

NIMS Materials Database: Current Status and Future Prospects

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ABSTRACT In addition to experiment, theory and computation, data-driven research is becoming be the fourth method of materials science. The new approach of materials development starts from analyzing a large, comprehensive and systematic data set, by statistical or machine learning methods, discover the relationships between materials process, structure and properties, and then design and optimize the material component and structure in order to obtain the properties required. Materials data and databases are the fundamental of this new approach. During the past tens of years, National Institute for Materials Science has developed a federal materials database system MatNavi, which contains more than 10 materials databases covering the basic and engineering properties of inorganic materials, polymers and structure materials. We have successfully set up a process of data collection and verification from literatures, calculation and experiments, and developed a series of database techniques to fit various types of materials data. To meet the needs of data-driven materials research, a new data platform integrating the conventional database and data analysis and simulation tools is under development. In the presentation, our experiences will be shared, and the challenges and outlook of materials database will be discussed.



Yibin Xu is Group Leader of the Materials Database Group, National Institute for Materials Science, Japan. She earned her first doctor degree of Materials Engineering in 1994 from Shanghai Institute of Ceramics, Chinese Academy of Science, and second doctor degree of Information Science in 2007 from Nagoya University. After working at Shanghai Institute of Ceramics, National Industrial Research Institute of Nagoya, and CTI Co., Ltd., she joint National Institute for Materials Science in 2002. Since then she has been involved in the development and management of NIMS Materials Database System (MatNavi). She is now the Sub Project Leader of Materials Research by Information Integration Initiative (MI²I), a national project funded by MEXT and JST. Meanwhile, as a materials scientist, her expertise focuses on measurement, calculation and prediction of thermophysical property of various materials. Much of

her current research centers on heat transportation and thermal engineering of nanostructured materials.