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Survey of Challenges in Chemistry and Materials Science Research

1.1 Introduction

Chemistry and materials science constitute a profoundly complex and ancient discipline that has faced entirely distinct challenges across different eras. Without delving into the distant past, let us consider the scenario 20 years ago when the author was engaged in undergraduate research within a chemistry laboratory at the University of Science and Technology of China. A formidable challenge at that time was the complete unpredictability of experimental outcomes, which sometimes left the researchers in the dark about the nature of their work. The standard procedure involved mixing prepared solids and liquids in a hydrothermal autoclave, followed by heating in an oven at 180 °C for approximately 24 hours. Subsequently, the mixture was extracted, separated, washed, and prepared for analysis. This involved observations under various electron microscopes to examine the morphology, along with routine completion of other tests, such as X-ray diffraction (XRD) and spectroscopy. Occasionally, tests for lithium-ion battery performance were also conducted. Perhaps one of the most gratifying experiences at that time was observing the artistic beauty of transmission electron microscopy (TEM) images.

Today, we have grown accustomed to the ubiquity of artificial intelligence, big data, and robotics in our daily lives. Looking back at academic papers from the field of chemistry and materials science twenty years ago, especially those concerning nanomaterials, they appear as collections of data interspersed among images, text, tables, and references. During that era, the publication of, or contribution to, an academic paper was often a source of great joy for many. This retrospective underscores not only the dramatic evolution of technology and methodology within the field but also highlights the fundamental nature of scientific inquiry, which remains constant: a quest for understanding and innovation. The transition from manual experimentation and analysis to the integration of advanced computational tools and methodologies has significantly enhanced the capacity for prediction, analysis, and application in materials science. Yet, the essence of discovery, characterized by moments of joy and frustration, the painstaking gathering of data, and the meticulous interpretation of results, continues to define the discipline. This evolution reflects a broader narrative of progress in science and technology, where the accumulation of knowledge and the development of new

tools mutually reinforce each other, driving the boundaries of what is possible ever forward.

1.2 Energy Form

When we discuss “new energy” today, it is invariably linked to another term, “new materials,” and vice versa. The relationship between materials chemistry and energy is one of mutual promotion and complementarity. The generation, storage, transport, and utilization of energy are all reliant on specific functional materials, while more advanced energy systems have enhanced the precision of our observations of the world, significantly propelling the technological progress of materials science. Concurrently, the continuous accumulation of human scientific and technological knowledge further promotes the emergence and application of new technologies. As described by the “materials big data” projects in recent years, combined with the current “generative” artificial intelligence technologies, we seem to have discovered a new domain for more efficient exploration and discovery from existing data toward incremental innovation. Of course, this is predicated on having sufficient computational power, which is itself a part of energy, underscoring the growing importance of technology in the new energy sector. Thus, we observe that today’s materials science can be viewed as the process where theory or algorithms drive data through energy to achieve incremental innovation, which represents our primary competitive direction. This improved and expanded version positions the interdependence of new energy and new materials within a broader scientific and technological context, emphasizing the role of computational power and artificial intelligence. It sets the stage for a detailed historical analysis, hinting at the evolution of these fields and their impact on contemporary scientific research and technological development. I will proceed to analyze this process from a historical perspective.

1.2.1 Steam Power

In analyzing the trajectory of materials chemistry within the broader context of societal development and energy paradigms, it becomes evident that the evolution of this field is deeply intertwined with the predominant energy sources of its respective eras. The progression from a society reliant primarily on human and animal labor to one powered by steam, and eventually to our current age of electricity and emerging renewable energies, has had profound implications for the advancement of materials chemistry.

During the pre-industrial era, characterized by manual labor, the field of materials chemistry was in its nascent stages. The absence of sophisticated instrumentation and analytical techniques meant that researchers’ understanding of chemical phenomena was limited to observable reactions and processes that could be achieved without the aid of advanced technology. This period’s knowledge base was foundational yet primitive by today’s standards, focusing on the basic properties of materials and their simple transformations.



Figure 1.1 The revolutionary invention of the steam engine marked a monumental leap from manual labor to mechanized production, symbolizing a pivotal moment in human history. The Steam Age stands as a crucial milestone in human history, catalyzing industrialization and modernization, reshaping production methods, social structures, and lifestyles, exerting profound and enduring influence on the world.

The Industrial Revolution marked a pivotal shift, with the invention and widespread adoption of the steam engine catalyzing an unprecedented expansion in industrial capabilities and scientific inquiry. The steam engine, a marvel of engineering and materials science, necessitated the development of materials that could withstand high pressures and temperatures. This requirement spurred significant advancements in metallurgy, exemplified by the Bessemer process, which revolutionized steel production by making it more efficient and cost-effective. The ability to produce stronger, more durable materials was not just a technological achievement but also a cornerstone in the edifice of modern industrial society, enabling the construction of railroads, bridges, and machinery that powered the nineteenth century's economic expansion (Figure 1.1).

Furthermore, the steam era's influence extended into the realm of chemical production and analysis. The coal industry, a key driver of the steam engine, became a vital source of raw materials for the burgeoning chemical industry. Coal tar, a byproduct of coal gasification, was the precursor for an array of chemical dyes, initiating a new era in the textile industry and laying the groundwork for synthetic organic chemistry. The development of analytical chemistry was equally crucial, with innovations such as spectroscopy and chemical thermodynamics emerging in response to the industrial and scientific challenges of the time.

The establishment of dedicated research institutions and the systematic approach to materials chemistry research were also hallmarks of this era. The professionalization of chemistry as a distinct scientific discipline, coupled with the enhanced collaboration between scientists and engineers, led to a more methodical and empirical approach to research. This collaborative ethos was instrumental in bridging the gap between theoretical chemistry and its practical applications, fostering a culture of innovation that would pave the way for the next century's scientific breakthroughs. The steam power era's legacy is its role in promoting the global

spread of chemical knowledge. The advent of steam-powered printing presses made scientific literature more accessible, while improved transportation facilitated the exchange of ideas and materials between researchers across the globe. This era laid the foundational principles of materials chemistry as we understand it today, setting the stage for the subsequent development of polymers, composites, and nanomaterials that are essential to modern technology.

As steam technology advanced, scientists gained a deeper understanding of thermodynamics, marking a period of significant progress in the field. This era was also characterized by burgeoning theoretical research in reaction kinetics, reflecting an increasing sophistication in the comprehension of the forces and principles governing chemical reactions. Concurrently, the chemical engineering industry experienced sustained growth, driven by these scientific advancements and the demand for industrial applications of chemical processes. In parallel, the field of reaction kinetics emerged, focusing on the rates at which chemical reactions occur and the factors influencing these rates. This area of study is vital for understanding how reactions can be optimized for industrial processes, including those used in the chemical engineering industry. Theories related to reaction kinetics, such as the Arrhenius equation (Arrhenius 1889), which describes how reaction rates increase with temperature, became instrumental in the design and improvement of chemical reactors and processes.

The expansion of the chemical engineering industry during this time can be attributed to the integration of these scientific insights into practical applications. Chemical engineers leveraged the principles of thermodynamics and reaction kinetics to develop processes that are more efficient, cost-effective, and capable of producing materials and chemicals at a larger scale. This not only facilitated the growth of the chemical industry itself but also had a wide-reaching impact on sectors such as pharmaceuticals, energy, and materials science, contributing to the advancement of society as a whole. Thus, the advancement of steam technology and the deepening understanding of thermodynamics and reaction kinetics played pivotal roles in the scientific and industrial growth of the 19th and early 20th centuries, marking a period of remarkable innovation and expansion in the chemical engineering field.

1.2.2 Electricity Power

The transition from steam to electric power marked a revolutionary period in human history, heralding the second industrial revolution. This era, spanning the late 19th and early 20th centuries, was not just about the adoption of electricity as a primary energy source but also about the profound impact it had on materials chemistry. The electrification of society demanded new materials with specific properties, fostering a wave of innovation in chemistry and material science.

An understanding confined solely to gases is significantly inadequate for the field of materials chemistry, which also heavily involves the study of condensed phases such as solids and liquids. These phases arguably represent a more prevalent subject of research. In the domain of solid-state physics, electrons emerge as one of

the pivotal research subjects. The study of electrons is indissolubly linked to the understanding of electricity and the socio-economic context of the era. By the late nineteenth century, the exploration and application of electricity had made considerable strides, with the advent of technologies like the light bulb, telephone, and electrical power distribution witnessing a qualitative leap and achieving widespread practical application. Many scientists of that period began to leverage electricity as a tool for scientific investigation. For instance, in 1895, Röntgen (1896) discovered X-rays while experimenting with a Crookes tube – an early experimental electrical discharge tube – during his studies on cathode rays. This discovery underscored the pivotal role of electrical technology in facilitating scientific breakthroughs.

The unveiling of X-rays opened the door to observing the microscopic structure of materials, further broadening the horizons of material chemistry through the advent of quantum mechanics. Quantum mechanics has introduced concepts such as momentum space into contemporary solid-state physics, significantly expanding our cognitive and exploratory scope in materials chemistry. This progression underscores the interdisciplinary nature of materials science, highlighting how advances in one area can propel understanding and innovation across multiple scientific domains. It exemplifies the profound impact of electrical studies and technological advancements on the evolution of materials chemistry, enabling the detailed examination of material properties at the atomic and molecular levels. Consequently, these insights have paved the way for the development of new materials and technologies, underscoring the integral role of a comprehensive understanding of all states of matter – solid, liquid, and gas – in the advancement of materials science and engineering (Figure 1.2).

With the maturation of solid-state physics (Ashcroft and Mermin 1976) and the conceptual framework of momentum space, the intricate relationship between



Figure 1.2 The advent of electricity ushered in an era of unprecedented innovation and connectivity, fundamentally transforming human civilization and laying the groundwork for the modern technological landscape. The Electrical Era represents a paradigm shift in human history, sparking revolutions in communication, transportation, and industry, fostering global interconnectedness, and fostering the birth of countless inventions that continue to shape our daily lives.