and the understanding of factors that lead to the breakdown of reversible reactions.

2.3.2.1 Lithium-organic batteries

Utilising organic materials in the cathodes for lithium-ion batteries could lead to significant advantages for sustainability and materials availability. (M. Armand and J.-M. Tarascon, 2008). Currently, inorganic heavy metals such as cobalt and nickel are used in the electrodes of Li-ion batteries, raising environmental contamination and sustainability concerns. Organic compounds such as conductive polymers, organo-sulphur compounds and quinone compounds have shown the potential to be used as cathode materials, bringing advantages such as greater sustainability, high performance and greater flexibility than their inorganic counterparts (Delaporte *et al.*, 2020). However, several materials challenges, including the intrinsically poor electronic conductivity of organic materials, their high level of solubility in non-aqueous electrolytes and their relatively lower energy density, as well as the ability to manufacture at scale and low-cost, will need to be addressed before commercialisation (Lyu *et al.*, 2021).

2.3.2.2 Lithium-sulphur batteries

Sulphur is a promising material to replace cobalt in lithium batteries due to its high abundance, low cost, nontoxicity and higher energy density (Bruce, Freunberger, *et al.*, 2011; Salim *et al.*, 2022). Sulphur electrodes have the theoretical ability to provide an energy density several times that of a Li-ion battery, though practical demonstrations have not yet reached this level. While the concept has been around since the 1960s, practical issues caused development to halt until the recent demand for high-density batteries renewed research interest (ibid). Lithium-sulphur (Li-S) batteries have several key challenges to overcome in the battery chemistry. Firstly, sulphur is a natural insulator, leading to poor electrode rechargeability and requiring other materials such as carbon to increase conductivity at the cost of larger electrodes and reduced energy density (Ji & Nazar, 2010; C. Li *et al.*, 2017). Secondly, sulphur is transformed into polysulfides dissolved in the electrolyte, which via a 'shuttle' mechanism between the electrodes ends up severely degrading the battery cell capacity through an irreversible loss of active sulphur (W. Ren *et al.*, 2019). Considerable research has been undertaken to reduce the shuttle effect via the design of porous cathodes to trap sulphur and searching for electrolytes which will inhibit the transfer of polysulfides. However, it is expected that successful commercialisation of Li-S batteries with high energy densities is still some way off.

2.3.2.3 Lithium-oxygen batteries

The lithium-oxygen pairing shows a very high theoretical energy density, and significant efforts have been made to develop batteries based on this principle. Lithium-oxygen batteries involve oxygen from the air entering a porous cathode. The oxygen is then reduced, forming an oxide with lithium ions as the cell discharges. The anode of the cell is formed of solid lithium metal, which possesses a higher energy density than the graphite anodes of a Li-ion battery. Both aqueous (water) and non-aqueous electrolytes have been considered for these batteries (Bruce, Hardwick, *et al.*, 2011). Although the theoretical energy density of these batteries is very high, similar to Li-S batteries they have significant materials challenges to overcome before commercialisation, relating to the solid metal anodes, porous cathodes and electrolytes (Y. Li & Lu, 2017). The solid lithium metal anode will form dendrites from its surface as lithium is deposited, leading to a loss of capacity as well as potential safety issues due to short-circuiting caused by the formation of dendrites on the surface. In addition, lithium metal reacts violently with water, and therefore needs to be separated from aqueous electrolytes via a coating, which reduces the conductivity of the anode. Non-aqueous electrolytes can lead to clogging at the porous carbon cathode as contaminants develop from unwanted water vapour (Liu *et al.*, 2020). A membrane is also required to block carbon dioxide and water from the ambient air from entering and clogging the cathode through preferential reactions.

Lithium-oxygen batteries therefore have significant challenges before mass commercialisation will become viable. There are also other metal-oxygen pairings that show promise for high-density batteries including sodium-oxygen and zinc-oxygen, though these face similar materials challenges including preventing degradation of the metal anode and locating a suitable electrolyte (Y. Li & Lu, 2017).

2.3.2.4 Solid-state batteries

Solid-state batteries replace the liquid or gel electrolyte with a solid material. This has several advantages: batteries would be safer due to the lack of a flammable electrolyte and lower levels of heat generation; they could be stable and usable at a greater range of temperatures and conditions than a liquid electrolyte, have longer lifetimes with less decay from repeated cycles and they could be lighter and more flexible due to the solid electrolyte requiring fewer packaging materials (C. Li *et al.*, 2021). The non-flammable nature and lighter weight have made these batteries especially appealing to EV manufacturers. The only currently commercialised battery with a solid electrolyte is the sodium-sulphur cell, which due to an operating temperature of 300oC and the use of molten sodium is only suitable for stationary grid scale deployment (Breeze, 2019). The development of a solid electrolyte for lithium chemistries with high levels of conductivity, electrochemical stability and mechanical longevity has been a major materials research priority over the last decade, with substantial advances reported (Tan *et al.*, 2020). However, significant challenges in moving from laboratory to commercial development remain, including the electrochemical instability of many of the electrolyte candidates, difficulties in perceiving and characterising the reaction dynamics occurring inside a solid-state battery cell and challenges in upscaling manufacturing, due to the brittle nature of the electrolytes (ibid). Several organisations are predicting commercialisation happening in the second half of this decade, starting with small-scale, high value applications (S&P Global Market Intelligence, 2021b).

2.3.3 Conclusions

Battery technology has seen somewhat slower rates of development in recent decades than areas which require battery power, such as technology miniaturisation, wireless data capacities and electric vehicle design. This has led to an increased demand for batteries with higher energy densities and charge/discharge rates than the currently dominant lithium-ion technology. As this section has explored, there are key fundamental science challenges with developing new battery chemistries, including the composition of the electrodes and electrolyte, the challenge of ensuring the cell reaction is fully reversible and to minimise the build-up of contaminants, and the characterisation of reaction dynamics at the cell interfaces. Scale-up and commercialisation challenges will also need to be addressed, as several technologies will require the development of new manufacturing methods and supply chains and will face price competition from the more established Li-ion ecosystem. However, there are significant efforts to commercialise next-generation batteries, initially focusing on the electric vehicle and aviation market (Robinson *et al.*, 2021; Zhu *et al.*, 2019), with Toyota currently planning to launch hybrid cars with solid-state batteries by 2025 (The Washington Post, 2022).

2.4 Novel Materials for Hydrogen and other Energy Carriers

2.4.1 Introduction

Hydrogen has long been seen as an important part of the drive to a low-carbon economy, as it can be used as an energy carrier, substituting for oil and gas in sections of the energy system where electrification is difficult or expensive. Hydrogen is not in itself a primary fuel and needs to be produced by various methods prior to use. Currently, the vast majority of global production of hydrogen (around 95%) comes from the steam methane reforming process (Royal Society, 2018). This is known as grey hydrogen and due to its use of fossil fuels is not low carbon. In order to produce low-carbon hydrogen, either carbon capture and storage (CCS) would have to be deployed at scale or alternative methods will need to be used. Alternative methods include:

- Electrolysis of water – breaking water into hydrogen and oxygen using electricity;
- Biological methods – using bacteria or algae to convert biomass to hydrogen via anaerobic digestion;
- Photoelectrolysis/solar fuels – using sunlight directly to split water into hydrogen and oxygen.

Electrolysis of hydrogen from water using low-carbon electricity is currently the most promising technology to deploy at the significant scales that could be required in the near-medium term. The other two technologies are at a more basic stage of development but could prove disruptive in the longer term. The UK has research groups working on all three technologies. This section will only consider electrolysis due to its greater readiness compared to the other two methods.

There is also growing interest in the use of ammonia as an energy carrier. Ammonia is produced using hydrogen and is relatively stable and easy to transport. It can be used directly in some fuel cells, decomposed to generate hydrogen, or combusted directly (Xue *et al.*, 2021).

2.4.2 Electrolysis

Electrolysis of hydrogen from water is not a new technology – alkaline electrolysis is a well-established technology, first demonstrated in 1789. Nonetheless, its high cost in energy consumption compared to steam reforming has meant that it so far has had limited commercial application (Shiva Kumar & Himabindu, 2019). It is well-positioned to be a major growth technology in a low-carbon transition, however, due to its potential to produce green hydrogen if powered by low-carbon electricity. There are several materials challenges in making hydrogen electrolysis more efficient and to reduce the intensity of critical materials. There are two major types of electrolysis technologies in commercial use – Alkaline Water Electrolysis and Proton Exchange Membrane Electrolysis (Y. Guo *et al.*, 2019).

2.4.3 Materials Challenges for Low-temperature Electrolysis

2.4.3.1 Alkaline Water Electrolysis

Alkaline electrolysis of water (AWE) to produce hydrogen is the oldest and most mature electrolysis technology and has been demonstrated up to the 100MW scale. Commercially, it has been used for hydrogen production for industrial uses since 1920, and are well-understood, with low capital costs, little use of expensive critical metals and relatively durable components (Schmidt *et al.*, 2017). However, it has limitations surrounding operating pressure and current density, and has trouble working with variable renewable sources due to issues with varying current input and frequent shut down-restart cycles affecting operation and output purity (Zeng & Zhang, 2010). There has been relatively limited development of AWE over the past few decades. Materials challenges for this technology include the improvement of membrane stability, both for temperature range and operational lifetime, as well as improvement of catalysts to allow higher current density and development of materials to allow higher temperature operation (Royce Institute, 2020a). The UK currently has little research or commercial activity in AWEs, which would need to change, either through market-pull or a government/industry backed push, for significant UK investment in this technology.

2.4.3.2 Proton-exchange Membrane Electrolysis

Proton-exchange membrane electrolysis (PEMWE) was developed in the 1960s by General Electric to attempt to overcome some of the drawbacks of alkaline electrolysis (X. Zhang *et al.*, 2015). It is a less mature technology than AWE and is usually used for small-scale applications (Schmidt *et al.*, 2017). However, it can produce high-purity hydrogen quickly and at higher pressures and is more suitable for the dynamic operation needed to operate with variable renewables. PEMWE currently has a higher capital cost than alkaline electrolysis partly due to the use of platinum-group metals in the catalyst. Materials challenges for this technology involve increasing the efficiency and lifetime of these precious-metal catalysts or finding acceptable lower-cost substitutes, as well as improving the lifetime and stability of cell membranes, transport layers and structural materials (Royce Institute, 2020a). The UK has key academic strengths in basic electrochemical research and modelling, as well as electrochemical diagnostics and systems optimisation (Royal Society, 2018). UK companies in this area include Johnson Matthey and ITM Power.

2.4.4 Materials Challenges for High-temperature Electrolysis

At higher temperatures (above 700oC), electrolysis of hydrogen from water (steam) becomes a more thermodynamically efficient process, leading to a smaller amount of electrochemical energy required per unit of hydrogen. A high amount of thermal input is required to heat the water to the appropriate temperature, however, making high-temperature electrolysis currently more suitable to be co-located with industrial processes or used for high-value applications. High-temperature electrolysis of hydrogen coupled with nuclear energy to provide electrical and thermal inputs has been considered as a method of producing low-carbon hydrogen (IAEA, 2021). This technology is currently at demonstration phase, with no large-scale commercial production of hydrogen as of yet.

The most promising technology to carry out high-temperature hydrogen electrolysis is by solid-oxide fuel cells (SOFC), which were originally designed to act as electrolysers, producing electricity by combining hydrogen and oxygen into water. These need to operate in a reverse mode to split water into its constituents, meaning that the materials used in the SOFC will need to be optimised for this reverse process (Revankar, 2019). Materials challenges in this area include improving the durability and performance of the electrolytes, electrodes and interfaces over longer periods of time, developing techniques to manufacture at scale and providing standardised testing for materials properties and degradation (Royce Institute, 2020a). The UK has strong basic scientific R&D capabilities in this area, but little industrial capacity, which is mostly in the domain of small, innovative start-ups. A more integrated programme between academia and industry may help to accelerate the commercialisation of this technology and position the UK well in this space to realise future gains (Royce Institute, 2020a).

2.4.4.1 Ammonia as an energy carrier

Ammonia has been typically used as a fertiliser in the agricultural sector, as well as in industrial processes and as a refrigerant. It has several advantages as an energy carrier – it has a relatively high energy density, it is easy to transport, store and utilise compared to hydrogen, it has a mature storage and transportation infrastructure due to its use in fertiliser and it burns cleanly, producing nitrogen, water and oxygen. Transportation costs are significantly cheaper – as much as ten times – compared to hydrogen by ship, rail or road (Royal Society, 2020). It can be utilised as a replacement for gasoline and other transport fossil fuels in internal combustion engines or turbines (Erdemir & Dincer, 2021). The key downside is the efficiency loss from the conversion of hydrogen to ammonia – making ammonia a less efficient way to utilise energy than hydrogen or direct low-carbon electricity. For this reason, ammonia is likely to be used in applications where energy needs to be stored for long periods of time or transported long distances by land or sea (Giddey *et al.*, 2017).

Ammonia is traditionally made using the Haber-Bosch process, an energy-intensive high-pressure and -temperature industrial method that consumes more than 1% of global energy production (J. Guo & Chen, 2017). Hydrogen for this process is generated utilising steam methane reformation from fossil fuels. More sustainable methods of producing ammonia are required for a net-zero world, both to produce fertiliser and also for potential usage as an energy carrier. One sustainable route to ammonia is hydrogen electrolysis coupled with the Haber-Bosch process powered by low-carbon electricity. Research on downscaling the Haber-Bosch process and integrating direct electrolysis of water in order to provide more localised generation of ammonia is underway, with demonstration projects at the RAL in Oxfordshire and Fukushima in Japan (Royal Society, 2020). Materials challenges include the degradation of catalysts under intermittent operation and overcoming the lower efficiencies seen at smaller scales.

Novel methods of ammonia production are at more basic research stages. Direct electrochemical synthesis of ammonia has been demonstrated and has been investigated utilising a variety of electrolyser cells at various temperatures. However, the reaction efficiencies are currently extremely low compared to the Haber-Bosch process, and significant work will need to be carried out on improving catalysis efficiency and cell materials before the technology can be scaled to commercial levels (Kyriakou *et al.*, 2017).

2.4.5 Conclusions

Electrolysis as a method to produce hydrogen could potentially play a significant part in the net-zero energy transition, if hydrogen is adopted as an energy carrier on a large scale. While there are key challenges with supplying low-carbon electricity to power the process, novel materials advances could make electrolytic cells more efficient, longer lasting and cheaper to manufacture and maintain. The UK has strong research capabilities and recent growth in start-up companies in this area, but as Section 3, below, will elaborate, has a need for stronger industrial partnerships and demonstration facilities to bring research advances to commercial viability. The use of ammonia as an energy carrier is promising, but research is currently at a more basic level and substantial advances will need to be made to make this a commercially viable energy vector.

3. Research and Policy Recommendations

3.1 Overview

A workshop was held with representatives from the UK academic and industrial sectors to explore the UK materials R&D space in January 2021. The purpose of the workshop was to understand the strengths of the UK's novel materials for energy R&D capability, the challenges currently facing this field, and the policy decisions which need to be made to support researchers and commercialisers. This work was intended to build on the conclusions of the Royce Institute's roadmaps (Royce Institute, 2020b), as well as provide an update for UKRI's Energy Prospectus Electrochemical Energy document, published in 2014 (Rhodes *et al.*, 2014).

The workshop asked attendees to describe what they considered to be the strengths and weaknesses of the UK materials for energy ecosystem. They were then asked for their priorities for policymakers to build on the UK's strengths and challenge the weaknesses. The answers of the attendees have been condensed and summarised below.

3.1.1 Strengths of the UK Materials R&D Sector

The UK has excellent modelling, simulation and theoretical design capabilities located across academia in addition to well-established fundamental research groups. This gives the UK a world-leading role in fundamental materials research, backed up with strong international links and collaborations with overseas research groups. This helps to bring in a great deal of international talent and expertise to the UK. There is also a strong history of collaborative working across different disciplines and academic groups, giving UK researchers the opportunity to develop wide and holistic skillsets.

UK research groups also have access to state-of-the-art materials characterisation facilities, including the Diamond Light Source synchrotron and the ISIS muon and neutron source.

3.1.2 Challenges facing the UK Materials R&D Sector

The UK has an exceptional capability in basic materials research and development. However, there are challenges in moving discoveries to the applied R&D stages and further through the innovation chain towards demonstration and commercialisation. The UK currently has no standardised national facilities to test, benchmark and certify the properties of novel materials, and scaling-up facilities, testbeds and other capabilities are often inconsistent and unavailable. Further challenges in developing, demonstrating and commercialising novel materials emerge from technology transfer and knowledge sharing. There were concerns about the difficulties for companies of working with academia due to slow processes, administration hurdles and associated charges, which in some cases especially for smaller companies can prove prohibitive. Open access, not just of journal articles but also of datasets, is important for knowledge sharing between academia and companies, but hurdles in the high cost of OA publishing and the unavailability of datasets remain. Concerns were also raised about universities in some cases potentially overestimating the value of their IP, with their priorities to get as high a price as possible for their IP instead of building stronger links and lasting relationships with partners. There was perceived to be a conflict in university priorities between IP being viewed as a source of income or a source of longer-term impact. More widely, there is a perception that there are few incentives to scale-up industrial activity and commercialise new technologies in the UK.

Workshop attendees also expressed concerns over the levels of 'low-risk, low reward' basic research projects being funded, with a corresponding lack of exploratory blue-sky research being carried out. Material properties can be non-intuitive and breakthroughs can come from unusual areas. There is often a tension in research funding as to the focus of research between maximising performance or minimising the use of critical materials. The example of the iridium catalyst for PEM cells was given. In this, the focus of funding could be in improving the performance of iridium or in replacing iridium, with a corresponding potential major drop in performance. There was seen to be too much focus on improving today's solutions and not enough on developing tomorrow's, with a lack of research into unexplored materials areas and more radical thinking. A related challenge is that of research continuity – ensuring that research teams and technical support staff are able to be kept together after the end of a grant to prevent the loss of institutional knowledge and skillsets.

3.1.3 Research Policy Recommendations

The workshop found a dynamic, impactful and internationally recognised UK novel materials research community, producing significant, high-quality basic R&D. However, leveraging this research was often inefficient, with a lack of platforms for characterisation and testing, difficulties in navigating technology transfer and partnerships with private industry, and access to support for demonstration and commercialisation. There were also concerns that research funders were prioritising short-term impact over speculative research. The following five proposals aim to improve these shortfalls.

Testing and Standardisation: A dedicated UK resource for testing including degradation testing, benchmarking, standardisation, and certification should be funded. This would certify materials to a new UK standard, with the aim for this to be recognised globally.

Technology Transfer: It needs to be made easier for companies and academia to work together to transfer R&D up the technology readiness chain. This would include streamlining admin hurdles and charges, improving open access to reports, articles and datasets and encouraging universities to consider the value of long-term relationships as well as short-term IP valuation.

Commercialisation Incentives: Though the quality of basic materials R&D in in the UK is very high, the incentives to further develop and commercialise materials are fewer than in other countries. Greater incentives could assist the development of novel materials industries in the UK - including greater access to venture capital and support, easy access to test-beds and demonstration platforms to provide the viability of materials, and further tax incentives for innovation and applied R&D.

Speculative Research: Materials is a field which benefits heavily from 'blue-sky' speculative research and testing, as material properties can be non-intuitive and breakthroughs can come from unusual areas. To ensure that the UK has a steady supply of future discoveries and disruptive impact, speculative research should be funded with fewer concerns about immediate results.

Research Continuity: To ensure greater consideration of research continuity, people with well-developed and relevant skillsets should be incentivised to stay in their roles and institutions. Successful teams, including technical support staff, should be supported to be able to be kept together after the end of a grant by providing continuity funding. Funding to train the next generation of researchers, including centres for doctoral training, should be continued and expanded.

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