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ADVANCED MATERIALS AND RESEARCH FOR THE GREEN FUTURE

NAPREDNI MATERIALI IN RAZISKAVE ZA ZELENO PRIHODNOST

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Environmental concerns, such as pollution, greenhouse-gas emissions, sustainability, global warming and climate change, are the biggest challenges of our times. In this respect, the more efficient use of energy and materials combined with technology optimization and innovation are playing a key role in the quest to become a green society with green industry. Multiple environmental and economic benefits can mostly be achieved through novel, lightweight energy-efficient designs. In order to develop and properly use new materials and new designs, complete understanding and information on their properties must be obtained. It is also vital to know how these properties are affected by the conditions of a specific application. Furthermore, as the design of components is pushed towards the limits, unsuitable and outdated measuring methods, measuring uncertainty and deviations from the defined material properties can lead to unexpected premature failure of the component and environmental problems.

For the green future, it is extremely important to develop new, advanced materials. However, it is often the changes of the production technology and to the surface of an already-existing material that can achieve great benefits to performance as well as the environment. It is all about modifying the material to perform better, last longer, be biocompatible and achieve different functionalities. Finally, besides high-tech equipment and research facilities, close cooperation between universities, research institutes and industry is needed to develop technologies, functional materials and solutions that can effectively support the journey of our society into a green future.

Keywords: environment, pollution, advanced materials, surface engineering, research

Okoljski problemi, kot so onesnaževanje, emisije toplogrednih plinov, trajnost, globalno segrevanje in podnebne spremembe, predstavljajo največje izzive našega časa. Ključno vlogo pri prehodu v zeleno industrijo in družbo ima učinkovitejša raba energije in materialov,povezano s tehnološko optimizacijo in inovacijami. Številne okoljske in gospodarske koristi je moč doseči z uporabo novih lahkih in energetsko učinkovitihkonstrukcij. Za razvoj in pravilno uporabo novih materialov in novih dizajnov je potrebno pridobiti popolno razumevanje in informacije o njihovih lastnostih. Pomembno je tudi, kako na te lastnosti vplivajo pogoji in parametri uporabe. Ker pa so zahtevane karakteristike in načrtovanje komponent potisnjeno do samih zmožnosti materialov, lahko že neustrezne in zastarele merilne metode, prevelika merilna negotovost in odstopanja od specifikacij povzročijo nepričakovano odpoved komponente in okoljske težave.

Za zeleno prihodnost je izjemno pomemben razvoj novih naprednih materialov. Vendar pa so pogosto spremembe proizvodne tehnologije in površine že obstoječega materiala tiste, ki lahko zagotovijo izjemne okoljskekoristi in izboljšanje funkcionalnosti. Vse se nanaša na spreminjanje materiala, da deluje bolje, traja dlje, je biokompatibilen in dosega najrazličnejše funkcionalnosti. Nenazadnje je poleg visokotehnološke opreme in raziskovalnih zmogljivosti potrebno tudi tesno sodelovanje med univerzami, raziskovalnimi inštituti in industrijo, kar omogoča razvoj novih tehnologij, funkcionalnih materialov in rešitev, ki lahko učinkovito podprejo prehod naše družbe v zeleno prihodnost.

Ključne besede:okolje, onesnaževanje, napredni materiali, inženiring površin, raziskave

1 ENVIRONMENTAL CONCERNS

Environmental concerns, such as pollution, greenhouse-gas emissions, sustainability, global warming and climate change, which are some of the biggest challenges of our times, have produced a variety of societal responses.[1] These include public policy measures such as the Geneva and Rio Conventions, the Paris Agreement, the U.S. Clean Air Act, the European Waste Electrical and Electronic Equipment Directive, the Japanese Home Electronics Recycling Law, and the latest European Green Deal, set to turn the EU into the first climate-neutral continent by 2050. [2] Actions are required across all sectors, including increased energy efficiency and renewable energy, low-emission mobility and decarbonized transport, minimized material use, recyclability, no hazardousness and no-waste production.

With transport contributing around 5 % to GDP and employing more than 10 million people in Europe alone, the transport system is critical to global businesses and supply chains, thus playing a vital role in society and the economy. At the same time, transport is not without costs to our society. It is a key source of environmental pressures, climate change, greenhouse gas (GHG) and pollutant emissions, noise, road crashes and congestion. It also takes up large strips of land and contributes to urban sprawl, the fragmentation of habitats and the sealing of surfaces. Transport consumes one-third of all final energy in the EU. The bulk of this energy still comes from oil. This means that transport is responsible for a large

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share of the EU's GHG emissions and a major contributor to climate change. It is also a significant source of air pollution, especially in cities. While most other economic sectors, such as power production and industry, have reduced their emissions and pollution since 1990, those from transport have risen.

Transportation accounts for more than one-quarter of the EU's total GHG emissions and for ≈ 16 % (≈ 8 gigatons CO_2e) of global GHG emissions.[3] The vast majority comes from road transport (75 %), i.e., cars and trucks, with most of the rest from aviation and ocean shipping (22.5 %). Only 1 % of the automobiles in operation globally are currently electric, with the number growing rapidly, encouraged by favourable government policy and incentives. EU targets for reducing the CO_2 emissions of cars and vans are a 50–55 % reduction by 2030 and zero emissions from new cars by 2035.[3] A low-carbon, zero-emission mobility system will thus require the near-complete replacement of the vehicle fleet. Passenger cars will likely be dominated by plug-in battery electric vehicles. Heavier trucks will likely see greater deployment of green hydrogen and fuel cells. Harder-to-abate sectors such as aviation and shipping could rely on technological advancements in biofuels and green hydrogen. The transition to a low-carbon mobility system will likely entail shifting production to electric and green hydrogen powertrains, including retooling manufacturing facilities, expanding battery and fuel-cell production, working with the mining industry to find new materials and sources of critical minerals, increase efficiency and reduce energy consumption and power losses. However, in all sectors, fully-recyclable, lightweight and CO_2-footprint materials will be required and will start to dominate.

Reducing GHG emissions also requires higher shares of renewable energy and greater energy efficiency. The production and use of energy, including transportation account for more than 75 % of the EU's GHG emissions. Thus, the binding target of renewable sources in the EU's energy mix by 2030 is set to 40 % and overall reduction of energy consumption to 36–39 %.[3] Energy production itself, primarily electricity generation and heating, accounts for ≈ 31% (≈ 15 gigatons CO_2e) of global GHG emissions.[4] Coal and natural gas are still the two largest sources of electricity generation, accounting for roughly 60 % of the total power produced. Nearly all the remainder comes from low-carbon sources, a mix of renewables (wind, solar, and hydropower) and nuclear. However, wind and solar growth has outpaced other generation sources and are forecasted to become the largest sources of installed global electricity generation capacity by 2025. [4]

The goal of a net-zero energy system will likely see nearly all electricity supplied by renewable energy, likely dominated by a mix of photovoltaic solar and onshore and offshore wind. A variety of other low-carbon power generation technologies potentially including bioenergy with carbon capture and sequestration, geothermal, modular nuclear, and natural gas with carbon capture could all play roles as well. However, solutions of problems related to energy transformation, storage, supply and efficiency, heat exchange, hydrogen storage, carbon capture and storage, etc., largely depends on materials and their properties.

Last but not least, also industrial manufacturing and materials production require a large amount of energy and is in many countries responsible for a large portion of environmental impacts and pollution, producing approximately 28 % (≈ 14 gigatons CO_2e) of global GHG emissions.[4] And the emissions trend is upward over the last decade. The bulk are the result of energy consumption during production across industries, although direct emissions as a by-product of cement and chemicals manufacturing are significant contributors too. Materials production and manufacturing also produce large volumes of waste, both in production and at end-of-life disposal. The carbon-intensive nature of many processes has challenged manufacturers seeking to transition towards lower-emission alternatives, increase efficiency, remove waste, and embrace circular approaches, especially in heavy industry. On the other hand, such hard-to-abate operations currently have few viable low-carbon alternatives and although environmental impacts and emissions of some pollutants may decrease over time due to increased efficiency in production and improved pollution controls, waste and GHG emissions typically go hand in hand with increasing materials production.

However, the more efficient use of energy and materials combined with technology optimization and innovation could play a key role in achieving multiple environmental and economic benefits. Although many opportunities exist, material efficiency is still not realized in practice to its full potential. In future steel, aluminium, cement, and other hard-to-abate heavy industries will see much wider use of green hydrogen and electrification, with on-site carbon-capture technology playing an important role. Furthermore, manufacturing should continue to obtain gains in efficiency, reducing emissions intensity, sensors deployment and analytics, digital transformation, etc. Additive manufacturing, lean production, circular design, and more robust material-recycling practices can reduce waste and emissions, at the same time providing low-weight, minimum-energy-demanding designs. Increased recycling leads to reductions in waste volume and generally leads to reduced GHG emissions.[4] Nevertheless, some advanced materials have limited recycling potential, although they can still be used in downgraded end-of-life applications.

Throughout their lifecycle, as materials are produced, converted to products, consumed, and discarded, the transformations use energy at every step. Industry is thus one of the largest energy-using sectors, emitting approximately 36 % of global GHG emissions associated with energy and processes (**Figure 1**). The production of bulk

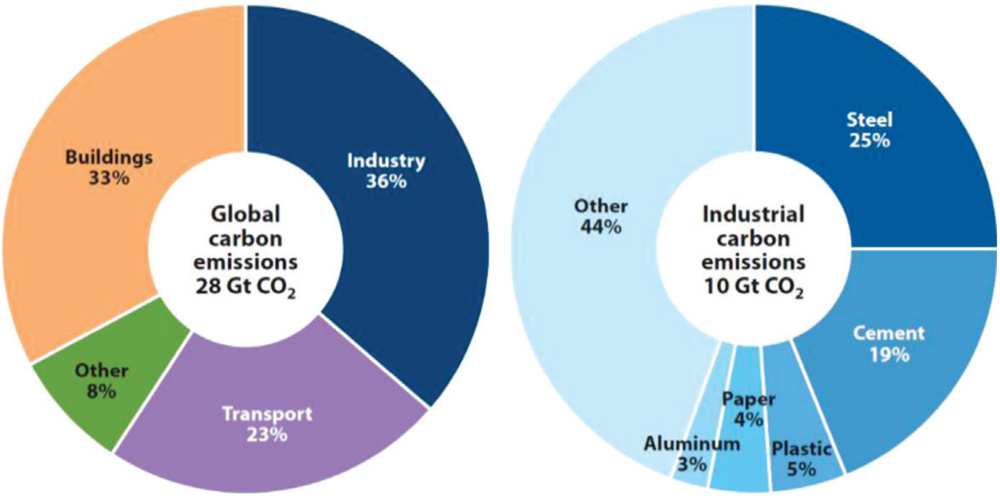

Figure 1: Distribution of global CO_2 emissions among sectors and materials production[4]

materials leads to approximately 25 % of all GHG emissions. This makes materials a key sector for climate, environmental, and economic policy. Although there is still considerable potential for reductions in the energy and GHG intensity of material production, ultimately there are limits.[5] Materials also play a key role in the planned transformation to a low-GHG-energy system. Sustainable energy technologies need novel materials as well as traditional materials such as steel, aluminium and copper, providing the highest level of re-use and recycling.[5,6] Hence, the transformation of the energy system is likely to lead to a changed and increased appetite for specific materials as a new energy infrastructure is built. Overall, the global consumption of materials such as aluminium and steel is likely to double if current developments continue. Simultaneously, there is a trend towards substitution with more energy-intensive and higher-CO_2 footprint materials (e.g., replacing steel with aluminium, polymers, or carbon fibres), which may lead to the increased use of energy and CO_2 emission in production, although they are reduced during the operation of the product. If current trends in global demand for materials continue, the environmental impact (GHG emissions, water withdrawals, pollution) of materials production is likely to increase. For the bulk materials, future relative improvements in the intensity of production are constrained given that the processes are already relatively energy efficient and are likely to be eclipsed by absolute growth in demand. For the critical materials, demand and performance needs may rise ahead of current trends driven by the development of new energy-supply and production technologies.

2 MATERIAL REQUIREMENTS

As shown, materials are central to most of the environment-protecting strategies, faced with the following challenges to[2]:

- reduce material intensity,
- reduce energy intensity,
- enhance material recyclability,
- reduce dispersion of toxic substances,
- maximize sustainable use of renewable resources,
- extend product durability.

To increase cost-effectiveness, efficiency, safety, performance, and to address environmental concerns there is an urgent need to develop advanced materials and manufacturing technologies that allow novel, lightweight energy-efficient designs. Lightweight designs mattes more now than ever before. The development and application of advanced lightweight materials, such as fibre-reinforced plastic composites, ceramic fibre composites and light metals, contributes to a significant reduction in weight with a simultaneous increase in performance. Especially in the automotive industry, aerospace, energy industry and construction, the most important impulses in the field of lightweight construction have been and are still being achieved. Another important issue is energy efficiency, requiring materials (i.e., electrical steel sheets) with minimum power losses. Advanced materials generally mean materials that have novel or enhanced properties that improve performance over conventional products and processes. They can boost the transition to greener technologies, with improved characteristics and enhanced performance, contributing to a more sustainable future. For each renewable technology to progress, the development and improvement of materials is needed to help us build a greener future. All renewable technologies face material challenges. Materials must be lighter, stronger and able to resist corrosion from demanding atmospheres and high temperatures.

Advanced materials are defined as multifunctional materials categorized into[7]:

- lightweight materials,
- smart materials,
- nanomaterials,
- self-healing materials,
- self-diagnostic materials,

- photonic materials,
- bio-inspired materials and designs.

Some representatives of advanced materials are carbon fibres, polymer composites, smart fibres, ceramics, intermetallic titanium aluminides, shape-memory alloys, carbon nanotubes, etc. A special group are bio-materials and bio-inspired design, known as bio-mimetics. Bio-mimetics has given rise to new technologies on the micro- and nano-scale, inspired by observing living organisms that have evolved well-adapted structures and materials over time through natural selection. Nature has solved engineering problems, such as self-healing abilities, environmental exposure tolerance and resistance, hydrophobicity, self-assembly, and harnessing solar energy. Some examples are shown in **Figure 2**.

The specific properties of advanced materials give them a lot of advantages over traditional materials, but specifics related to resource availability, energy and CO_2-footprint intensive production, degradability and recyclability, bio-compatibility, etc. may rise sustainability concerns and pose some serious environmental threats. With the environmental concerns now moved to the top of the engineering agenda, the development and selection of material is far from simple. Today, we see the huge proliferation of materials that were created over the last half-century. It is estimated that 32 % of the plastic produced annually goes into the oceans, while the production of carbon fibres is about 14 times as energy intensive as producing steel, and the creation process spews out a significant amount of GHGs (up to 20 times more than recycled steel[12]). Furthermore, to become the strong, light composite material carbon fibres are combined with a plastic polymer resin, with the manufacturing process being wasteful. By the time carbon fibre sheets are trimmed to size, almost one-third ends up on factory floors and one-fifth goes straight into the waste, without ever making it into a product. Where the material does make it into products, most of it will ultimately end up in landfill due to the fact that the recycling of carbon fibres is very limited[13]. Another problem with specific modern materials is their availability. For example, indium-tin-oxide is currently used as a conductor in most of our touch screens, yet indium is one of the rarest elements in the earth's crust, meaning supply is very limited and expensive to mine.

Metals on the other hand have excellent sustainable character. The growing importance of the consideration and use of sustainable materials depends on the relationship between the renewability of the natural resources and the material products that are generated from them. The risk of depleting a natural resource can make their use less desirable when other, more sustainable, alternatives exist. Metals such as iron (Fe) and aluminium (Al) are elements and therefore cannot be destroyed or depleted. The Earth's overall resource deposits of metallic elements have not decreased but simply change locations and present themselves in different forms. Aluminium and steel have many product applications, and once these product applications cease to function the material can be recycled and reused in the creation of another product. This cycle allows the aluminium and steel to remain a permanently accessible material through recycling, retaining the properties and thus making them one of the only truly cradle-to-cradle materials.[14] Metals may also possess exceptional properties if produced and processed properly. However, the applicability, capacity and potential of metals is still not fully exploited and realized in practice. This requires an advanced materials-research approach combined with digitalization and the introduction of green technologies.

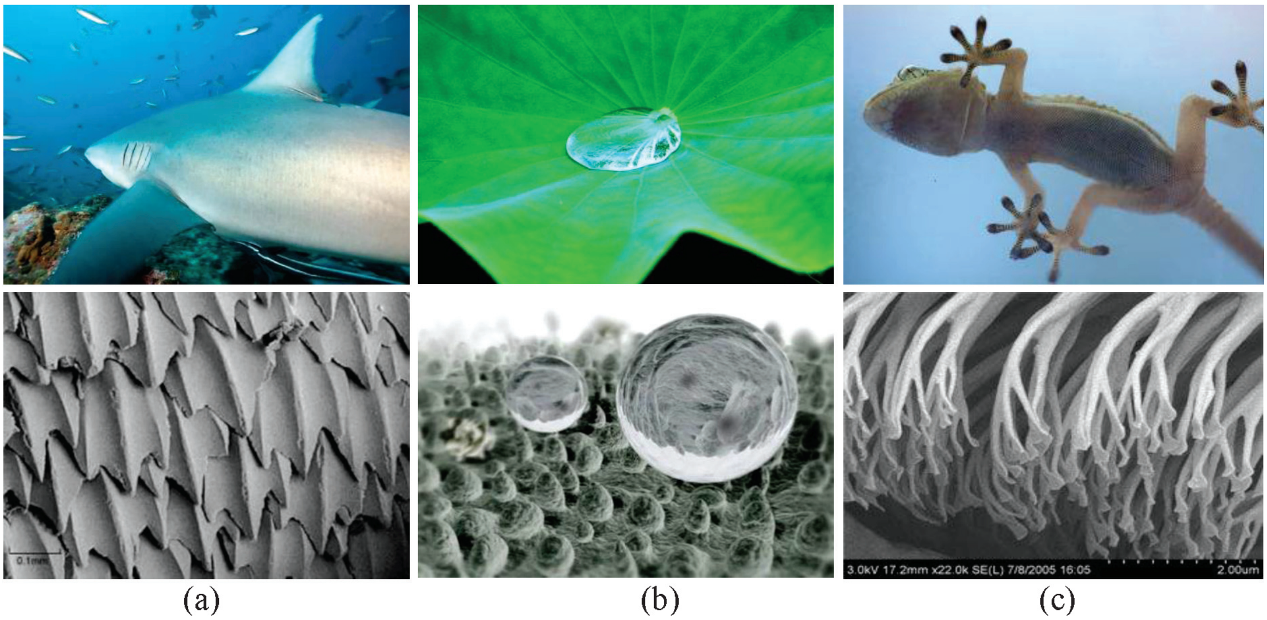

Figure 2: Examples of nature engineering: a) shark skin with reduced drag,[8] b) self-cleaning lotus leaf,[9] c) super adhesion of gecko feet[10,11]

The problem of many components, products and goods which society takes for granted, is they are quite difficult to recycle. Just a few decades ago, making durable products resulted in special, hard-to-recycle materials, which were also so bound together that during the recycling process, it was really hard to separate them. And even when it is technically feasible to take apart a product and recycle its parts, it is often that new, advanced materials are very technically challenging to recycle and not economically justified. To increase the potential and likelihood of products and materials being recycled, it is essential to consider recyclability during the design phase. Not only product design, but also the design of the material itself is crucial to increase recycling rate and sustainability. In parts design already a few simple steps can make a big difference, including the use of less impacting and easily recyclable materials, like metals, reduce the quantity and diversity of materials, not using materials which can reduce the quality of recycled ones, labelling parts that can be recycled, making them easy to dissemble and creating guides on how to take apart a product for recycling.[15] Although it is foreseen that research and development will lead to less energy required for both extracting and recycling materials, as well as an overall reduced carbon footprint, it is essential that companies are forced into recycling by design and to fully recycle their products, i.e., high quality recycling and ultimate reuse. By exporting products to regions where a subsequent high-quality recycling is rather unlikely to happen, the material loop will not be closed, subsequently decreasing resource efficiency and limiting sustainability.

Another issue is material production and recycling itself. Processing of materials is one of the most significant sources of energy consumption and GHG emissions globally, forcing the need for "green materials" with reduced direct emissions and energy needs. As part of this trend is increased interest in the recycling of materials and the development of materials being more recyclable by design. Historically, metals have higher rates of recycling, because scrap can more easily be collected and recycled. However, where there are challenges and physical difficulties with the collecting, sorting and separating of waste materials or involves technically challenging and a more energy-intensive process, recycling rate may be very low or even non-existant.[16] The higher the value of the constituents and the lower the complexity of a specific side stream or residue, the more of that material will be recirculated and recycled. There are several factors which make material less recyclable, including technical barriers and barriers linked to the traceability of materials due to their potential contamination.[17] However, when recycling is taking place in state-of-the-art processes, down cycling or materials quality issues can mostly be avoided. To make material more recyclable, it must maintain its mechanical and chemical properties after recycling and be able to be sorted prior to recycling, so it needs to be transformable and sortable with an acceptable cost-to-performance ratio and environment impact; recycling is not necessarily beneficial.[18] The main short-term efforts to increase recyclability of materials are related to waste-material sorting and separation, medium-term to information tools supplying all the essential information regarding overall production chain through the so-called digitized circular economy[19] and the use of biodegradable and bio-sourced materials, while long-term to increased material recyclability by design, also requiring the development of new technologies and research strategies.[18] Commonly downgrading of a certain material takes place by a common collection of different alloys. A separation afterwards is possible, but involving greater efforts. Even more critical is the mixing of residues from different processes. However, in some cases, the mixing of specific material streams can also lead to a higher recycling potential, if this improves the overall thermodynamic environment of the process.[18] Very complex are also recycling challenges related to critical metals, i.e., tantalum and indium, used in very low concentrations with respect to the overall composition, which are lost almost completely at present. An efficient and economical viable recovery and recycling of these metals is a major technological challenge, requiring multistage mechanical, thermal/metallurgical, and chemical treatment steps in multi-metal recovery processes[18], taken into account already during the material design phase. The growing complexity of the products also demands their full digitization.

In terms of environment protection an important challenge is how to reduce direct emissions during material production, i.e., the material CO_2 footprint. Currently the steel industry is among the three biggest producers of CO_2, with emissions being mainly produced by a limited number of steel plants. In response, decarbonisation measures such as blast-furnace efficiency improvement, use of biomass reductants, carbon capture and usage,[20] and establishing or switching to hydrogen-based (H_2) steel production can be implemented either in future (greenfield) sites or existing (brownfield) facilities.[21] Blast-furnace efficiency programs do not eliminate CO_2 emissions completely, biomass reductants are only feasible in certain regions, while carbon capture and usage is still in the early stages of development. Therefore, an approach combining scrap, direct reduced iron, electric arc furnace (EAF) and use of green hydrogen is currently considered the most viable option and the long-term solution to achieve carbon-neutral steel production.[21] However, the key challenge will be obtaining ssufficient amount of electricity from renewable energy to produce green hydrogen and run EAFs. Therefore, the optimal steps to steel-production decarbonisation will differ depending on the technical feasibility, the existing infrastructure, but mainly on the availability and price of renewable electricity and scrap.

Also, in the case of aluminium production the use of renewable energy as the source of the green electricity is the best way to improve the carbon footprint of the primary aluminium.[22] On average, 72 % of GHG emissions from the aluminium sector are from the primary production of aluminium. However, the electrolysis process still produces direct CO_2 emissions. Although they are on average only about one-tenth of those from the energy source, they are still significant. Globally, they account for about 300 million tonnes of CO_2.[23] These direct emissions could be reduced by using inert anodes and aluminium chloride process.[24] Other alternatives are to use bio-carbon in the anodes or to employ carbon capture and use. In the case of copper production, GHG emissions are typically associated with the consumption of fuel in the mining and materials transport processes, as well as indirect emissions from electrical energy use in extractive and beneficiation processes. This is due to the high energy demand requirement to crush and grind ore. The average energy and GHG intensity is 4.5 t CO_2-equivalent (CO_2e) per tonne of copper produced.[25] With the increase in secondary smelting a decreasing demand for copper-mining activities are taking place. Also, energy demands for secondary smelting are on average lower than the one of primary, leading to about a factor-of-2-lower specific CO_2 emissions.[26] However, the production of the electricity used in the copper-smelting process remains the major source of GHG emissions.

Last but not least, we should also discuss batteries-related GHG emissions. Lithium-ion batteries and electrical mobility play an important role in the world's decarbonisation and reduction of GHG.[27] However, climate impact, which derives from the mining and refining of battery materials, and manufacturing of cells, modules and pack must also be taken into account. The production of a battery cell requires sourcing of as much as 20 different materials from around the world, which will pass through several refining stages before entering an advanced and energy-intensive manufacturing process with very different climate impacts depending on which energy source is used.[27] In this respect climate impact related to lithium-ion battery manufacturing (mainly associated with energy requirements) may range from about 40 kg to 200 kg CO_2e/(kW·h), being equivalent to CO_2 emissions produced by a comparable diesel car in 1–7 years.[28] As much as 75 % of energy consumption comes from the cells production and 20 % of that for mining, conversion and refining of the active materials. However, the largest climate impact of the cell comes from the synthesis of the precursor and lithium compound into cathode powder, with the cathode production requiring 47 % of the cell energy demands.[27] For pack production the dominant energy consumption comes from the aluminium used, resulting in about 140 kg CO_2e/(kW·h).[29] As can be seen, the major environmental factor in many materials production, including batteries, is cumulative energy demand and its source. Using a less-carbon-intensive energy mix (mainly hydro and nuclear power in Sweden vs. coal and natural gas in Poland, **Figure 3**) will result in much lower CO_2 impact. To decrease the CO_2 impact, also recycling needs to be taken into account, making already-extracted material available for the production of new batteries. By using direct recycling where the cathodes and anodes retain its composition followed by different types of hydro metallurgic processing energy demand in material production can be reduced by as much as 48 %.[30]

3 RESEARCH NEEDS

Advanced metallic materials research should incorporate:

- materials testing and properties correlation,
- measurement uncertainty and innovations,
- modelling and simulation,
- advanced heat-treatment strategies and surface engineering,
- compatibility.

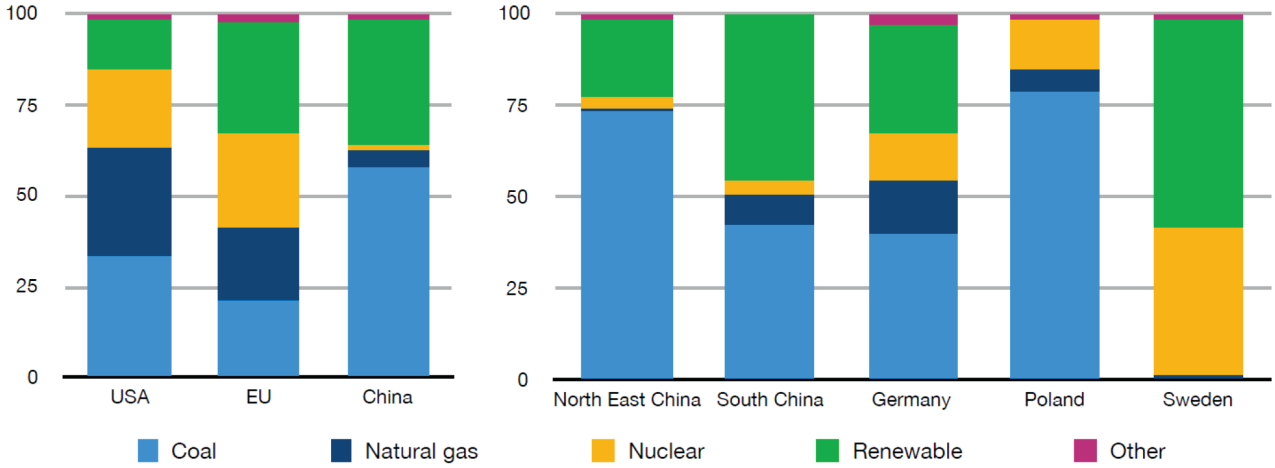

Figure 3: Average energy mix per region and country[27]

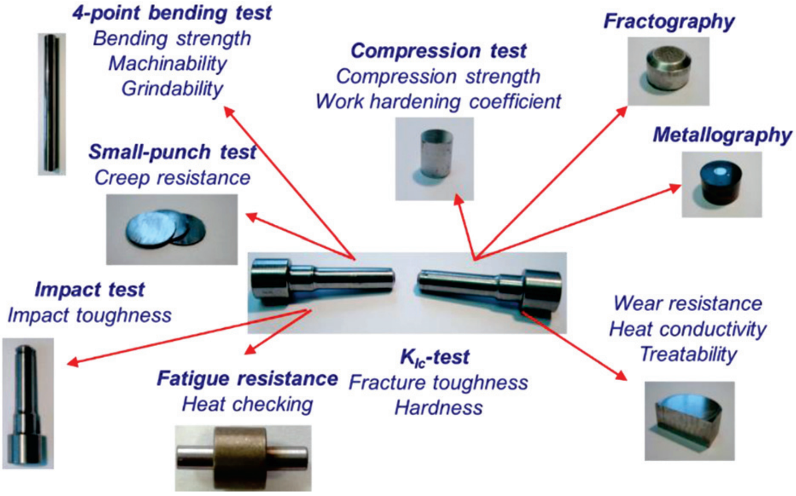

Figure 4: Characterization versatility of CNPTB test specimen

In general, the properties of metals depend not only on the balanced chemical composition and the processing route, but also greatly on the final heat-treatment process, which defines the final microstructure. With the industry being confronted with ever-increasing demands on higher productivity, lower production costs, more complex products, lightweight design and environmental restrictions, requirements on a material's properties are also becoming more demanding. Consequently, this means tougher property requirements for a large number of properties, which usually don't go hand in hand. Improvement in one property often results in another property's deterioration. Furthermore, although different material properties (strength, hardness, toughness, wear resistance, machinability, etc.) can be determined using standard test methods, each one requires specific and often unique test specimens, thus exposed to different conditions during manufacturing and heat treatment. This makes it practically impossible to evaluate and directly correlate multiple properties. On the other hand, a method based on circumferentially notched and fatigue-precracked tensile bar specimen – CNPTB[31] (**Figure 4**) has been found as a very promising research testing method, with the cylindrical geometry providing uniform microstructure and the. possibility of preparing different test specimens. In this way many different properties including fracture resistance, toughness, hardness, strength, fatigue and wear resistance, machinability etc. can be determined and mutually correlated, as shown in **Figure 5**.

In order to properly use materials in design, a complete understanding and information on their mechanical properties must be obtained. It is also vital to know how these properties are affected by the conditions of a specific application of the material. Factors such as the size of the part, surface condition, loading direction and loading rate may result in changes to these properties that must be considered in the design.[33] Furthermore, as the design of components, especially in automotive industry, is constantly pushed toward the limits of the material, unsuitable and outdated measuring methods as well as deviations from the defined material properties and excessive measuring uncertainty can lead to unexpected premature failure of the component and environmental problems[34]. Therefore, a sophisticated and reliable determination of material properties with low uncertainty is crucial in modern design aimed at a green future. Small deviations in testing specimen's diameter or unsuitable surface preparation may result in a large increase in measurement uncertainty and failure probability[35] (**Figure 6**).

With the modification of the composition and elements, the effect of heat-treatment conditions on the metal's microstructure evolution and properties, includ-

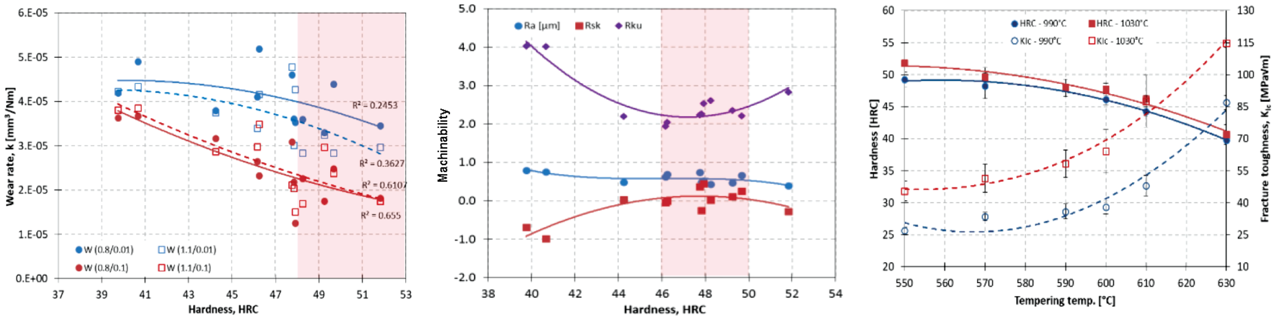

Figure 5: Examples of multiple tool-steel properties' determination and correlation[32]

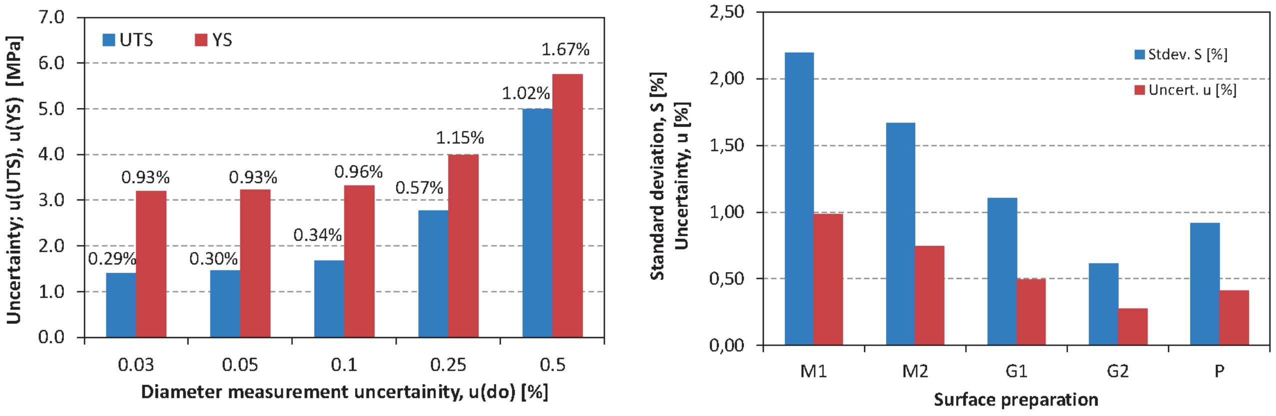

Figure 6: Effect of specimen size mismatch and surface condition on measurement uncertainty in tensile and hardness testing of Al alloys, respectively[35,36]

ing two the most important properties in material selection in automotive industry, fracture toughness and hardness, will change, thus requiring tremendous experimental work. Although the influence of chemical composition on phase transformations, hardenability, and strength have been studied since late 1960s, with several models and equations being deduced by analysing available data, they are too general and very seldom consider interactions of the alloying elements. Another technique of obtaining and optimizing material properties is based on processing and a trial-and-error approach. However, this requires an excessive use of resources. Therefore, there is a huge need for tools allowing the prediction of properties of metallic materials as a function of composition and heat-treatment process variables. This can be done by the mathematical modelling process and the calculation of phase diagrams, but this is not an easy task, especially in the case of multiphase systems. First of all, heat flow and phase-transformation kinetics are coupled, with the results relying on the knowledge of thermodynamic processes and used database. Furthermore, also minor modifications in the geometry or properties can

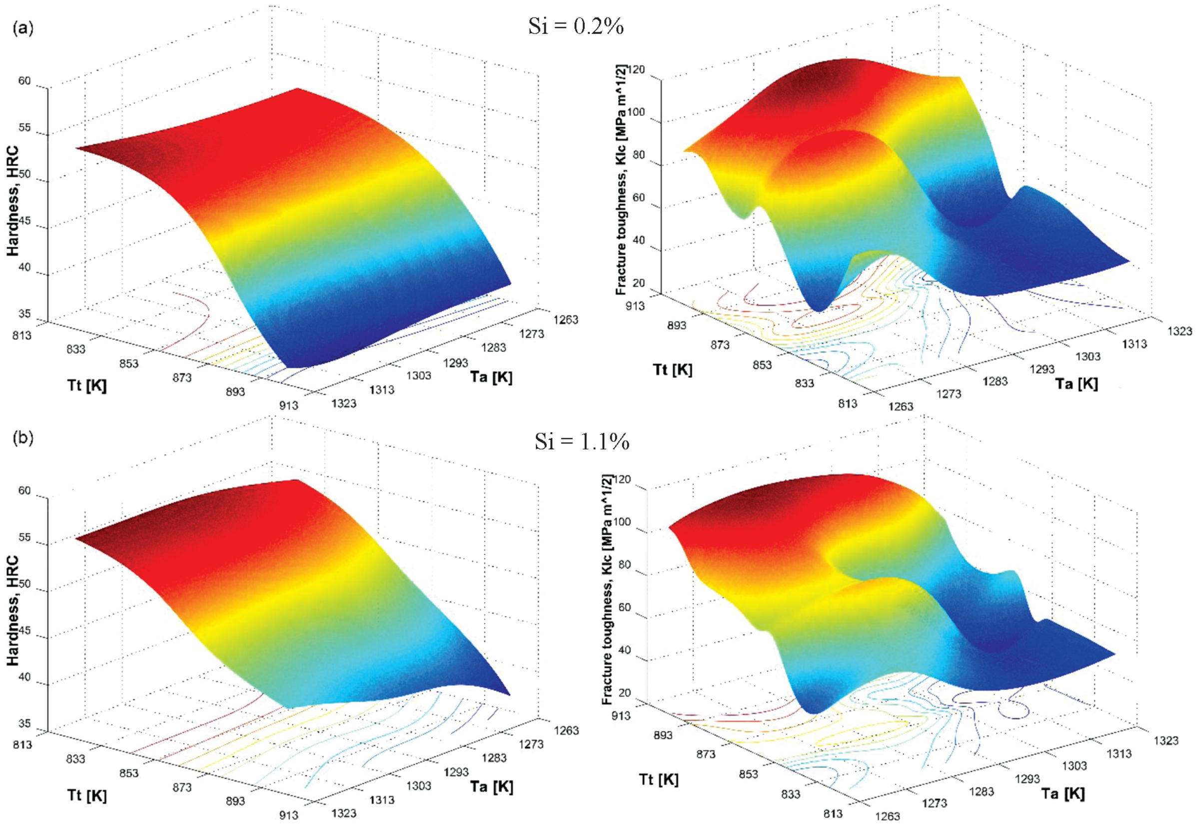

Figure 7: ANN based analysis of heat-treatment parameters and composition on steel properties[38]

result in large variations in prediction, with any simplification of a complex system leading to greatly reduced accuracy of the model. On the other hand, soft computing methods like genetic algorithms, fuzzy logic, artificial neural networks (ANN) and artificial intelligence (AI) have been found to be able to perform highly complex mappings of nonlinearly related data by inferring subtle relationships between input and output parameters, thus providing good predictions in materials science regardless of any relational knowledge of the nature of the analysed system.[37] AI and ANN are particularly suited to problems that involve the manipulation of multiple parameters and nonlinear interpolation, and as a consequence are therefore not easily amenable to conventional theoretical and mathematical approaches. With such an approach the multiphase analysis of different parameters and elements can be carried out, as exemplified in **Figure 7**, providing valuable guidelines for focused experimental research and shortening development and time-to-market phase. Of course, modelling results strongly depend on the training dataset provided. The larger it is, the better are the results and predictions.

Many materials have been developed to have specific properties, obtained through processing and heat treatments. However, although new processes, technologies and materials are developed constantly, their final treatments are not always up to date. The heat treatment of metals, for example, is an ancient art expanded down the ages from black art to science to improve mechanical properties. Furthermore, materials production is, in general, focused on bulk properties, without being particularly optimized for the surface properties. Recently, studies of sub-zero cooling cycles have gained attention, showing a huge potential for improving the working performance of a wide range of materials (steels, cast iron, cemented carbide, aluminium alloys, copper alloys, super-alloys, ceramic materials, composites, polymers, wood, etc.) and in countless applications (metal-mechanics, automotive and transportation, aerospace, mining, timber industry, agriculture, electric/electronics, chemical industry, medical, sports, music, etc.). One of the key factors contributing to the growth of advanced heat and thermo-chemical treatment strategies, involving sub-zero and deep cryogenic treatment, is the need to develop superior products with improved performance and properties, especially in tooling, automotive, aerospace and energy production industry. Through improved material properties (**Figure 8**), including wear resistance, toughness, corrosion and fatigue resistance,[39] cryogenic treatments are a very valuable tool for reducing the consumption of energy and strategic materials (steel, aluminium, light alloys, polymers) as well as their environmental footprint. Its use also enables shorter production times and savings, improved productivity and better quality. Furthermore, in contrast to conventional heat-treatment processes, which are specific for a particular material and mainly limited to ferrous metals, a deep cryogenic treatment is applicable to almost all engineering materials.

Superior material properties are getting more and more important as the high-performance expectations, required levels of reliability and environment protection increase. The limits of materials are stretched primarily through alloy design and the utilization of composite technology.[40] However, the development of traditional metallic alloys using one or two principal alloying elements has reached a saturation point.[41] Thus, multi-component alloy design and development is the way forward to realize a much wider spectrum of compositions with a superior combination of properties, as shown by high-entropy alloys (HEA).[42] These alloys contain multiple alloying elements (four or more) and are designed principally based on configurational entropy. Such alloys also have the potential to eliminate the need for heat treatment. Initially high-density elements such as Fe, Cu and Ni were used, targeting equi-atomic compositions and single-phase structures. Currently, multi-component high-entropy alloys with a different combination of elements and different combination of properties are explored.[43] These include low-density HEAs (i.e., $Mg_{43}(MnAlZnCu)_{57}$) with density values lower than 3 g/cm^3 targeting weight-critical applications and high-density HEAs (i.e., $V_{20}Nb_{20}Mo_{20}Ta_{20}W_{20}$) for harsh environment applications providing excellent specific strength, superior mechanical performance at high tem-

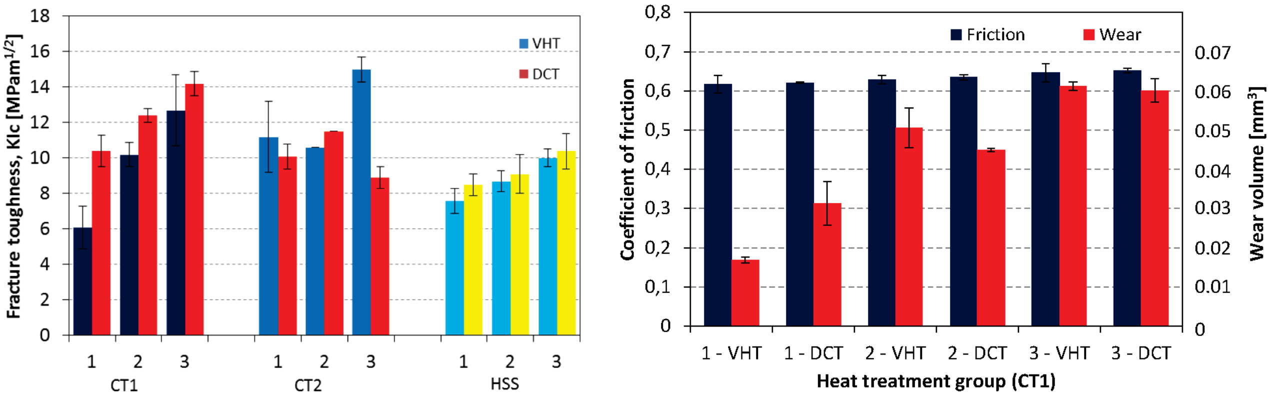

Figure 8: Properties comparison between conventional vacuum heat treatment (VHT) and deep cryogenic treatment (DCT) of tool steels[39]

peratures, exceptional ductility and fracture toughness at cryogenic temperatures, superparamagnetism and superconductivity.[44] From the perspective of enhancing properties, attention has to be placed on compositional control to develop multi-component alloys where the secondary phases are developed inherently during a processing step to exhibit a superior combination of properties without the need for heat treatment. However, there are still many fundamental issues related to the formation of different phases, which need the development of new theories, models and mechanisms. Furthermore, although an almost unlimited number of compositions are possible (10^{102} different alloy systems estimated that could potentially be useful to society) only a few may prove useful, requiring efficient high-throughput method for alloy screening.[45] Machine learning, showing fast and reasonably accurate property predictions combined with density function theory, is a promising approach to guide the new multicomponent alloy design.[46,47] In this way it can be determined whether a system is likely to be stable as well as to calculate many material properties. On the other hand, the inverse approach of choosing elements that can provide the needed specifications can be used when a specific combination of properties is needed for a given application.

Surface engineering (**Figure 9**), on the other hand, can solve surface-related demands and properties, and offer materials savings and environmental benefits by:

- implanting alloying atoms to different depths, thereby improving toughness and fatigue properties (surface modification),
- depositing surface layers, thick or thin, including solid lubricants (surface coating),
- redesigning the surface shape of the component to distribute stresses (surface texturing).

Many modern surface engineering processes also have low environmental impact.

For the green future, it is extremely important to develop new, advanced materials. However, it is often the changes to the surface of already-existing material that can achieve the greatest benefits to performance as well as environment. Surface engineering is about modifying the surface of what lies beneath, to make it perform better, last longer, or even achieve a different function entirely. So, surfaces can prevent or control the main "life-determining" characteristics of materials (such as wear, corrosion and fatigue). But they can also have a huge impact on sustainability, by ensuring optimized use of scarce materials, reducing energy losses due to friction, increasing wettability, providing tissue-compatibility, etc.[49]

A very important issue in materials research is environment friendliness, biocompatibility, non-toxicity, degradability, recyclability, sustainability, etc. However, from the functionality and performance points of view, compatibility with other materials, compounds and substances in the system is equally important. An example is the compatibility of coatings with lubricants. By improv-

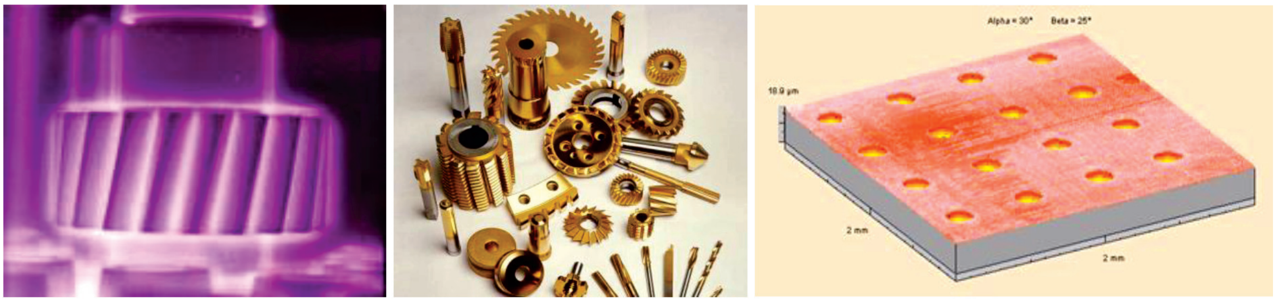

Figure 9: Examples of surface engineering by plasma nitriding, coating[48] and texturing

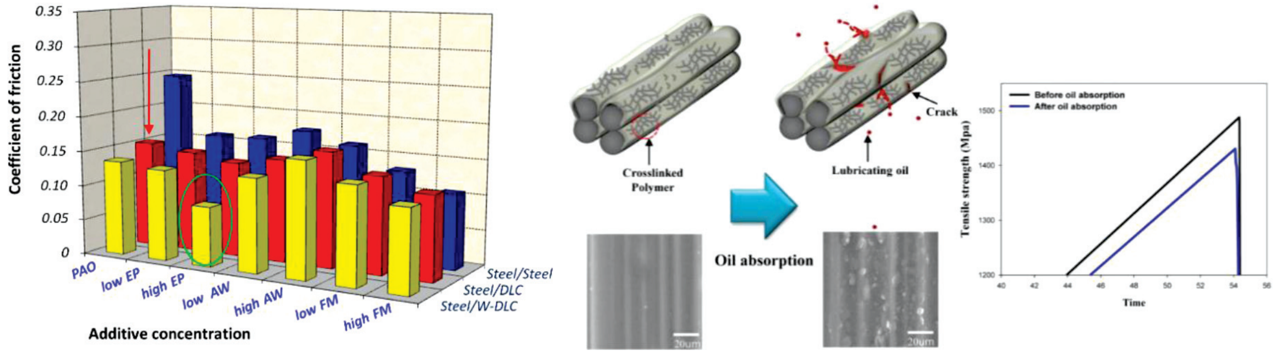

Figure 10: Friction reduction through combined action of DLC coatings and additives,[50] and negative effect of oil penetration on strength of carbon-fibre-reinforced composites[51]

Figure 11: Forgings from ultra-high-strength steel, die from hot work tool steel with improved thermal conductivity and light-weight design with new Al 6086 alloy[52]

ing tribological properties, i.e., reducing wear and coefficient of friction of contact surfaces, hard coatings provide great opportunity for further improving performance, durability and efficiency of tools and components, which can no longer be achieved by material selection, design or lubrication. At the same time, they even show the possibility of running components dry, thus potentially eliminating lubricants or at least replacing them with less hazardous ones. However, although certain coatings, especially carbon (DLC) and MoS_2-based coatings show low friction and wear under dry-sliding conditions, the majority of components and tools will remain lubricated using the same oils originally developed for uncoated metallic surfaces, at least for the near future. There are many reasons for this. Firstly, tribological properties of low friction coatings are sensitive to the surrounding and contact conditions, notably the relative humidity. Furthermore, the lubricant also serves other functions, such as cooling, insulation, wear-particles removal, etc. Therefore, the design of new materials and components for a green future needs to take into account also this aspect. As shown in **Figure 10,** certain combinations may result in further tribological improvements and superior performance, while others can have detrimental or even disastrous effect.

4 SLOVENIAN COOPERATIVE RESEARCH RESULTS

Besides advanced research and high-tech research facilities the close cooperation between universities, research institutions and industry is needed to develop advanced functional materials and solutions that can effectively support journey of our society into green future. A great example of such collaboration is Slovenian research program MARTINA (Materials and Technologies for New Applications),[52] involving 15 partners (2 universities, 6 research institutes and centres, 7 companies), where through the joint research and development the following materials with superior properties were developed and introduced (**Figure 11**):

- Three ultra-high-strength steels for automotive and transportation industry, providing 10–20 % higher strength at up to 5-times better fatigue resistance, reduced need for heat treatment and diminished heat affected zone influence. Two steels are aimed for forged load-bearing components and one for safety construction elements in light-weight designs.
- Two tool steels with reduced non-metallic inclusions, better fatigue and heat checking resistance, improved machinability and 60 % higher thermal conductivity, thus focusing on reduced energy consumption and material use.
- New high-strength Al alloy (registered as 6086 type) produced with a high share of scrap. This addresses requirements on light-weight design, reduced material CO_2-footprint, reduced energy use and raw material input.
- Completely new magnetic material and production process based on anisotropic magnetic particles in a thermoplastic matrix, allowing the production and magnetization in a single stage and magnets with up to 40 % better magnetic-field effectiveness.
- Application of metallic nanoparticles in different polymeric materials, providing completely new structural properties such as anti-bacteric and wear resistance, electrical conductivity, magnetic properties, etc.

5 SUMMARY

For a green future, the development and progress of materials are extremely important. For each renewable technology to progress, the development and improvement of materials is needed. The development and application of advanced lightweight materials, regarded as materials with novel or enhanced properties that improve performance over conventional products and processes, contributes to a significant reduction in weight and increase in performance. The specific properties of advanced materials give them a lot of advantages over traditional materials, but specifics related to resources availability, energy and CO_2-footprint intensive production, degradability and recyclability, bio-compatibility, etc. may raise sustainability concerns and pose some serious threats to the environment. Metals, on the other hand, have ann excellent sustainable character, without their true properties and applicability potential being fully exploited.

The limits of materials are stretched primarily through alloy design. However, the development of traditional metallic alloys using one or two principal alloying elements has its limits. These can be overcome by multicomponent alloy design (i.e., high-entropy alloys), allowing a much wider spectrum of compositions with a superior combination of properties, such as low-density alloys with density values much lower than aluminium and high-density alloys providing excellent specific strength and performance at high temperatures, etc. However, although almost unlimited number of compositions are possible only a few may prove useful. Machine learning combined with computational modelling is a promising approach to guide the new multicomponent alloy design. On the other hand, often already changes to the surface of the existing material can provide great benefits to performance and environment. Surface engineering is about modifying the surface through diffusion, coating or texturing processes to make material perform better, last longer, or even achieve a different function entirely.

The problem of many products and goods that society takes for granted, is they are quite difficult to recycle. Even when it is technically feasible to take apart a product and recycle its parts, it is often that new, advanced materials are very technically challenging to recycle and not economically justified. To increase the potential and likelihood of products and materials being recycled, it is essential to consider recyclability during the design phase. Not only product design but also design of the material itself is crucial to increase the recycling rate and sustainability. Materials need to be more recyclable by design. The main short-term efforts to increase the recyclability of materials are related to waste-material sorting and separation, medium-term to information tools and use of biodegradable and bio-sourced materials, while long-term to new technologies and research strategies.

In terms of environment protection an important challenge is how to reduce direct emissions and CO_2 footprint during material production. Steel, aluminium and copper production are the three biggest producers of CO_2. An approach combining recycling, electrification and the use of green hydrogen is currently considered the most viable option and the long-term solution to achieve carbon-neutral production. However, the key challenge will be obtaining sufficient amounts of green electricity from renewable energy. The same is true when it comes to electrical mobility, regarded as a major step toward the world's decarbonisation and reduction of GHG emissions. Climate impact which derives from manufacturing of cells, modules and pack, mining and refining of battery materials, as well as origin of the electricity must all be taken into account.

With the environmental concerns being at the top of the engineering agenda, the development and selection of materials is far from simple. In order to develop and properly use new materials in designs, complete understanding and information about their properties must be obtained, including how these properties are affected by the conditions of a specific application. Sophisticated and reliable determination of material properties and their correlations supported by computational methods, machine learning and artificial intelligence is crucial in modern design aimed for green future.

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