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Citation: Science Bulletin **60**, 1966 (2015); doi: 10.1007/s11434-015-0937-2

View online: http://engine.scichina.com/doi/10.1007/s11434-015-0937-2

View Table of Contents:http://engine.scichina.com/publisher/scp/journal/SB/60/22

Published by the Science China Press

Sci. Bull. (2015) 60(22):1966–1968
DOI 10.1007/s11434-015-0937-2

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www.springer.com/scp

News & Views

Remarks on the recent progress of Materials Genome Initiative

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Published online: 5 November 2015

The Materials Genome Initiative (MGI) has attracted great attention globally since June 2011, when the US President Obama announced Advanced Manufacturing Partnership (AMP), in which MGI is a key component. In June 2014, the US National Science and Technology Council published "Materials Genome Initiative Strategic Plan", describing in detail the strategy that guides and coordinates US Federal activities and provides a clear technical path for carrying out the MGI's vision and reaching the goal, i.e., discover, develop, manufacture and deploy advanced materials twice as fast, at a fraction of the cost. It is optimistic as successful cases and activities from early 2000s demonstrate that the integration of modeling tools and databases can significantly reduce design time and cost while improving quality.

In China, continuous discussions and researches have never paused since the launch of MGI. On December 21–23, 2011, honorably chaired by Prof. Changxu Shi and Prof. Kuangdi Xu, Chinese Academy of Engineering (CAE) and Chinese Academy of Sciences (CAS) jointly held the S14 Xiangshan Science Conference with the title of "Systematic materials science and engineering". The topics included: (1) high-throughput materials preparation and characterization tools; (2) development of computational methods and software; (3) MGI databases; (4) key materials research and breakthrough.

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On October 6–9, 2012, Prof. Liquan Chen, the member of CAE, presented "MGI—the opportunity and challenge for materials science in China", in the 9th Academic Conference of the Division of Chemical Engineering, Metallurgy and Materials of CAE.

In December 2012, CAE launched the key consultant project "Strategic research on systematic materials science and engineering—MGI in China", led by Prof. Liquan Chen. On June 12, 2014, the first version of the CAE consultant report was released at the Beijing Conference Center. In February 2015, CAE submitted the final consultant report to the State Council. The Vice-Premiers Yandong Liu and Kai Ma committed to support MGI-related research in China, and urged the Ministry of Science and Technology (MOST) and the Ministry of Industry and Information Technology to implement.

In January 2013, CAS also started a key consultant project organized by Profs. Chongyu Wang and Cewen Nan. It was finished at the end of 2014 and submitted to the State Council.

On November 22, 2014, the CAE MGI consultant team and the MOST consultant members for advanced materials (the National High Technology Research and Development Program of China) held a joint meeting. The main topic was to discuss the possibility of recommending the MGI project as one of the national key science and technology projects.

On March 23, 2015, CAE submitted a proposal of the MGI project to MOST, as one of the key special projects for the 13th 5-year-plan of China.

In the meantime, national MGI platforms for creative materials researches were planned in China. The high-throughput materials synthesis and characterization platform will strongly link with Shanghai Synchrotron Radiation Facility, Beijing Synchrotron Radiation Facility

(in plan) and Guangdong Spallation Neutron Source (under construction). The high-throughput computation platform aims to integrate various computational tools at the micro-, meso- and macroscopic levels. MGI database centers plan to improve the existing various materials databases (e.g., environmental corrosion and aging network) and integrate them to build a national materials database network. The MOST is to start large projects to develop key technology for MGI in 2016–2020. The National Natural Science Foundation of China is planning to create a national MGI research center for databases.

Currently, several MGI centers have been established by Chinese municipal governments. The following are among the first to inaugurate, i.e., the Shanghai Institute of Materials Genome (August 2014), the Beijing Key Laboratory for Materials Genome (March 2015) and International Institute of MGI in Ningbo (August 2015).

While one may try to find "real" entities of genome in materials, Kaufman and Ågren [1, 2] argued that the materials genome should be considered in analogy with biological genome, and defined as a set of information in the form of databases that allow prediction of materials' structures, as well as the responses to processing and usage conditions. Materials scientists systematically and continuously search for theoretically sound, quantitative relationships among materials composition/process, microstructure, property and performance. As a result, the rational materials design based on the relationships can significantly accelerate the materials development and deployment. We believe that the underlying "materials genome" can be considered as twofold, firstly the quantitative relationships with physical significance that can be coded in computational tools and relevant databases to predict materials properties and guide the materials design; secondly the basic building blocks such as atom cluster and phase.

By combining advanced experimental techniques, and dedicated databases built on the experimental data, the integrated computational tools at micro-, meso- and macroscale levels will speed up the realization of the goal of MGI. In the foreseeable future, the integrated multi-scale calculations are capable of simulating the whole processes of materials production and predicting the microstructure evolution and properties of materials, which enables a precise control of materials production processes during the design stage. This is a promising route of materials and process design pursued by MGI.

Chinese Science Bulletin published a special issue (Volume 59, 2014), the first academic monograph in China on MGI, to discuss the combination and integration of three means of the materials research and development, i.e., experiment, computation and data. The experimental techniques evolve from traditional and practical tools to measurements in a high-throughput scale and at sub-Ångstrom resolution and picometer precision [3, 4]. The computational methods include first-principles calculations [5, 6], molecular dynamic simulations [7], phase-field method [8, 9], computational thermodynamics [10, 11] and kinetics [12], computational mechanics, the finite element analysis and many more [13, 14]. The databases [15–17] for multi-component engineering materials are in fact a comprehensive summary and careful discrimination of all experimental and computational results, and in turn improve the efficiency of further experiments and promote the accuracy of calculations by implementing more reasonable model parameters. With these tools and databases, practical materials can be rationally designed [18–20].

MGI is now believed to be a unique opportunity to promote a culture or paradigm transfer in materials development and deployment, converting the research practice from the trial-and-error route to rational materials design by adopting seamless integration of experiment, computation and materials data. This integrated MGI platform allows educational, academic and industrial activities to operate on the same basis, which not only strengthens the collaboration between academia and industry, but also fosters the next generation of materials specialists and workforce with the new vision of MGI.

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