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Editorial

Editorial for Special Issue on Materials Genome Engineering

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With the rapid advancement of computing and information technology at the turn of the 21st century, the power of data collection and processing has multiplied tremendously. Based on this a game-changing advancement, science is at the advent of the "fourth paradigm" of massive data plus artificial intelligence, in which the efficiency of scientific research is continuously improved, research time is shortened, and research cost is reduced [1]. These advances happen to coincide very well with the long-term pursuit of material science. Within the scientific fourth paradigm, the Materials Genome Initiative (MGI) announced in 2011 by the US government [2] offered a forward-looking new path. Through the integration of computation, experiments, data technology, and theory, MGI aimed to create a data-centric prediction-based new model of material research to eventually replace the trial-and-error method centered on experimental observation. Soon afterwards, many similar plans were set off around the world. For example, in order to speed up the research and development (R&D) of high-performance alloys and other new-generation materials, the European Union launched several plans including the Seventh Framework plan of Accelerated Metallurgy (ACCMET), Metallurgy Europe—A Renaissance Program for 2012–2022, Horizon 2020, and the Graphene Flagship. In Germany, plans such as Matfo (1984–1993), MaTech, Material Innovation WING for Industry and Society, the Recommendations for Implementing the Industry 4.0 Strategy white paper, and Digital Strategy 2025 were successively promulgated and implemented to encourage various social forces to participate in the R&D of new materials. Japan launched Element Strategy Research (2007), Element Strategy Research Base (2012), the Innovative Laboratory Construction Support Initiative—Materials Research by Information Integration (2015), the Materials Research by Information Integration Initiative (MI^{2}I), and the 2015 White Paper on Manufacturing. Around the same period, plans such as the Future Growth Momentum Plan, the Nano Fusion 2020 Project, the Third Basic Science and Technology Plan, the Future Growth Engine Plan, and the South Korea 3D Printing Industry Revitalization Plan (2017–2019) were implemented in Republic of Korea. Meanwhile, Russia released the Material and Technology Development Strategy 2030 and the Technology Development Forecast to 2030.

In 2016, China officially launched the Key Technology and Support Platform for Materials Genome Engineering (MGE), with the strategic target of reducing both R&D cycle time and R&D cost by half (i.e., "double half"). This program supports R&D in four key technologies: high-throughput calculation methods, high-throughput preparation and characterization, in-service performance evaluation, and material big data technology. The results will lead to a demonstrative MGE infrastructure consisting of three platforms: high-throughput computing, high-throughput synthesis and characterization, and a materials database. In the meantime, the program provides funding to build up application use cases of MGE in five material categories—energy materials, biomedical materials, rare earth functional materials, catalytic materials, and special alloy materials—with the aim of demonstrating the power of the new approach and establishing a foundation for paradigm transformation.

Though still in its infantry, MGE has demonstrated its game-changing potential, which is badly needed to revolutionize the way in which materials R&D is conducted today. Looking ahead, MGE is on the way to becoming a worldwide movement that is increasingly being adopted by the materials science community. However, it is difficult to imagine that such a fundamental paradigm shift could happen overnight. In that sense, the "long march" has just begun.

This special issue on MGE assembles six papers that discuss several key aspects of this general theme. Zi-Kui Liu's paper "View and Comments on the Data Ecosystem: The Ocean of Data" offers viewpoints on the need for new tools to connect data repositories and provide feedback to create an ocean of data for the sustainable

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ecosystem of materials data and the new "materials genome" beyond individual phases to predict emergent behaviors.

In their opinion paper "On the Data-Driven Materials Innovation Infrastructure," Hong Wang et al. argue that as a new routine of materials research, MGE requires a whole new data-centric infrastructure consisting of data facilities, high-throughput experiments, and high-throughput computation to cover both the generation and the utilization of data. Data facilities include databases, a library of artificial intelligence (AI)-based modeling tools, and an integrated platform. Ideally, data should be generated rapidly via high-throughput experimentation and computation through Data Fab, a centralized or virtually linked platform capable of batch production, in order to ensure that the data is highly integrated, systematic, consistent, and comprehensive.

The data identifier (DID) is an essential tag or label in all kinds of databases, and is particularly important in this era of a paradigm shift to data-centric materials informatics. William Yi Wang et al. contribute an article titled "DID Code—A Bridge Connecting Materials Genome Engineering Databases and Inheritable Integrated Intelligence Manufacturing," which proposes a universal DID format consisting of a set of build chains. The proposed DID is flexible and convenient for extending and sharing data in and between various cloud-based platforms. With this DID, classical two-dimensional (2D) codes can be constructed and precisely recognized and decoded by smart phones or specific machines. By utilizing these 2D codes as the fingerprints of a dataset linked with its cloud-based platforms, progress and updates in the composition–processing–structure–property–performance workflow process can be tracked spontaneously.

Combinatorial materials science allows streamlining of the synthesis process and data management using multiple characterization techniques. In their research paper "Combinatorial Synthesis and High-Throughput Characterization of Microstructure and Phase Transformation in a NiTiCuV Quaternary Thin-Film Library," Ichiro Takeuchi et al. synthesize a composition spread of a NiTiCuV thin-film library by means of magnetron co-sputtering on a thermally oxidized silicon (Si) wafer. The composition-dependent phase transformation temperature and microstructure of NiTi-based shape memory alloys (SMAs) are investigated and determined using high-throughput wavelength dispersive spectroscopy, synchrotron X-ray diffraction, and temperature-dependent resistance measurements. Phase maps for the quaternary system and the correlations of functional properties are discussed with respect to the local microstructure and composition of the thin-film library.

Macroscopic materials are heterogeneous, multi-elementary, and complex. No material is truly homogeneous or isotropic at a certain small scale. Parts of a material that differ from one another can be viewed as "natural chips." Lei Zhao et al. contribute the paper "A State-of-the-Art Review of High-Throughput Statistical Spatial-Mapping Characterization Technology and Its Applications," which presents a review of research on the high-throughput statistical spatial-mapping of characterization technology at multiple scales and demonstrates several applications for materials such as steels, superalloys, galvanized materials, and ferrosilicon alloys.

Computer simulation has been an important component of the MGE concept and is a rapid growing area in materials science. In the paper by Zhong Yu et al. titled "Investigation of the Creep Resistance in Grade 91 Steel through Computational Thermodynamics," simulation results explain the mechanisms that can affect the creep resistance of Gr. 91 steel. These researchers offer a possible solution for increasing creep resistance within this steel at elevated temperatures by optimizing the steel composition, welding, and heat-treatment process parameters, thus providing guidance for future alloy development to improve creep resistance and prevent type IV cracking.

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