III. Chemical, Metallurgical, and Materials Engineering

1 Engineering research fronts

1.1 Trends in top 11 engineering research fronts

The top 11 engineering research fronts assessed by the Field Group of Chemical, Metallurgical, and Materials Engineering include the fields of energy, materials, chemistry, and biotechnology (Tables 1.1.1 and 1.1.2). Among these top research fronts, “renewable energy systems,” “membrane bio-reactor and membrane fouling control technology,” and “applications of porous organic materials for CO_2 capture” are based on the popular topics suggested by *Clarivate Analytics*. The other eight are recommended by the domain experts working in these research areas.

“Renewable energy systems,” “catalyst design by artificial intelligence (AI),” and “membrane bio-reactor and membrane fouling control technology” are the more emerging research fields based on the data for the mean year of publications (Table 1.1.1). Notably, “catalyst design by AI” is a rapidly rising field according to the increasing number of core papers published annually (Table 1.1.2) even though the citation numbers are not high (Table 1.1.1). “Catalytic biomass conversion” and “applications of porous organic materials for CO_2 capture” are hot research areas as the number of citations per publication is greater than 90 citations (Table 1.1.1).

(1) Renewable energy systems

Renewable energy is the energy that is generated from natural processes that are continuously replenished. Renewable energy systems (RES) such as those utilizing wind, solar, biomass, hydropower, geothermal, and ocean energy play critical roles in realizing the energy sector that is clean, low-carbon, safe, and efficient. Although the RES have developed rapidly in recent years, they are still limited by relatively high cost, low reliability, and unsatisfactory synergy among multiple systems, resulting in challenges in terms of global energy transition.

Currently, the main goal of the studies researching RES is to utilize the energy more cleanly and efficiently, and thereafter introduce advanced coordination among a variety of RES

Table 1.1.1 Top 11 engineering research fronts in chemical, metallurgical, and materials engineering

No.	Engineering research front	Core papers	Citations	Citations per paper	Mean year
1	Renewable energy systems	26	1 232	47.38	2016.2
2	High-temperature alloy	500	16 602	33.20	2014.6
3	Material life cycle engineering	240	18 703	77.93	2014.8
4	Catalyst design by AI	50	352	7.04	2016.7
5	High-performance C/C composites for aerospace and aeronautics	139	4 482	32.24	2014.7
6	Membrane bio-reactor and membrane fouling control technology	38	1 401	36.87	2015.9
7	Catalytic biomass conversion	110	10 116	91.96	2014.3
8	Chemical biotechnology	226	19 594	86.70	2014.4
9	Applications of porous organic materials for CO_2 capture	80	7 663	95.79	2014.8
10	High-performance adsorption-catalytic materials for separation and purification	84	6 539	77.85	2014.8
11	Artificial nitrogen fixation under ambient conditions	80	4 873	60.91	2014.9

Table 1.1.2 Annual number of core papers published for the top 11 engineering research fronts in chemical, metallurgical, and materials engineering

No.	Engineering research front	2013	2014	2015	2016	2017	2018
1	Renewable energy systems	1	3	5	4	8	5
2	High-temperature alloy	126	115	139	73	38	9
3	Material life cycle engineering	57	61	47	42	23	10
4	Catalyst design by AI	2	4	5	10	10	14
5	High-performance C/C composites for aerospace and aeronautics	36	26	35	33	7	2
6	Membrane bio-reactor and membrane fouling control technology	6	4	4	6	8	10
7	Catalytic biomass conversion	27	44	26	12	0	1
8	Chemical biotechnology	73	61	43	40	8	1
9	Applications of porous organic materials for CO_2 capture	18	22	13	14	12	1
10	High-performance adsorption-catalytic materials for separation and purification	14	23	22	15	9	1
11	Artificial nitrogen fixation under ambient conditions	21	18	16	5	10	10

for optimizing the production, transportation, distribution, conversion, storage, and consumption of energy with the life cycle view. In general, the major aspects of the research can be categorized into four points: 1) from a macroscopic point of view, the proposal of strategies and paths for the development of the RES; 2) from a microscopic point of view, the improvement of the technical performances such as economics, reliability, and effectiveness of the RES; 3) in terms of energy generation, the optimization of hybrid renewable and traditional energy systems; 4) from the perspective of energy consumption, the integration of the RES into the energy, industrial, and transport sectors.

(2) High-temperature alloy

A high-temperature alloy based on iron, nickel, and cobalt, is a metal material that can withstand the working conditions at a high temperature of 600 °C for a long time. It is also called "super alloy" and exhibits a comprehensive performance such as excellent high-temperature strength, good oxidation resistance and hot corrosion resistance, and good fatigue performance and fracture toughness, as well as high alloying characteristics. Super alloys are the key materials for the manufacture of aeroengine hot components, and are widely used in the fields of electric power generation, metallurgy, glass manufacturing, and atomic energy, as well as in ship and automobile industries. Known as the "cornerstone of advanced engines" and accounting for 40%–60% of the total engine weight, super alloys are important in the development of engine technology. Currently, the research of super alloys include the development of new alloys and the surface treatment and welding of alloy materials. In particular, the high-temperature properties, together with the demand for new aeroengines and expansion of alloy applications in recent years have accelerated the development of new super alloys.

(3) Material life cycle engineering

Material life cycle engineering (MLCE) is an eco-design-oriented applied engineering field to meet the performance requirements, protect the environment, and conserve the resources. Through the application of technological and scientific principles including hazardous substance substitution, green process planning, clean production, and resource recycling in the complete industrial supply chain, MLCE can allow a systematic optimization of material products during the entire life cycle. Material ecological design plays an important role in alleviating the issues of resource scarcity and environmental pollution as the related issues are comprehensively considered in the early product design stages. Furthermore, the application of MLCE can reduce or even eliminate the negative effects of material products on the environment in the industrial supply chain.

MLCE has developed into an international research frontier based on the multidisciplinary intersection of materials, manufacturing, and environmental sciences. MLCE studies mainly include the material ecological design theory and methods, material life cycle evaluation theory and methods, development of assessment database of material environmental impact and analysis software, and recycling technology in MLCE.

The application of life cycle engineering in the field of materials should be further strengthened in future. By means of eco-design, life cycle assessment, and life cycle optimization technologies, a green development model of eco-environment materials industry can be established, which can gradually decrease the significant imbalance between the material production and resources, thereby allowing sustainable development in the field of materials.

(4) Catalyst design by AI

AI involves establishing an artificial neural network and utilization of machine learning. Currently, machine learning is used to address the clustering and regression problems. The first step in the application of machine learning to the field of catalysis is the identification of the problem as either clustering or regression. Then, the artificial neural network is developed by executing the learning and testing processes. After the artificial neural network is trained, it can be adopted to predict the catalytic performances of some simple catalysts and reactions. The decisive factors in determining the catalytic performances under these conditions are the adsorption energy values of one or two reactants. Although machine learning has already been applied to various types of problems in catalysis, there is no publication reporting the literature mining or image recognition of catalysis data such as infrared (IR) spectra by machine learning. We expect that these gaps will be filled in future.

(5) High-performance C/C composites for aerospace and aeronautics

C/C composites consist of continuous carbon fibers (as reinforcing phase) and carbon materials (as matrix). C/C composites have excellent properties such as low specific gravity, high specific strength, high specific modulus, low thermal expansion coefficient, ablation resistance, and thermal shock resistance. For the leading edges of the wing, nose cones, rocket nozzles, re-entry vehicles, and thermal protection system applications, C/C composites have unparalleled advantages compared with other materials. In recent years, with the rapid development of the aerospace industry, there is an urgent need for the development of long-term, high-temperature-resistant, and oxidation-resistant C/C composites. Material modification and coating protection are the two effective oxidation resistant strategies for C/C composites. The pursuit of long-life, anti-oxidation coating on the C/C composites is one of the main research areas for C/C composites. However, owing to the long production cycle, high cost, and difficulties in batch production, the applications of C/C composites are limited to aerospace and military. Therefore, it is necessary to develop new processing methods for the preparation of advanced C/C composites, which can reduce the preparation time and production cost.

(6) Membrane bio-reactor and membrane fouling control technology

Membrane bio-reactor (MBR) is a new waste water treatment technology which combines membrane separation and biological treatment. Currently, the solid/liquid separation membrane bio-reactor (SLSMBR) is the most widely studied and used reactor in MBR technology. The secondary sedimentation tank in the conventional activated sludge process is replaced by a membrane, which allows the coupling of high-efficiency membrane separation and traditional activated sludge method. Owing to the retention of microorganisms and macromolecular organics by the membrane, the biological concentration and organic oxidation efficiency in the reactor are high. Compared with the conventional activated sludge method, the MBR technology has advantages such as high effluent quality, low sludge production, small floor space, and low operation cost. The MBR technology has attracted significant worldwide attention for waste water treatment. However, as the membrane in MBR is directly contacted with the mixture solution, the particles and macromolecule solutes are inevitably absorbed and deposited onto the membrane surface or into the pores under physical, chemical, or biological actions, leading to the membrane pore blocking, reduction of water flux, and increase in the transmembrane pressure. Membrane fouling is one of major issues that restricts the extensive application of MBR technology. The studies regarding the control of membrane fouling and regeneration of membrane are important, and can be mainly focused on the membrane material and properties, type of pollutant, and operation conditions.

(7) Catalytic biomass conversion

Biomass is a general term for various organisms produced by photosynthesis using atmosphere, water, and soil. It is the major organic and renewable carbon resource in nature. Owing to its widespread resources, abundance, and carbon neutrality, the biomass is extensively used to synthesize fuels and prepare a variety of fine chemicals, which are considered an alternative to petrochemical resources. Catalytic biomass conversion is an effective method to achieve efficient usage. Representative biomass resources currently studied are lignocellulose (including cellulose, hemicellulose, and lignin), oils, sugars, and microalgae. Components such as sugar and cellulose can be catalytically converted into products of higher alcohols and platform compounds. Catalytic conversion of lignin produces aromatic hydrocarbons, aromatic aldehydes (carboxylic acids), phenols, and alkane fuels. Oils and fats can be used for producing biodiesel. All these aspects are interesting research directions in the field of biomass conversion. Owing to the complexity and difficulties in pretreatment as well as the reaction and separation of the biomass components, the development of more economic and green separation processes and catalytic systems is the main goal in the near future. In addition, the complete utilization of the multiple components of biomass and the co-production of high-value-added H_2, fuels, and chemicals are also the emerging trends in the catalytic biomass conversion field.

(8) Chemical biotechnology

Chemical biotechnology employs chemical methods to regulate cellular growth, metabolism, and product formation for the production of biochemicals, biofuels, and biomedicine. To generate chemical signals, the cells reshape their metabolism, leading to a more favorable phenotype resulting in additional products, reduced by-products, and improved stress-resistance. The chemicals may affect the cellular transcription, translation, or enzyme catalysis, and consequently alter the biosynthesis of macromolecules and small metabolites. After the engineered cells are successfully constructed by genetic engineering and genome editing tools, an additional phenotype space can be explored by applying a chemical biotechnology strategy. The results are of significance in the areas of both biotechnology and biological sciences. A particularly emerging area is the implantation of abiogenic-chemicals or those from the traditional petrochemical industry into the cellular metabolism to obtain useful products that can lead to more innovations in future.

(9) Applications of porous organic materials for CO_2 capture

The rapid increase in the atmospheric CO_2 concentration in recent years has caused a serious threat to the sustainable development of human society because of the accompanying greenhouse effect. Therefore, the development of cost-effective and environmentally friendly technologies for CO_2 capture are necessary to mitigate this problem. The CO_2 capture mainly includes pre-combustion capture (H_2/CO_2 separation), post-combustion capture (CO_2/N_2 separation), and oxy-fuel combustion (H_2O/CO_2 separation). The most widely used method in industry for CO_2 capture, i.e., amine adsorption, requires a high energy penalty to regenerate the adsorbent and results in many environmental problems. Compared with amine adsorption, the porous organic materials for CO_2 adsorption and separation are more energy efficient and easier to utilize and regenerate. Porous organic materials such as metal-organic frameworks (MOFs) and porous organic polymers (POPs) are promising for CO_2 capture applications owing to their exceptional properties including high surface area, easily tunable structure, and reproducibility. The CO_2 uptake capacity, CO_2 selectivity, physical/chemical stability, and production/regeneration cost are the four commonly used indicators to evaluate the performance of porous organic materials for CO_2 capture. The CO_2 capacity or selectivity can be realized by the pre/post-synthetic modifications of MOFs/POPs to introduce CO_2-philic functionalities. Using this method, the researchers have developed MOFs/POPs with high CO_2 adsorption performance and some MOFs can even be produced on a large scale. More research should be focused on improving the stability of these porous organic materials under relevant industrial conditions (in the presence of H_2O, CO, NO_x, and SO_x) and reducing the production cost of these materials. By overcoming these issues, the porous organic materials can be considered as promising candidates for the next-generation CO_2 capture technology in industry.

(10) High-performance adsorption-catalytic materials for separation and purification

Volatile organic compounds (VOCs) cause various problems such as photochemical smog, greenhouse effect, ozone layer destruction, and adverse effects to human health, which have threatened the survival and development of human beings. In terms of VOC abatement technologies, adsorption is a mature one, with small energy consumption and high treatment efficiency. The catalytic combustion technology has many advantages including large processing capacity, no secondary pollution, and ease of dealing with flammable and explosive gases. The main factors in the development of these two efficient waste gas treatment technologies are the adsorbents and catalysts. The development of high-performance adsorption-catalytic materials for separation and purification is the key to achieve energy conservation and reduction of emissions in the chemical processes. For VOC adsorbents, the activated carbon materials and zeolites have been widely used in industry. The development target for the high-performance adsorbents is selective adsorption, large adsorption capacity, and easy desorption. Currently, the noble metal catalysts are widely used as combustion catalysts. However, the development of noble metals is limited by disadvantages such as easy sintering, poor heat resistance, and high cost. The development of universal combustion catalysts with low cost and good stability is an urgent issue that should be addressed in the field of catalytic combustion.

The following points need to be considered in the research and development of high-performance adsorption-catalytic materials for separation and purification. 1) A deep analysis of the interaction between VOCs and adsorbents/catalysts should be performed through the development of material characterization and computational simulation. 2) Research on a mixture of VOCs, involving water vapor, SO_x, and NO_x should be carried out to simulate the real conditions of VOC emission. 3) The development of dual-function materials with both high-efficiency adsorbent and catalyst functions is optimal, i.e., the VOCs with low concentration in the exhaust gas can be concentrated by selective adsorption at the adsorption site on the material and then completely removed by the catalytic oxidation activity in the same material.

(11) Artificial nitrogen fixation under ambient conditions

Niterogen fixation through the conversion of atmospheric nitrogen into ammonia is regarded as one of the most significant processes in industry as ammonia not only plays a key role in the production of fertilizers to sustain the rising global population, but also serves as a green energy carrier and an alternative fuel. Since 1913, ammonia is mainly synthesized on an industrial scale by the traditional Haber–Bosch process at a high pressure (15–20 MPa) and high temperature (300–500 °C). This process is highly energy-consuming and accounts for more than 1.4% of the world's energy consumption and 1.6% of world's CO_2 emissions. Therefore, it is necessary to develop a green, sustainable, and alternate artificial niterogen fixation process to synthesize ammonia by employing renewable resources at ambient conditions. Possessing eco-friendly and sustainable characteristics, nitrogen-to-ammonia conversion through nitrogenase enzymes, photochemical reduction, and electrochemical reduction are considered as promising candidates for artificial niterogen fixation under mild conditions. Moreover, the electrocatalytic process using water as a sustainable proton source to substitute the raw material hydrogen used in the Haber–Bosch process is feasible for lowering the energy demand and decreasing the CO_2 emissions, which can allow the sustainable development of human society and alleviate the global energy and environmental crises. As the core components of the artificial niterogen fixation system, the rational design of efficient nitrogen reduction reaction (NRR) catalysts with high activity, high selectivity, and good stability, and the development of reaction process can promote the advancement of the NRR as a green and more sustainable method with low energy consumption are needed. Research efforts directed toward the electrocatalysts designed for NRR under ambient conditions have attracted worldwide interest.

1.2 Interpretations for three key engineering research fronts

1.2.1 Renewable energy systems

One of the greatest challenges in future is the sustainable generation and utilization of energy, and the RES play the most significant role in the realization of a sustainable energy system. In recent years, there is an increasing trend toward the studies on the RES, particularly the wind, solar, and biomass energy systems, among which, four emerging trends are discussed as follows. First, from a macro perspective, the researches should aim at understanding if and how the energy sector can be decarbonized by utilizing the RES. For instance, some European countries such as Denmark have proposed long-term plans for the energy transition, which employ renewable energy resources to replace the fossil fuels.

To build a clean, low-carbon, safe, and efficient energy system for China, it is necessary to promote the utilization of the renewable energy (particularly, the wind and solar energy) in the end-use energy sectors for enhancing the energy efficiency in the end-use consumption (primarily, the industry and transport sectors) and developing the distributed RES. Second, the popularization of the renewable energy relies heavily on the technical progress of the RES. Therefore, improving the conversion/utilization efficiency, strengthening the economic competitiveness, and developing advanced energy storage systems to enhance the reliability of the RES will be crucial in future researches. Third, the energy systems in future will consist of different types of energy sources from renewable energy to fossil fuels, implying that the collaborative planning and operational optimization of the hybrid energy systems, particularly the renewable energy-based systems, will be the new trends. The methods for the creation of a hybrid energy system based on the characteristics of different energy sources and improvement of the utilization ratio of the renewable energy in the hybrid system are some areas that can be investigated. Finally, the RES offer an opportunity to utilize sustainable sources in the traditional energy, industrial, and transport sectors. Among the various research directions, the integration of renewable sources into hydrogen production will be continually pursued, to not only afford a feasible way for the utilization of renewable energy, but also realize clean hydrogen manufacturing. The renewable-based hydrogen can be applied in the fields beyond the electric power sector, i.e., (1) for linking hydrogen to cooling, heating, and electricity for synthesizing and optimizing different energy networks and sectors; (2) utilizing hydrogen as an industrial gas to promote the development of industrial sectors as low-carbon units by employing it in smelting, metallurgy, chemical engineering, and other industries as high-efficiency raw material, reducing agent, and heat source; (3) employing renewable hydrogen for decarbonizing the transport sector, where a sustainable transportation system can be built by integrating the renewable energy, hydrogen, fuel cells, and new energy vehicles from a life cycle view.

By reviewing the core papers regarding the RES published after 2013, the countries/regions and institutions that mainly focus on the studies in this area are listed in Tables 1.2.1 and 1.2.2, respectively. Denmark, Germany, and Finland are the top three countries in terms of publications, accounting for 61.54%, 42.31%, and 19.23% of the total number of the core papers, respectively, whereas Aalborg University and Aarhus University have made the most significant contributions in this research field. As shown in Figure 1.2.1, Denmark and Germany have the best collaborative relationship, and the collaboration network between Germany–Finland and Denmark–USA is also well-developed. Figure 1.2.2 exhibits that the most active collaboration is observed among Aarhus University, Frankfurt Institute for Advanced Studies, and Goethe University, Frankfurt. According to Table 1.2.3, the core papers are mostly cited by the researchers from Germany, Denmark, and the USA in the descending order, whereas the data listed in Table 1.2.4 indicates that Aalborg University, Lappeenranta University of Technology, and Aarhus University are the top three institutions that include the core literature as references.

Table 1.2.1 Countries or regions with the greatest output of core papers on “renewable energy systems”

No.	Country/Region	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	Denmark	16	61.54%	944	76.62%	59.00
2	Germany	11	42.31%	594	48.21%	54.00
3	Finland	5	19.23%	161	13.07%	32.20
4	USA	4	15.38%	307	24.92%	76.75
5	Australia	3	11.54%	72	5.84%	24.00
6	Pakistan	1	3.85%	8	0.65%	8.00
7	Spain	1	3.85%	36	2.92%	36.00
8	Croatia	1	3.85%	11	0.89%	11.00
9	Netherlands	1	3.85%	13	1.06%	13.00
10	South Africa	1	3.85%	13	1.06%	13.00

Table 1.2.2 Institutions with the greatest output of core papers on "renewable energy systems"

No.	Institution	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	Aalborg Univ	8	30.77%	433	35.15%	54.13
2	Aarhus Univ	7	26.92%	315	25.57%	45.00
3	Lappeenranta Univ Technol	5	19.23%	161	13.07%	32.20
4	Frankfurt Inst Adv Studies	4	15.38%	83	6.74%	20.75
5	Goethe Univ Frankfurt	3	11.54%	214	17.37%	71.33
6	Stanford Univ	2	7.69%	80	6.49%	40.00
7	Australian Natl Univ	2	7.69%	41	3.33%	20.50
8	Karlsruhe Inst Technol	2	7.69%	20	1.62%	10.00
9	Forschungszentrum Julich	1	3.85%	6	0.49%	6.00
10	Rhein Westfal TH Aachen	1	3.85%	6	0.49%	6.00

Figure 1.2.1 Collaboration network among major countries or regions in the engineering research front of "renewable energy systems"

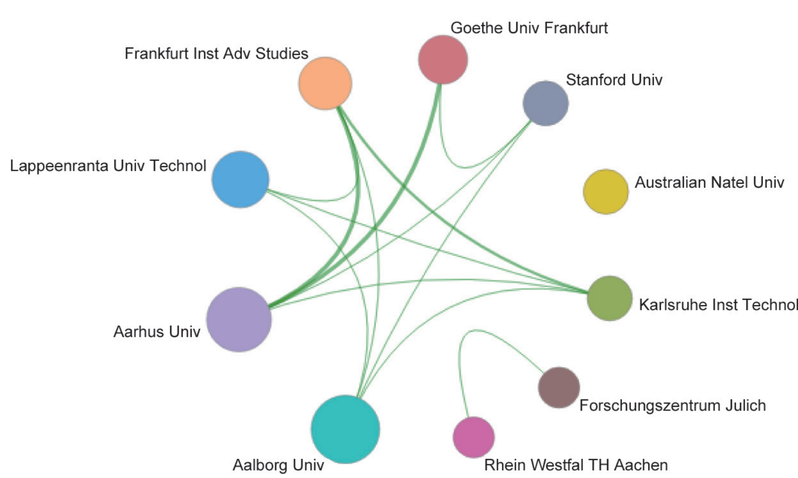

Figure 1.2.2 Collaboration network among major institutions in the engineering research front of "renewable energy systems"

Table 1.2.3 Countries or regions with the greatest output of citing papers on "renewable energy systems"

No.	Country/Region	Citing papers	Percentage of citing papers	Mean year
1	Germany	132	16.92%	2017.0
2	Denmark	121	15.51%	2017.0
3	USA	120	15.38%	2016.3
4	China	77	9.87%	2017.4
5	Finland	65	8.33%	2017.3
6	UK	57	7.31%	2017.0
7	Italy	53	6.79%	2017.4
8	Australia	47	6.03%	2016.9
9	Spain	38	4.87%	2017.1
10	Switzerland	35	4.49%	2017.1

Table 1.2.4 Institutions with the greatest output of citing papers on "renewable energy systems"

No.	Institution	Citing papers	Percentage of citing papers	Mean year
1	Aalborg Univ	52	19.40%	2017.3
2	Lappeenranta Univ Technol	46	17.16%	2017.3
3	Aarhus Univ	39	14.55%	2016.8
4	Stanford Univ	23	8.58%	2015.3
5	Tech Univ Denmark	21	7.84%	2016.4
6	Univ Zagreb	18	6.72%	2016.8
7	Forschungszentrum Julich	16	5.97%	2017.5
8	Univ Sydney	14	5.22%	2016.6
9	Karlsruhe Inst Technol	14	5.22%	2017.4
10	Frankfurt Inst Adv Studies	13	4.85%	2017.1

1.2.2 High-temperature alloy

Super alloy is a metal material developed in the 1930s and was first used in the aviation industry by the UK, Germany, and the USA. After the second world war, owing to the rapid development of the aviation industry and high performance of super alloys, many countries developed new high-temperature alloys. In addition to the wide use of high-temperature components, super alloys have been applied in thermal and nuclear power generation, metallurgy, and glass manufacturing, as well as in ship and chemical industries.

The composition of super alloy is complex, containing active elements such as chromium and aluminum, and is unstable under oxidation or hot corrosion environments. Additionally, the surface defects of the machined parts, caused by work hardening and residual stress, have a negative impact on its chemical performance and mechanical properties. Because of high alloying, super alloy materials are prone to the segregation of components, which has a significant impact on the micro-structure and properties of the cast super alloys and deformed super alloys. With different characteristics from those of ordinary metal materials, the preparation of super alloys includes the casting of high-temperature alloy (conventionally cast super alloy, directional solidification columnar super alloy, and single crystal super alloy), deformed super alloy, and powder super alloy.

With advances in alloy theory and production process, the performances of super alloys have been enhanced through alloy strengthening and process improvement. Alloy strengthening includes alloy solid solution strengthening and grain boundary strengthening with a second phase hardening agent. Process strengthening includes improvement in smelting, solidification, crystallization, thermal processing, heat treatment, and surface treatment to improve the microstructure. The preparation technology and process for super alloy materials are still undergoing improvement and innovation, for example, the adoption of the triple-melt process of vacuum induction melting, electroslag remelting, and vacuum arc remelting (VIM-ESR-VAR), improvement of high-temperature strength by using the directionally solidified alloy and single crystal alloy, and utilization of powder metallurgy to reduce the segregation of alloying elements and increase the material strength. In addition, the oxide dispersion-strengthened super alloys and high-temperature inter-metallic materials are also under development.

The countries/regions and institutions with the greatest output of core papers in the field of "high-temperature alloy" since 2013 are listed in Tables 1.2.5 and 1.2.6, respectively. The collaboration networks among major countries/regions and institutions are shown in Figures 1.2.3 and 1.2.4. The countries/regions and institutions with the greatest number of citing papers are included in Tables 1.2.7 and 1.2.8.

The majority of the core papers are published by the top four countries, China, the USA, Germany, and the UK. Among these, the Chinese output of the core papers accounts for 40.2% of the total, whereas the number of core papers from the USA accounts for 20.6%, and those from Germany and the UK both exceed 10%. The top four countries of average citation are Sweden, Japan, China, and the UK (Table 1.2.5). The USA and

Table 1.2.5 Countries or regions with the greatest output of core papers on "high-temperature alloy"

No.	Country/Region	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	China	201	40.20%	7174	43.21%	35.69
2	USA	103	20.60%	3269	19.69%	31.74
3	Germany	62	12.40%	1955	11.78%	31.53
4	UK	53	10.60%	1824	10.99%	34.42
5	India	30	6.00%	875	5.27%	29.17
6	France	28	5.60%	725	4.37%	25.89
7	Canada	27	5.40%	881	5.31%	32.63
8	South Korea	16	3.20%	457	2.75%	28.56
9	Sweden	14	2.80%	628	3.78%	44.86
10	Japan	13	2.60%	480	2.89%	36.92

Table 1.2.6 Institutions with the greatest output of core papers on "high-temperature alloy"

No.	Institution	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	Chinese Acad Sci	39	7.80%	984	5.93%	25.23
2	Cent S Univ	33	6.60%	1862	11.22%	56.42
3	Northwestern Polytech Univ	28	5.60%	912	5.49%	32.57
4	State Key Lab High Performance Complex Mfg	28	5.60%	1701	10.25%	60.75
5	Univ Erlangen Nurnberg	20	4.00%	641	3.86%	32.05
6	Univ Birmingham	14	2.80%	602	3.63%	43.00
7	Harbin Inst Technol	14	2.80%	521	3.14%	37.21
8	Ruhr Univ Bochum	13	2.60%	376	2.26%	28.92
9	Univ Oxford	13	2.60%	384	2.31%	29.54
10	Max Planck Inst Eisenforsch GmbH	12	2.40%	362	2.18%	30.17

Figure 1.2.3 Collaboration network among major countries or regions in the engineering research front of "high-temperature alloy"

Germany have the highest level of collaboration, followed by China, France, and Canada. This shows that these countries focus more on collaboration in this field (Figure 1.2.3). The institutions that account for the highest output of the core papers in this area are the Chinese Academy of Sciences, Central South University, and Northwestern Polytechnical University (Table 1.2.6).

The percentages of citing papers from China and the USA are 46.93% and 16.54%, respectively. According to the data analysis, the highest number of core papers are cited by Chinese institutions, which indicates that the Chinese scholars are at the forefront of this research area (Table 1.2.7). The institution that accounts for the highest output of the citing papers is the Chinese Academy of Sciences, followed by Northwestern Polytechnical University and Beijing University of Science and Technology (Table 1.2.8).

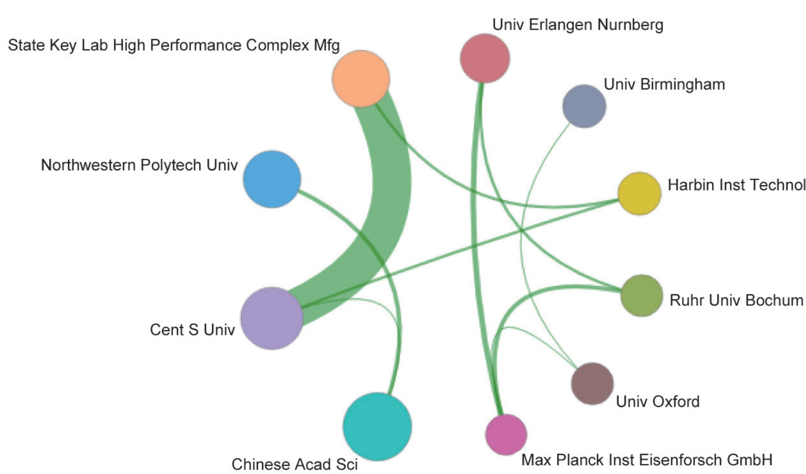

Figure 1.2.4 Collaboration network among major institutions in the engineering research front of "high-temperature alloy"

Table 1.2.7 Countries or regions with the greatest output of citing papers on "high-temperature alloy"

No.	Country/Region	Citing papers	Percentage of citing papers	Mean year
1	China	4652	46.93%	2017.1
2	USA	1639	16.54%	2017.0
3	India	623	6.29%	2017.3
4	Germany	583	5.88%	2017.0
5	UK	555	5.60%	2017.0
6	South Korea	369	3.72%	2017.0
7	France	345	3.48%	2016.9
8	Japan	334	3.37%	2017.0
9	Iran	307	3.10%	2017.1

The output of core papers and citing papers in China and the USA are among the highest in the world, and the number of core papers cited by the Chinese institutions is high.

1.2.3 Material life cycle engineering

Faced with the increasing resource scarcity and environmental pollution, sustainable development through the harmonization of materials, resources, and environment has become a global consensus. MLCE is considered to be important for alleviating these issues. Therefore, the life cycle engineering research has attracted significant attention and has been extensively developed since the beginning of the 21st century. MLCE requires material design during the entire life cycle process. Systematic optimization of the complete industrial chain can be achieved through the quantitative analysis of the material performance, resource consumption, and environmental performance. Furthermore, the environmental impact of the material products during the complete life cycle can be effectively reduced by continuous technological innovation and optimization of process parameters during the manufacturing, management, and recycling processes. Currently, the research on MLCE mainly includes the material ecological design theory and methods, material life cycle evaluation theory and methods, development of assessment database of the material environmental impact and analysis software, and recycling technology in MLCE.

Table 1.2.8 Institutions with the greatest output of citing papers on “high-temperature alloy”

No.	Institution	Citing papers	Percentage of citing papers	Mean year
1	Chinese Acad Sci	591	20.61%	2017.0
2	Northwestern Polytech Univ	418	14.58%	2017.1
3	Univ Sci & Technol Beijing	307	10.71%	2017.0
4	Cent S Univ	273	9.52%	2017.1
5	Harbin Inst Technol	263	9.17%	2017.1
6	Tsinghua Univ	205	7.15%	2016.8
7	Beihang Univ	202	7.05%	2017.0
8	Shanghai Jiao Tong Univ	171	5.96%	2017.0
9	Oak Ridge Natl Lab	148	5.16%	2017.1
10	Northeastern Univ	147	5.13%	2017.4

Table 1.2.9 Countries or regions with the greatest output of core papers on “material life cycle engineering”

No.	Country/Region	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	USA	46	19.17%	2923	15.63%	63.54
2	Italy	29	12.08%	2002	10.70%	69.03
3	UK	28	11.67%	3683	19.69%	131.54
4	China	22	9.17%	1623	8.68%	73.77
5	Spain	21	8.75%	1401	7.49%	66.71
6	Netherlands	12	5.00%	1478	7.90%	123.17
7	Switzerland	12	5.00%	539	2.88%	44.92
8	Belgium	11	4.58%	1415	7.57%	128.64
9	Germany	11	4.58%	1343	7.18%	122.09
10	Portugal	11	4.58%	861	4.60%	78.27

The main countries/regions and institutions with maximum number of core papers in MLCE research during the period between 2013 and 2018 are listed in Tables 1.2.9 and 1.2.10, respectively. As shown in Table 1.2.9, the USA and Italy are the two countries with the maximum output of core papers, accounting for 19.17% and 12.08% of the total output, followed by the UK with 11.67%. Among the institutions, the Technical University of Denmark has the highest percentage (3.33%) of published core papers as shown in Table 1.2.10. Figure 1.2.5 shows the collaboration network among the countries or regions with maximum output in this research field. China and the USA collaborate most frequently. The collaborations between the Chinese Academy of Sciences and the University of Nottingham as well as that between University Catania and Politecnico di Milano are relatively less frequent (Figure 1.2.6). China and the USA are ranked first and second among various countries for citing core papers, accounting for 30.08% and 16.81%, respectively, as shown in Table 1.2.11. According to Table 1.2.12, the top three institutions with maximum output of citing papers are the Chinese Academy of Sciences, Tsinghua University, and University of Chinese Academy of Sciences, with the corresponding percentages of citing papers of 26.32%, 12.42%, and 9.87%, respectively.

Table 1.2.10 Institutions with the greatest output of core papers on “material life cycle engineering”

No.	Institution	Core papers	Percentage of core papers	Citations	Percentage of citations	Citations per paper
1	Tech Univ Denmark	8	3.33%	512	2.74%	64.00
2	Univ Lleida	5	2.08%	516	2.76%	103.20
3	Univ Perugia	5	2.08%	368	1.97%	73.60
4	Univ Catania	5	2.08%	197	1.05%	39.40
5	Univ Nottingham	5	2.08%	195	1.04%	39.00
6	Delft Univ Technol	4	1.67%	1033	5.52%	258.25
7	Univ Coimbra	4	1.67%	492	2.63%	123.00
8	Chinese Acad Sci	4	1.67%	172	0.92%	43.00
9	Politecn Milan	4	1.67%	150	0.80%	37.50
10	Univ Pittsburgh	3	1.25%	208	1.11%	69.33

Figure 1.2.5 Collaboration network among major countries or regions in the engineering research front of “material life cycle engineering”

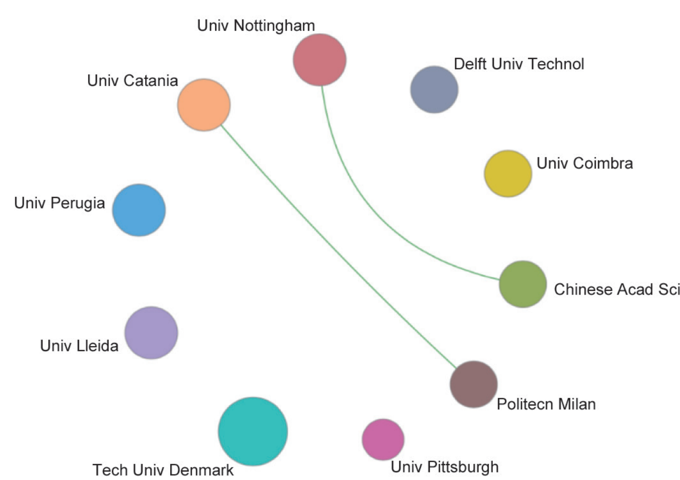

Figure 1.2.6 Collaboration network among major institutions in the engineering research front of “material life cycle engineering”

Table 1.2.11 Countries or regions with the greatest output of citing papers on "material life cycle engineering"

No.	Country/Region	Citing papers	Percentage of citing papers	Mean year
1	China	3864	30.08%	2017.5
2	USA	2160	16.81%	2017.2
3	Italy	1052	8.19%	2017.2
4	UK	1004	7.82%	2017.3
5	Spain	919	7.15%	2017.3
6	Germany	852	6.63%	2017.3
7	France	677	5.27%	2017.2
8	India	631	4.91%	2017.5
9	Australia	624	4.86%	2017.5
10	South Korea	582	4.53%	2017.6

Table 1.2.12 Institutions with the greatest output of citing papers on "material life cycle engineering"

No.	Institution	Citing papers	Percentage of citing papers	Mean year
1	Chinese Acad Sci	464	26.32%	2017.5
2	Tsinghua Univ	219	12.42%	2017.3
3	Univ Chinese Acad Sci	174	9.87%	2017.6
4	Tech Univ Denmark	133	7.54%	2016.9
5	Katholieke Univ Leuven	129	7.32%	2016.9
6	Hong Kong Polytech Univ	127	7.20%	2017.6
7	Natl Univ Singapore	117	6.64%	2017.1
8	Zhejiang Univ	109	6.18%	2017.6
9	Shanghai Jiao Tong Univ	100	5.67%	2017.6
10	Univ Sci & Technol China	97	5.50%	2017.7

2 Engineering development fronts

2.1 Trends in top 12 engineering development fronts

The top 12 engineering development fronts assessed by the Field Group of Chemical, Metallurgical, and Materials Engineering are shown in Table 2.1.1. Among them, "combination of AI with chemical engineering," "biomass substitution of polymer materials," "development of microreaction system," "wearable flexible electronic devices," "biorefinery for chemical products from biomass renewable resources," "key fabrication technology for advanced structural and functional integrated ceramic materials for major national defense demands," and "intelligent bionic self-healing coating technology" are based on the published patents provided by *Clarivate Analytics*. The other five are recommended by the experts. The annual numbers of patents published from 2013 to 2018 are listed in Table 2.1.2.

"Combination of AI with chemical engineering," "targeting the function design of materials with the assistance of computer simulation technology" (Table 2.1.1), and "catalyst design by AI" (Table 1.1.1) are in development for accurate production operations, efficient and smart manufacturing processes, and system-optimized design.

(1) Combination of AI with chemical engineering

With the increasing scarcity of resources and energy supplements, the requirement for the safe and environmentally friendly chemical engineering processes and the design, production, and control of the conventional chemical

Table 2.1.1 Top 12 engineering development fronts in chemical, metallurgical, and materials engineering

No.	Engineering development front	Published patents	Citations	Citations per patent	Mean year
1	Combination of AI with chemical engineering	506	1 326	2.62	2015.9
2	Biomass substitution of polymer materials	859	3 331	3.88	2014.5
3	Military refractory metal material	491	2 398	4.88	2014.3
4	Development of microreaction system	442	3 660	8.28	2014.3
5	Wearable flexible electronic devices	696	4 374	6.28	2014.9
6	Coal conversion to chemicals	669	4 655	6.96	2014.1
7	Targeting the function design of materials with the assistance of computer simulation technology	664	7 642	11.51	2014.9
8	Performance and response behavior detection and characterization technology under extremely harsh in-service environments	325	4 091	12.59	2012.7
9	Biorefinery for chemical products from biomass renewable resources	368	1 341	3.64	2014.5
10	Key fabrication technology for advanced structural and functional integrated ceramic materials for major national defense demands	1016	3 793	3.73	2014.4
11	Intelligent bionic self-healing coating technology	474	1 437	3.03	2015.7
12	Polymer materials with excellent biodegradability and multiple recyclability	947	10 767	11.37	2013.7

Table 2.1.2 Annual number of core patents published for the top 12 engineering development fronts in chemical, metallurgical, and materials engineering

No.	Engineering development front	2013	2014	2015	2016	2017	2018
1	Combination of AI with chemical engineering	60	79	64	93	93	117
2	Biomass substitution of polymer materials	223	210	226	138	60	2
3	Military refractory metal material	71	67	45	63	66	79
4	Development of microreaction system	146	133	85	58	17	3
5	Wearable flexible electronic devices	148	138	157	126	102	25
6	Coal conversion to chemicals	229	210	151	73	6	0
7	Targeting the function design of materials with the assistance of computer simulation technology	108	191	144	117	82	22
8	Performance and response behavior detection and characterization technology under extremely harsh in-service environments	41	32	24	23	27	39
9	Biorefinery for chemical products from biomass renewable resources	101	98	95	51	19	4
10	Key fabrication technology for advanced structural and functional integrated ceramic materials for major national defense demands	309	287	220	155	41	4
11	Intelligent bionic self-healing coating technology	75	70	66	80	91	92
12	Polymer materials with excellent biodegradability and multiple recyclability	114	135	104	110	124	107

engineering processes cannot be fully satisfied by the modern industry. Recently, the "AI + chemical engineering" approach has shown promising implications in the revolution of production, management, and marketing of the chemical industry, which can enhance the core innovation and competitiveness. The application of AI in chemical engineering in recent years can be divided into two aspects: the abstraction of the problems and the development of specific techniques in chemical engineering processes. Currently, the combination of AI with chemical engineering has already been applied in the following fields: 1) catalysts design, 2) equipment detection and fault diagnosis, 3) digital twin, 4) optimization of the controlling and warning processes, and 5) management of resources and energy.

(2) Biomass substitution of polymer materials

Polymer materials such as plastics, rubber, and fibers have extensive applications. The pace of development and application range of the polymer materials have exceeded those of the traditional metal and inorganic materials, and these have become an indispensable in industry, agriculture, national defense, science and technology, and daily life. However, most of the polymer materials are currently derived from the non-renewable petrochemical resources (oil, coal, and natural gas) and their sustainable development is challenging. The development of new polymer materials in accordance with the sustainable development goals is a common concern of researchers and industry worldwide.

The biomass substitution of polymer materials involves the use of renewable resources such as natural plants and animals as synthetic raw materials to replace the original petroleum-based raw materials. Currently, the main research will focus on the following aspects. 1) A new type of green polymerization reaction system suitable for industrial scale production will be developed from low-cost biobased monomers, which can be used to synthesize biobased polymer materials with controllable structures and excellent performances. 2) Various types of polyhydroxyalkanes will be synthesized by fermentation with microorganisms from various carbon sources. 3) Biobased polymer materials will be prepared by chemical or physical modification directly using starch, cellulose, chitin, and various agricultural and forestry wastes as raw materials. In future, the cost reduction and improvement of the comprehensive performances of biobased polymer materials will be the key issues to be addressed for their large-scale industrial applications.

(3) Military refractory metal material

Military refractory metal materials such as W, Mo, Ta, and Nb have melting points higher than 2000 °C. Owing to their high melting point, low thermal expansion coefficient, low vapor pressure, excellent corrosion resistance against liquid metals, and high-temperature strength, the refractory metal materials have been widely applied in aerospace, electrical and electronics, national defense, and nuclear sectors.

With the rapid development of the these high-tech fields, demands for refractory metal materials with high performances are increasing. A significant amount of research has been carried out on the methods for strengthening and toughening of refractory metal materials together with high performance. Because of the highest melting point of 3420 °C and small thermal neutron capture cross section, W and its alloys were selected as the most promising candidate materials for first wall and divertor of International Thermonuclear Experimental Reactor (ITER). However, limitations including low-temperature brittleness and high-temperature oxidation have hindered the engineering applications of W. Therefore, the strengthening and toughening of refractory metal materials in combination with their high performance in extreme servicing environment is a critical research issue to be resolved. In addition, the combination of powder preparation of refractory metal materials and additive manufacturing is another research field with significant potential. Refractory metal products with complex shapes for applications in extreme servicing environments can be fabricated using 3D printing technology, which has considerable advantages compared to the traditional powder metallurgy. Moreover, these 3D refractory metal products with high performances can satisfy the strategic demands in manufacturing, aerospace, and national defense sectors.

(4) Development of microreaction system

Microchemical engineering and technology is a new discipline and frontier in the field of chemical engineering. It focuses on the study of the behaviors and principles of the chemical engineering process with characteristic scales in the microscale range (within submillimeter scale).

Owing to the small channel characteristic scale, low reactant holdings, and modular structure of the microreactor system, it possesses excellent heat and mass transfer performance, good safety, easy control, and direct amplification (numbering-up) of the process, which can significantly improve the safety and production efficiency of the rapid and highly exothermic reaction process, and accelerate the practical applications of the laboratory results. This system has broad application prospects in fine chemicals such as medicine, pesticides, and energetic materials, as well as in the fields of polymers, petrochemicals, biochemicals, medical detection, and synthesis of micro and nanomaterials. The optimization design of the microreaction process and the development of engineering system equipment are urgently needed including the optimization design of microreactor structure, development of reaction process, process intelligent control, system integration, and manufacture of microreaction equipment. This involves the transfer process mechanism, transfer–reaction coupling mechanism, optimization of microstructural components, process safety control strategy, parallel scaling-up law, and system integration and optimization.

It is important to upgrade the traditional chemical industry and improve the chemical process safety and environmental protection. Microreactor technology can realize chemical process intensification, process safety, energy conservation, and reduction of emission.

(5) Wearable flexible electronic devices

Wearable flexible electronic devices are the electronic devices that are in direct or indirect contact with the skin and are mechanically flexible. To adapt to different working environments and human body requirements for device deformation, flexible wearable electronic devices often require good mechanical flexibility, but high technical difficulty limits the development of wearable flexible electronic devices. First, the wearable flexible electronic devices require good stretchability and flexibility without damaging the electronic properties, which puts higher demands on the circuit materials. Second, the preparation conditions and performances of the flexible electronics currently show a gap from the traditional electronics. The applications of flexible wearable electronics are observed in all aspects of human life. The research in this area mainly focuses on electronic skin, wearable physiological monitoring and treatment devices, flexible conductive fabrics, thin film transistors, and flexible gate circuits with transparent film.

(6) Coal conversion to chemicals

In terms of the petroleum resources, crude oil refining and petrochemical industry are very important for the rapid development of the national economy. With increasing dependence on foreign oil resources, the energy security can be severely challenged. Based on China’s natural endowment of energy resources, the clean and efficient utilization of coal resources is important for solving environmental problems and supporting high-quality and rapid economic and social development. In the modern coal/chemical industry, significant breakthroughs have been made in the commercialization of technologies such as coal-to-olefins, coal-to-ethylene glycol, and coal-to-liquifaction oil. These successful developments have opened the pathway for producing chemicals and clean fuels from coal with syngas/methanol as intermediates. Further developments include the utilization of innovative technologies to extend the applications of coal-based chemical processes, eliminate the technical bottlenecks of coal-based olefins, coal-based aromatics, and coal-based oxygenates, and improve economical efficiency of the process. The coupled and coordinated development of coal-to-chemical conversion with petrochemicals, power generation, and biomass conversion will be significant in the further enhancement of the efficiency of resource/energy utilization and will be useful for the sustainable development of the chemical industry.

(7) Targeting the function design of materials with the assistance of computer simulation technology

The traditional materials research and development involves repeated trial and error processes that not only waste significant manpower and material resources, but are also time-consuming due to the long research and development cycle. Computer molecular simulation technology can provide a qualitative prediction and simulate the quantitative results of some structures and properties of molecular systems. With the help of computer technology and theoretical calculation methods, the approach toward materials research has gradually changed from the traditional “experience-guided experiment” to “theoretical prediction and experimental verification.” In particular, high-throughput computational screening techniques developed for a large number of samples can significantly accelerate the discovery of excellent materials. In the research and development process of new materials, high-throughput screening, big data, and high-performance computer development have afforded the possibility of designing materials with "targeted" function.

(8) Performance and response behavior detection and characterization technology under extremely harsh in-service environments

Advanced structural ceramic materials are commonly used at high temperatures, where the in-service environments are extremely harsh. To accurately reflect the practical response of the structural ceramic materials under these harsh environments, the adopted simulation method must appropriately reflect the actual in-service environment. However, the existing relevant simulating environments are generally different from the actual conditions. Hence, the simulation method and technologies need to be further improved. According to the basic properties of the advanced structural materials and the in-service response and testing in harsh conditions, it is necessary to improve the performance testing and evaluation of the components and structural parts. Promotion of the research and development processes, industrialization of major products, and provision of uniform testing standards and specifications are the important developmental trends that can facilitate the wide application of advanced structural ceramic materials.

(9) Biorefinery for chemical products from biomass renewable resources

Biorefinery is an emerging industrial model for the production of energy and chemicals from the biomass renewable resources. It is a process integration for the sustainable conversion of biomass into energy, chemicals, and materials, involving food, feed, paper, and textiles in many important industrial fields. Biorefineries can allow deep processing and recycling of renewable biomass resources. In theory, most traditional petrochemicals can be obtained from the biorefinery processes. Additionally, owing to the recyclability of the raw materials and combination with many biological processes, the biorefineries can significantly reduce the energy consumption and air and water pollution in industrial processes, and support the current green development trend. Therefore, the biorefineries for materials and chemicals have a wide scope for development.

(10) Key fabrication technology for advanced structural and functional integrated ceramic materials for major national defense demands

Due to the rapid development of the high-tech aerospace industry, there is an urgent need for advanced ceramic materials that combine specific structural and functional characteristics. However, because of limitations such as difficulty in molding and machining and low fracture toughness, the development of the processing technology is important for applications in high-tech aerospace industry. Currently, the national defense sector urgently requires high-performance advanced ceramic materials with complex shapes. In this context, the low-cost green manufacturing techniques for the near net sizes and complex shapes should be developed. To improve the preparation techniques for multi-functional ceramic fiber composite films, high-strength porous ceramics resistant to high-temperature corrosion, and ceramic substrates with high thermal conductivity, the reliable evaluation criteria and lifetime prediction model must be established. With the aim of industrial development and international cooperation, it can effectively promote the research and development of advanced ceramic materials and provide support for the national key projects and strategic new industries.

(11) Intelligent bionic self-healing coating technology

Intelligent bionic self-healing coating technology refers to the use of self-healing capabilities derived from medicine and biology in the field of materials science, which means that the coating can be automatically repaired after the generation of cracks. There are many methods to develop self-healing coatings such as the introduction of microcapsules into a polymer matrix to form a healing agent and an initiator. When cracks are generated under an external force, the embedded microcapsules are torn and the polymerization is initiated, followed by re-bonding and repairing of the crack. A hybrid organic–inorganic nanocomposition can also be assembled as a cell wall to form a microtube, and the coating can be spontaneously repaired and healed after damage. The current research focuses on polyethylene terephthalate coatings, automotive paint finishes, mobile phone back cover coatings, and some rubber materials.

(12) Polymer materials with excellent biodegradability and multiple recyclability

Polymers are widely applied materials and are irreplaceable in almost all national economic fields. Most of the polymers are chemically stable and nondegradable, which are processed mainly by incineration or land filling after abandonment, and only very few of them are recycled. Moreover, the properties of the recycled commercial polymers, which are typically obtained by physical reprocessing, inevitably deteriorate and therefore, multiple recycling of polymers cannot be performed. With increasing interdependence between the human society and polymers, the proliferation of polymer waste results in serious global problems such as environmental pollution and wastage of resources. For example, the white pollution, marine microplastic, and oil crises, which are directly related to the polymer applications, have become one of major hindrances to sustainable development of human society.

In view of these urgent challenges, the development of a new generation of polymer materials with comparable performances to those of commercial polymers, excellent biodegradability after abandonment, and multiple recyclability has attracted considerable attention from scientists and engineers. Under suitable recycling conditions, these novel polymers can be effectively pyrolyzed into monomers for further polymerization, resulting in highly efficient multiple recycling. For polymers that are unsuitable for recycling, these can be biodegraded into small molecules that are harmless to the environment, i.e. water and carbon dioxide. Therefore, this approach provides a novel, comprehensive, and effective solution for the global problems arising from the components derived from polymer applications.

2.2 Interpretations for three key engineering development fronts

2.2.1 Combination of AI with chemical engineering

Limitation of resources and energy supplements have necessitated the requirement of safe and environmentally friendly chemical engineering processes, and the design, production, and control of the conventional chemical engineering processes cannot be satisfied by the modern industry. Recently, the successful applications of AI in the fields of man–machine game and machine vision have opened a new pathway for updating the chemical engineering processes. The “AI + chemical engineering” approach is showing promising results in the production, management, and marketing of the chemical industry, which can enhance the innovation and competitiveness in these fields.

The applications of AI in chemical engineering in recent years can be divided into two aspects: the abstraction of the problems and the development of specific techniques in chemical engineering processes. The abstraction of the problems in chemical engineering is mainly focused on the generation of problems from traditional chemical processes by classical AI methods followed by the development of their solutions with well-established AI techniques. The development of specific techniques in chemical engineering processes is mainly focused on the expansion of the classical AI techniques by adding special elements from chemical engineering processes, followed by development of specific intelligent algorithms and software that satisfy the chemical processes.

These two aspects should be studied in depth for the application of AI in not only the basic research and development, but also in applied research of chemical engineering. The combination of AI with chemical engineering has been applied in the following fields.

(1) Catalyst design. The design of chemical catalysts requires large amount of experimental data and professional knowledge. Their combinations and correlations can be rapidly determined by the application of AI. As a result, the research and development cycle of the catalysts and small molecules can be shortened. By the prediction of the active binding sites of the small molecules, the synthetic route and reverse molecular design can help in improving the efficiency of catalyst design. (2) Equipment detection and fault diagnosis. Based on the big data processing and knowledge inference, AI algorithm models have been applied to the signals of vibrations, sound, images, and electricity of the operational chemical equipment, for online monitoring of the processes and predictions of the faults and errors. (3) Digital twin. By combining the big data in industry and applying the AI techniques to the mechanisms, the models for characterizing the operational state of the chemical engineering processes can be developed, the parallel of manufacturing can be realized in a visualized manner, and management and optimization of the chemical processes can be achieved. (4) Optimization of the controlling and warning processes. Big data and AI techniques show promising prospects in multi-objective collaborative optimization and control. The safety,

stability, and effectiveness in complex chemical processes can be improved by controlling and warning processes. (5) Management of resources and energy. Developing man-machine cooperation and knowledge-driven decision system for intelligent production plan, based on the industrial internet, big data, and knowledge-based work automation, can allow the optimization of a production plan that fuses the demand-driven and device operation characteristics. Then, the resources and energy demand in chemical engineering processes can be optimized.

The countries/regions with the highest output of core patents on the "combination of AI with chemical engineering" are mainly from the USA and China, followed by Japan and South Korea; some European countries, Germany, Sweden, Switzerland, and France, have also contributed significantly (Table 2.2.1). The USA and Germany have close collaboration in this front (Figure 2.2.1), but there is no collaboration from the institutions with the highest output of core patents (Table 2.2.2 and Figure 2.2.2); most of these are American institutions.

2.2.2 Biomass substitution of polymer materials

Environmental pollution, resource wastage, and strong dependence on the petrochemical resources caused by

Table 2.2.1 Countries or regions with the greatest output of core patents on "combination of AI with chemical engineering"

No.	Country/Region	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	USA	165	32.61%	640	48.27%	3.88
2	China	131	25.89%	235	17.72%	1.79
3	Japan	64	12.65%	79	5.96%	1.23
4	South Korea	45	8.89%	22	1.66%	0.49
5	Germany	22	4.35%	15	1.13%	0.68
6	Sweden	14	2.77%	47	3.54%	3.36
7	Taiwan of China	14	2.77%	15	1.13%	1.07
8	Switzerland	12	2.37%	24	1.81%	2.00
9	France	9	1.78%	8	0.60%	0.89
10	Israel	8	1.58%	26	1.96%	3.25

Table 2.2.2 Institutions with the greatest output of core patents on "combination of AI with chemical engineering"

No.	Institution	Country	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	KLAT	USA	12	2.37%	44	3.32%	3.67
2	GENE	USA	10	1.98%	37	2.79%	3.70
3	SKFK	Sweden	9	1.78%	37	2.79%	4.11
4	BOEI	USA	8	1.58%	25	1.89%	3.13
5	FICO	USA	7	1.38%	23	1.73%	3.29
6	DANH	USA	6	1.19%	52	3.92%	8.67
7	ASHF	UK	6	1.19%	19	1.43%	3.17
8	HONE	USA	5	0.99%	32	2.41%	6.40
9	UNAC	USA	5	0.99%	22	1.66%	4.40
10	SIEI	Germany	5	0.99%	4	0.30%	0.80

KLAT: KLA-Tencor Corp.; GENE: General Electric Co.; SKFK: SKF AB; BOEI: Boeing Co.; FICO: Fisher Controls International, Co., Ltd.; DANH: HACH Co.; ASHF: Ashford Tech Software Inc.; HONE: Honeywell Int. Inc.; UNAC: United Technologies Corp.; SIEI: Siemens AG.

Figure 2.2.1 Collaboration network among major countries or regions in the engineering development front of “combination of AI with chemical engineering”

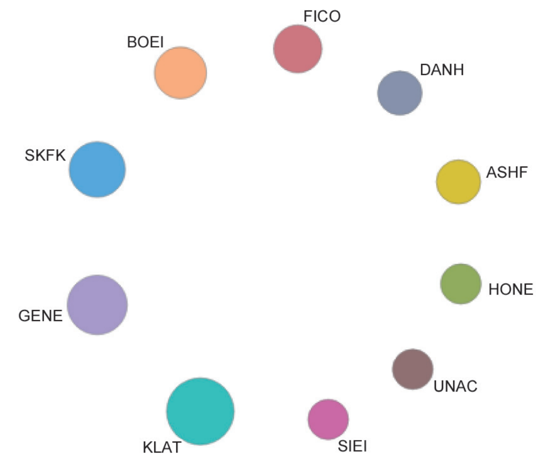

Figure 2.2.2 Collaboration network among major institutions in the engineering development front of “combination of AI with chemical engineering”

the extensive use of polymer materials have attracted the attention of researchers and industries worldwide since the 21st century. Using the renewable biomass derived from nature to prepare biobased polymer materials can not only effectively resolve the issues of resource and energy security, but also alleviate the environmental and climate problems caused by the rapid increase of carbon emissions. The key challenges in the biomass substitution of polymer materials are large-scale preparation of monomers from the biomass sources, polymerization with high efficiency, improvement of the properties of biobased polymers, and reduction in the cost of biosynthetic polymer materials. Currently, the industrial products from biobased polymer materials including polylactic acid and polyhydroxyalkanoate are available, but some limitations such as low yields, high cost, and properties that are not comparable to the petroleum-based polymers are observed. Therefore, the research and development of biobased polymer materials with high cost–performance ratio or performance reaching or exceeding those of some petroleum-based products are the important directions of development for the biobased polymers in future.

The major countries/regions and institutions with greatest core patents in biomass substitution of polymer materials since 2013 are listed in Tables 2.2.3 and 2.2.4, respectively. The collaboration networks between the major countries/regions and institutions are shown in Figures 2.2.3 and 2.2.4, respectively. The research in biobased polymer materials mainly focuses on the preparation of polymers from biomass monomers or biofermentation and the preparation of biobased polymer materials by chemical and physical modifications using starch, cellulose, chitin, and various agricultural and forestry wastes as raw materials. The top three countries with maximum core patents are China, the USA, and Japan. The percentages of core patents and citations from China are 68.34% and 59.95%, respectively, whereas those from the USA are 10.24% and 19.63%, respectively, and Japan are 10.24% and 9.07%, respectively. The USA has the most extensive collaboration with other countries including Japan, the UK, the Netherlands, and Germany. In addition, Germany collaborates with Switzerland, Japan, and the USA, but China, Austria, and France do not collaborate with other countries. The China Petrolum and Chemical Corporation, Dow Global Technologies LLC, BASF SE, Changchun Institute of Applied Chemistry of Chinese Academy of Sciences, Toray Industries, LG Chem., and other institutions have core patents on biobased polymers, among which the China Petrolum and Chemical Corporation has the greatest number of core patents.

2.2.3 Military refractory metal material

Military refractory metal materials such as W, Mo, Ta, and Nb have melting points higher than 2000 °C. Owing to their high melting points, excellent high-temperature mechanical properties, and unique physical and chemical properties, the refractory metal materials have been widely applied in aerospace, electrical and electronics, national defense,

Table 2.2.3 Countries or regions with the greatest output of core patents on "biomass substitution of polymer materials"

No.	Country/Region	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	China	587	68.34%	1997	59.95%	3.40
2	USA	88	10.24%	654	19.63%	7.43
3	Japan	88	10.24%	302	9.07%	3.43
4	South Korea	40	4.66%	140	4.20%	3.50
5	Germany	22	2.56%	96	2.88%	4.36
6	Switzerland	8	0.93%	34	1.02%	4.25
7	France	7	0.81%	32	0.96%	4.57
8	Netherlands	6	0.70%	41	1.23%	6.83
9	UK	4	0.47%	38	1.14%	9.50
10	Austria	4	0.47%	31	0.93%	7.75

Table 2.2.4 Institutions with the greatest output of core patents on "biomass substitution of polymer materials"

No.	Institution	Country	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	SNPC	China	11	1.28%	48	1.44%	4.36
2	DOWC	USA	9	1.05%	76	2.28%	8.44
3	BADI	Germany	9	1.05%	49	1.47%	5.44
4	CAAC	China	8	0.93%	24	0.72%	3.00
5	TORA	Japan	8	0.93%	13	0.39%	1.63
6	GLDS	South Korea	7	0.81%	78	2.34%	11.14
7	ASAH	Japan	6	0.70%	32	0.96%	5.33
8	SABI	USA	5	0.58%	39	1.17%	7.80
9	CPCH	USA	5	0.58%	31	0.93%	6.20
10	ESSO	USA	5	0.58%	30	0.90%	6.00

SNPC: China Petroleum and Chemical Corporation; DOWC: Dow Global Technologies LLC; BADI: BASF SE; CAAC: Changchun Institute of Applied Chemistry of Chinese Academy of Sciences; TORA: Toray Industries, Inc.; GLDS: LG Chem. Co. Ltd.; ASAH: Asahi Kasei Chem. Co.; SABI: SABIC Global Technologies B.V.; CPCH: Chevron Phillips Chem Co. LP.; ESSO: Exxonmobil Chem Patents Co., Ltd.

and nuclear sectors. The USA, Japan, European countries, and some other countries consider the refractory metals as important strategic materials because of their vital roles in various high-tech fields. With the continuous development of high-tech fields and extreme servicing environments, the demand for refractory metal materials with high performance is rapidly increasing. Extensive research has been performed to strengthen and toughen the refractory metal materials and improve the performance. The strengthening and toughening methods mainly include elemental doping, severe plastic deformation, and dispersion strengthening. The low-temperature brittleness and high-temperature oxidation resistance can be improved by refining the grain size or introducing second nanoscale particles. With the development of 3D printing, the refractory metal products with complex shapes for applications in extreme servicing environments can be fabricated using 3D printing technology, which is a significant advantage in comparison to the traditional powder metallurgy. Moreover, these 3D refractory metal products with high performances can meet the strategic demands in manufacturing, aerospace, and national defense sectors.

Tables 2.2.5 and 2.2.6 include the countries/regions and institutions with the greatest output of core patents in the field

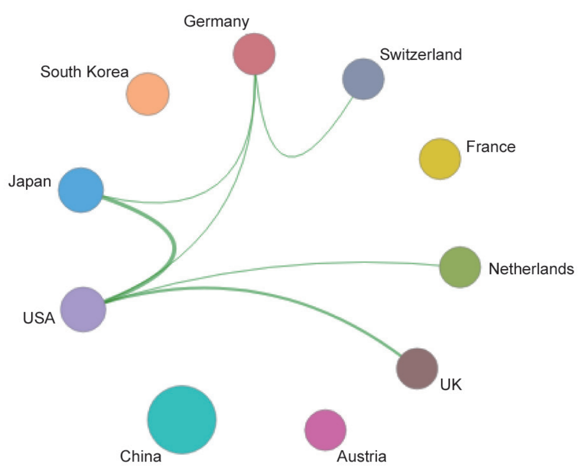

Figure 2.2.3 Collaboration network among major countries or regions in the engineering development front of “biomass substitution of polymer materials”

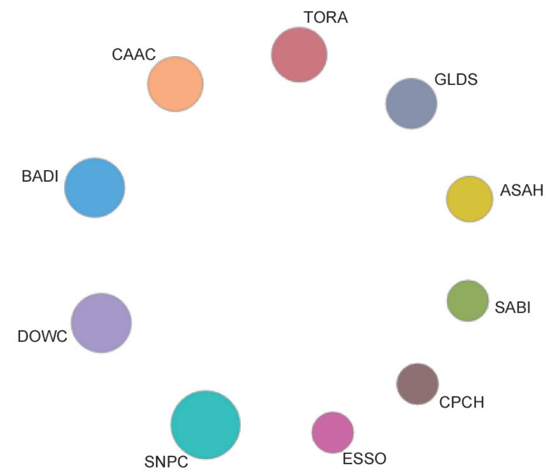

Figure 2.2.4 Collaboration network among major institutions in the engineering development front of “biomass substitution of polymer materials”

Table 2.2.5 Countries or regions with the greatest output of core patents on “military refractory metal material”

No.	Country/Region	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	China	292	59.47%	343	14.30%	1.17
2	Japan	116	23.63%	1309	54.59%	11.28
3	USA	20	4.07%	282	11.76%	14.10
4	South Korea	18	3.67%	10	0.42%	0.56
5	Germany	13	2.65%	230	9.59%	17.69
6	Switzerland	5	1.02%	36	1.50%	7.20
7	France	5	1.02%	24	1.00%	4.80
8	Taiwan of China	4	0.81%	1	0.04%	0.25
9	Sweden	3	0.61%	118	4.92%	39.33
10	Brazil	3	0.61%	21	0.88%	7.00

of military refractory metal materials. As shown in Table 2.2.5, China and Japan rank first and second among these countries in terms of core patents, and their published core patents account for 59.47% and 23.63%, respectively. Although China has the most published core patents in the field of military refractory metal materials in the world, the average citation of core patents is relatively low, approximately 1.17. The top three institutions for maximum core patents are Nihon Parkerizing Co., Ltd. of Japan, Chongqing Runze Pharm. Co., Ltd. of China, and JX Nippon Mining & Metals Corp. of Japan. Their corresponding percentages of published core patents are 6.31%, 3.05% and 2.85%, respectively (Table 2.2.6).

Figure 2.2.5 shows the collaboration network among major countries or regions with the most core patents in the field of military refractory metal materials. The collaboration between Japan and Germany is the most frequent, followed by the collaboration between the USA and Germany. Figure 2.2.6 shows the collaboration network among major institutions. According to Figure 2.2.6, Chemetall GmbH of Germany and Nippon Paint Co., Ltd. of Japan have the closest collaboration. In addition, the collaboration between Nippon Stell & Sumitomo Metal Corp. of Japan, Henkel AG & Co. KGaA of Germany, and Nihon Parkerizing Co., Ltd. of Japan is relatively frequent.

Table 2.2.6 Institutions with the greatest output of core patents on “military refractory metal material”

No.	Institution	Country	Published patents	Percentage of published patents	Citations	Percentage of citations	Citations per patent
1	HOOL	Japan	31	6.31%	512	21.35%	16.52
2	CQRZ	China	15	3.05%	14	0.58%	0.93
3	NIHA	Japan	14	2.85%	41	1.71%	2.93
4	YAWA	Japan	10	2.04%	127	5.30%	12.70
5	CMTL	Germany	9	1.83%	240	10.01%	26.67
6	NIPA	Japan	9	1.83%	206	8.59%	22.89
7	ANSH	China	8	1.63%	18	0.75%	2.25
8	KUNS	China	6	1.22%	20	0.83%	3.33
9	SHAO	China	5	1.02%	2	0.08%	0.40
10	HENK	Germany	4	0.81%	78	3.25%	19.50

HOOL: Nihon Parkerizing Co., Ltd.; CQRZ: Chongqing Runze Pharm. Co., Ltd.; NIHA: JX Nippon Mining & Metals Corp.; YAWA: Nippon Steel & Sumitomo Metal Corp.; CMTL: Chemetall GmbH; NIPA: Nippon Paint Co., Ltd.; ANSH: Pangang Group Panzhihua Iron & Steel Research Institute Co., Ltd.; KUNS: Kunshan Qiaorui Metal Prod. Co., Ltd.; SHAO: Shaoxing Wancheng Metal Sheet Co., Ltd.; HENK: Henkel AG & Co. KGaA

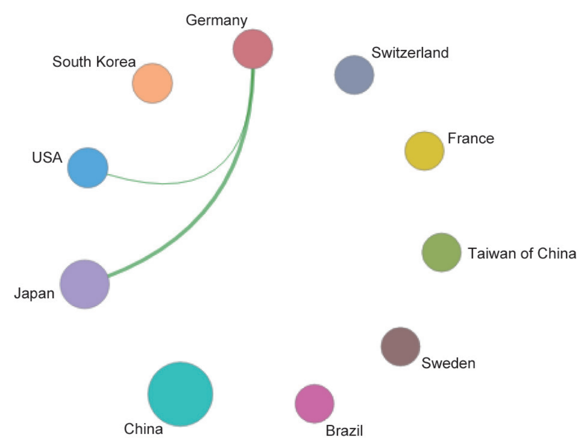

Figure 2.2.5 Collaboration network among major countries or regions in the engineering development front of “military refractory metal material”

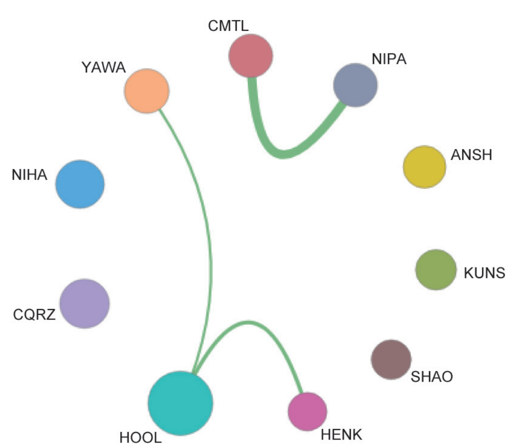

Figure 2.2.6 Collaboration network among major institutions in the engineering development front of “military refractory metal material”

Participants of the Field Group

Leaders

WANG Jingkang, LIU Jiongtian

Deputy Leaders

LI Yanrong, LIU Zhongmin, MAO Xinping, NIE Zuoren, TAN Tianwei, ZHOU Yu, QU Lingbo, YUAN Yingjin

Members of the Working Group

CHEN Biqiang, LIU Xingzhao, XI Xiaoli, YANG Zhihua, YAO Changguo, YE Mao, CAI Di, LI Daxin, WANG Man, WANG Jing, WANG Jingtao, CHENG Luli, GAO Yanjing, HUANG Yaodong, SUN Xiuliang, ZHU Xiaowen

Report Writers

CAI Di, CHEN Guangwen, DING Ya, GUO Xiaojia, HUANG Yaodong, KANG Guodong, LI Daxin, LI Jinzhe, LIU Lin, SHAN Meixia, WANG Dan, WANG Man, WANG Meng, WANG Xiuli, WANG Feng, XU Di, YAO Changguo, ZHU Xiaowen

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Wuhan Branch of Baosteel Central Research Institute

WANG Yuan, GU Haifang, SUN Zhu

Beijing University of Technology

LIU Yu, MA Liwen, WEN Shengping, YANG Jianshen

Beijing University of Chemical Technology

LIU Jingjing, ZHANG Huili, ZHANG Weidong

Dalian Institute of Chemical Physics, Chinese Academy of Sciences

LIU Huifang, MA Huaijun, QI Yu, SUN Jian, WANG Sheng, XIE Feng, ZHAO Zongbao, ZHU Hejun, ZHU Xuefeng

University of Electronic Science and Technology of China

JIANG Shuwen, YAN Jing, YAN Yichao, ZHANG Wanli, ZHU Bin

Harbin Institute of Technology

LI Qian, NIU Bo, QIU Baofu

Sichuan University

CHEN Sichong, WANG Yuzhong

East China University of Science and Technology

QIAN Feng, ZHONG Weimin

Tianjin University

LI Yanni, QIAO Jianjun, YANG Zuguo