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Views & Comments

A Vision of Materials Genome Engineering in China

Jianxin Xie, Yanjing Su, Dawei Zhang, Qiang Feng

Beijing Advanced Innovation Center for Materials Genome Engineering & Institute for Advanced Materials and Technology & State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, Beijing 100083, China

In the new round of global scientific and technological revolution and industrial transformation, one of the biggest bottlenecks we are facing is the lack of adequate materials technology. It is urgently hoped that there can be a major revolution in the materials research and development (R&D) field, rather than gradual and slow development [1]. Under this background, materials genome engineering (MGE) has been developing rapidly, and its key technologies and engineering applications have become the frontiers of materials research [2]. The goal and mission of MGE is to establish a new R&D mode and a new technology system with deep integration and collaborative innovation of rational design, efficient experiment, and big data technology in the whole chain of materials R&D, manufacturing, and application, thereby significantly improving the R&D efficiency, promoting the engineering applications, and meeting the increasingly urgent demand for new materials in economic and social development.

MGE is systematic engineering that leads to the revolution of materials science and technology in many ways, including the transformation of the traditional paradigm in materials research, the development and application of disruptive innovation technologies and equipment, and the cultivation of the next-generation materials workforce with creative minds and skills. China has laid out a comprehensive plan for MGE research in order to accelerate the development of advanced materials technology and industry with enhanced innovation capability and international competitiveness, relying on an integrated implementation of the R&D on cutting-edge technologies, the construction of innovation platforms, the training of high-quality innovative personnel, and the promotion of engineering applications.

The National Key R&D Project on Critical Technologies and Supporting Platforms for MGE

The National Key R&D Project on Critical Technologies and Supporting Platforms for MGE was established by China's Ministry of Science and Technology in 2015, with an investment of 840 million CNY. The project aims to build three types of leading platforms (i.e., computing, experiments, and databases) to support MGE research and collaborative innovation, and four critical technologies (i.e., high-throughput materials computation and design, high-throughput materials processing and characterization, high-efficiency materials service and failure evaluation, and materials big data technology). To promote the development and application of MGE methodology and technology, five categories of materials—namely, energy materials, biomedical materials, rare-earth functional materials, catalysts, and specialty alloys—are the focus of demonstrations of accelerated materials insertion. A unique feature of this project is its emphasis on the optimization of materials processing technologies and the development of high-efficiency evaluation techniques for materials service performance. The primary tasks of the project are as follows:

(1) Rapid discovery of composition–structure–property relationships in advanced materials via high-throughput and automated process algorithms; development of integrated computational materials engineering (ICME) methods to overcome bottlenecks in multiscale and cross-dimensional computation; and optimization of materials design and processing by establishing a comprehensive materials composition–processing–structure–property relationship. The overall goal of these tasks is to integrate high-throughput materials computation with ICME to establish a technological foundation and supporting tools for rational materials design, while taking advantage of China's powerful supercomputing resources.

(2) Development of high-throughput techniques and equipment for materials fabrication in different forms (thin-film, powder, and bulk materials) based on thin-film preparation, three-dimensional (3D) printing, diffusion multiples, directional solidification, and gradient thermal treatment, among others; and development of high-throughput experimental techniques for the characterization of materials composition and structure by exploiting analytical algorithms suitable for the rapid processing of massive experimental data obtained from advanced scientific facilities (e.g., synchrotron radiation sources and spallation neutron sources). The overall goal of these tasks is to develop revolutionary high-throughput experimental techniques for the high-efficiency verification of rational materials design and for the rapid screening and optimization of materials composition, processing, and microstructure.

(3) Development of key technologies for the engineering applications of advanced materials, including multiscale simulation, high-efficiency evaluation, equivalent accelerated tests, and big data technologies for the study of materials service performance

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and failure behaviors. These tasks aim to solve bottleneck issues such as the long cycles and high costs associated with research on materials service and failures, and represent a unique engineering-application-oriented feature of the MGE program in China.

(4) Development of intelligent databases capable of automatic data collection, archiving, mining, and application to serve high-throughput computation and experiments and to achieve the automatic processing and accumulation of massive materials data; and construction of materials data platforms with the integrated functions of data collection, sharing services, data analysis, advanced materials discovery, and new industrial products design, in order to promote the application of big data technologies and artificial intelligence in the R&D of advanced materials.

Active investments from local government and enterprises

Guided by the National Key R&D Project, local governments and enterprises have been actively investing and participating in MGE research. For example, the Beijing municipal government and the Chinese Academy of Sciences jointly invested 570 million CNY to build a large-scale MGE research facility in 2017. The Beijing municipal government also invested 500 million CNY to establish the Beijing Advanced Innovation Center for Materials Genome Engineering, which is dedicated to inviting top-class materials scientists all over the world to collaborate on interdisciplinary MGE research and education. In 2017, the Shenzhen municipal government invested 710 million CNY to build large-scale scientific facilities for the high-throughput characterization of materials composition and structure. Since 2018, Yunnan Province has invested over 400 million CNY to build an MGE research platform in order to support its flagship industry in rare and precious metals, transferring the technological breakthroughs of the national key projects to the R&D for new products. In addition, provinces and municipalities, such as Shanghai and Guangdong, along with numerous large-scale enterprises, have provided major funding for MGE projects and platforms.

A collaborative innovation framework guided and supported by the central government

The National Key Project supports the R&D on critical generic MGE technologies, software and equipment, and the building of collaborative platforms covering the whole chain of materials design, R&D, manufacturing, and application. Under guidance from the central government, local governments and industry sectors are becoming the key drivers promoting the engineering application of the key technologies and equipment of MGE. To support the sustainable development of critical MGE technologies and applications, China is placing strong emphasis on the coordination of technological R&D and standards development in MGE. In 2019, the Chinese Society for Testing and Materials (CSTM) established an MGE standards committee and published the first global MGE-specialized standard [3], specify the content, structure, and essential information of data in an MGE database, which sets a foundation for widespread applications of data-driven approaches in materials research.

New culture and environment to foster MGE research

Beginning in 2017, the Chinese Academy of Engineering launched its national annual forum on MGE in order to promote MGE concepts, strengthen international academic communication, and facilitate the development and application of the fundamental theories, advanced techniques, and critical equipment required for MGE research. Moreover, an MGE symposium is held annually at the Chinese Materials Conference organized by the Chinese Materials Research Society (C-MRS), and an annual MGE seminar series is organized by the Chinese Society for Metals (CSM). Many universities have redesigned their undergraduate and graduate curricula and now offer to teach computational materials, materials informatics, high-throughput materials experiments, and materials big data technology, which are essential courses for the cultivation of a specialized workforce for MGE research.

Significant impacts of MGE technologies on engineering applications

After five years of development, synergy has formed from the intensifying collaboration among universities, institutes, industries, and customers to conduct fundamental MGE research and work on its potential industrial applications. A number of innovative research breakthroughs have been achieved, and the effectiveness of MGE approaches is being manifested in various engineering applications, which exhibit high development momentum and magnificent prospects for industrialization. According to a report titled *Creating the Next-Generation Materials Genome Initiative Workforce* that was published by the Minerals, Metals, and Materials Society (TMS) in 2019, China's MGE is demonstrating a particularly comprehensive integration between industry and academia [4].

R&D of critical generic technologies, software, and equipment

Numerous software programs for high-throughput, concurrent, automated, and multiscale computation have been developed for MGE research. A throughput magnitude of up to 10^4 has been realized in high-throughput concurrent computation. This process was deployed on a supercomputer platform and has been opened for sharing. High-throughput processing techniques and equipment for materials in different forms (i.e., thin-film, power, and bulk materials) have also been invented, as well as high-throughput experimental techniques for materials heat treatment, solidification, and processing optimization. Multiscale, cross-dimensional algorithms have been developed to evaluate materials service performance and failures under complex environments more efficiently. Finally, an integrated and extensible data framework, including data collection, databases, and data mining, has been established to enable the personalized description, convenient combination, and mining and analysis of complicated materials datasets with MGE concepts [5].

Development and industrialization of advanced materials

Some typical examples of the development and industrialization of advance materials are as follows. A novel high-temperature bulk metallic glass (Ir–Ni–Ta–(B)) [6], which possesses the highest glass transition temperature and mechanical strength on record and exhibits an excellent thermoplastic shaping performance, has been developed, relying on combinatorial high-throughput fabrication techniques, high-throughput X-ray diffraction, and electrical resistance measurements. As another example, a chemical short-range order was discovered among the interstitial elements in a TiZrHfNb high-entropy alloy. Ordered interstitial compounds can improve both the strength and the ductility of the alloy (which are increased by 48.5% and 95.2% when doped with 2 at% interstitial oxygen (O) atoms, respectively) by changing the dislocation shear mode, which presents a new idea for strengthening and toughening metallic materials [7]. In a different study, cone dislocations were found to be an effective plastic carrier in magnesium (Mg) alloys. The nucleation and slip of the cone dislocations can be promoted to improve the plasticity of Mg alloys by increasing the applied stress and decreasing the grain size, which provides a new technical approach for the development of high-toughness Mg alloys [8]. As another example, through the alloying of sodium (Na) and silver (Ag) and the doping of a trace amount of elemental bismuth (Bi), a stable lead-free double perovskite $Cs_2AgInCl_6$ with highly efficient white luminescence was developed, breaking the record for the efficiency limit of white phosphor for nearly half a century and providing a new research strategy for lead-free perovskite luminescence materials [9]. Moreover, a property-oriented design approach for high-performance alloys has been proposed that involves machine learning compositional design models. Based on these models, next-generation high-strength (i.e., a mechanical strength of up to 800 MPa) and high-conductivity (i.e., an electrical conductivity of up to 50% International Annealed Copper Standard (IACS)) [10] copper alloys have been developed for the fabrication of large-scale electrical circuits. Furthermore, high-throughput experiments and screening methods have been used to develop high-performance catalysts for benzene and ethylene liquid-phase alkylation and new-generation nanoscale molecular sieves with MFI structure and morphology, which have already been massively industrialized and have generated significant economic output.

Future perspectives on MGE in China

Within the next 10–15 years, China will implement the National Materials Genome Engineering Program in order to meet the surging demands for the R&D of high-end advanced materials, industrial upgrading, and the improvement of independent support capacity and original innovation capacity. The major objectives of this program will focus on four aspects. The first aspect is the development of critical generic technologies, which include high-efficiency materials computation methods and software, high-throughput/automated/intelligent materials experimental technology and equipment, materials big data technology, and intelligent technology for materials R&D. The second aspect is the construction of MGE infrastructure and innovation platforms, which include ICME platforms, databases, and big data technology platforms, as well as technological innovation platforms for materials design, processing, characterization, and evaluation. The third aspect is the wide application of key MGE technologies in the field of emergent advanced materials and high-end key materials in order to promote the transformation of the traditional trial-and-error materials research mode. Finally, the fourth aspect is the cultivation of a large number of innovative talents with comprehensive knowledge and skills by incorporating MGE modules into the materials science and engineering curricula in Chinese universities.

References

[1] Shechtman D. Current challenges in materials science and engineering [presentation]. In: 2018 World Forum on Scientific and Technological Innovation; 2018 Aug 10–12; Beijing, China; 2018.
[2] Group on Advanced Materials. Materials Genome Initiative for global competitiveness. Washington, DC: White House Office of Science and Technology Policy; 2011.
[3] Wang H, Zhang LT, Yang ML, Su YJ, Liu Q, Xiang XD, et al. T/CSTM 00120–2019: General rule for materials genome engineering data. Chinese standard. Beijing: Chinese Society for Testing and Materials; 2019. Chinese.
[4] The Minerals, Metals, and Materials Society (TMS). Creating the next-generation Materials Genome Initiative workforce. Pittsburgh: TMS; 2019.
[5] Su YJ, Fu HD, Bai Y, Jiang X, Xie JX. Progress in materials genome engineering in China. Acta Metall Sin 2020;56(10):1313–23. Chinese.
[6] Li MX, Zhao SF, Lu Z, Hirata A, Wen P, Bai HY, et al. High-temperature bulk metallic glasses developed by combinatorial methods. Nature 2019;569(7754):99–103.
[7] Lei Z, Liu X, Wu Y, Wang H, Jiang S, Wang S, et al. Enhanced strength and ductility in a high-entropy alloy via ordered oxygen complexes. Nature 2018;563(7732):546–50.
[8] Liu BY, Liu F, Yang N, Zhai XB, Zhang L, Yang Y, et al. Large plasticity in magnesium mediated by pyramidal dislocations. Science 2019;365(6448):73–5.
[9] Luo J, Wang X, Li S, Liu J, Guo Y, Niu G, et al. Efficient and stable emission of warm-white light from lead-free halide double perovskites. Nature 2018;563(7732):541–5.
[10] Wang C, Fu H, Jiang L, Xue D, Xie J. A property-oriented design strategy for high performance copper alloys via machine learning. npj Comput Mater 2019;5(1):1–8.