Spin-Current Thermoelectric Conversion – Informatics-Based Materials Development and Scope of Applications

ISHIDA Masahiko, IWASAKI Yuma , SAWADA Ryohto , KIRIHARA Akihiro , SHIRANE Masayuki

Abstract

Since the energy conversion technology that makes use of a new physical property called the spin current was reported in 2008, conversion efficiencies have been improved significantly, being helped by the discovery of new materials. This improvement has been backed not only by the accumulation of discoveries of new materials and mechanisms but more importantly, by efforts aimed at improving the efficiencies of materials development processes by taking a completely new approach. This paper introduces the creation of a new materials development process that combines an attempt at large-scale data acquisition in the field of materials development and an informatics approach for analyzing the acquired data by using machine learning. The potential benefits of its utilization are also discussed. In addition, the paper discusses the application domains of the spin-current thermoelectric conversion technology that are currently being put into practical use.

Keywords

Spin Seebeck effect, thermoelectric conversion, materials development, materials informatics, machine learning, heterogeneous mixture learning

1. Introduction

There are many cases in which the discovery of a material or device possessing new functionality changes not only the structures of individual enterprises but also exerts a very great impact on leading to the reform of the entire society. Some such examples include the neodymium magnet, the high-temperature superconductor and the blue LED. All of which have achieved significant success due to the extensive committed research, as well as the impact of chance events.

However, the environments that surround material and device development are changing continually. The need for results has now reached a very high level of urgency in the fields that are experiencing severe competition. Consequently, attention is drawn to approaches that can develop materials and devices more efficiently by the maximum use of advanced technologies. Particularly, the materials informatics (MI) gathers special attention as a new technique for accelerating development by utilizing the knowledge obtained via informatics.

In the present paper, section 2 describes the trends of MI technology development, section 3 reports on an actual usage case of MI for the development of a material for use in the new technology known as spin-current thermoelectric conversion. Section 4 introduces the possible applications of this technology.

2. Trends in MI Technology Development

Most R&D in the material science field has targeted physical properties such as the strengths of steel materials or the carrier mobility of semiconductors, which are expressed simply and quantitatively. Topics dealing with data involving millions of types or quantities have thereby been limited. As a result, there was rarely a need to use informatics that surpassed the level of sophistication of mathematical statistics used traditionally in R&D. However, considering that the progress of experimentation and simulation technologies has led to an increase in the types and quantities of data and the use of informatics has achieved success in the bioscience and drug discovery fields that had launched the use of informatics earlier. The Materials Genome Initiative (MGI) was started in 2011 in the United States. This triggered the general rise in an interest in informatics. The MGI has the objective of developing materials more efficiently by advancing research under the initiative of data analysis that uses artificial intelligence (AI). Consequently it is currently advancing the preparation of a materials database and building an open platform equipped with various innovative analysis tools. In Japan also, the development of platforms and key technologies similar to those of the MGI has been started by various associations including the "Materials research by information integration" Initiative (Mi^2i) started in 2015 and other projects.

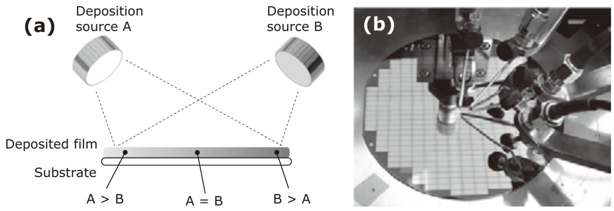

Fig. 1 (a) Composition-gradient sample preparation method using the glancing-angle deposition process. (b) Automatic electrical property measuring system utilizing a semi-automatic probe system.

3. Development of Spin-Current Thermoelectric Converted Materials Utilizing MI

NEC is conducting the R&D into a thermoelectric conversion technology that can mutually convert between the charge and the heat current using a phenomenon called the spin current[1]. This research belongs to a relatively new academic theme[2]. As NEC's original efforts aimed at improving efficiency in the search for new materials, and the ongoing positive trends have both already achieved certain successful results[3][4][5]. Various innovative approaches using MI are therefore currently being advanced.

3.1 Data initiative applied to Materials Science developments

What is important in the R&D of material science is to clarify the causal relationships that exist behind the new physical properties or phenomena. To make this possible, a deductive approach that defines the orientation of a development base on understanding the factors and mechanisms affecting the targeted physical property is regarded as being the accepted orthodox method.

On the other hand, when dealing with a completely new academic field for which the accumulation of fundamental knowledge is as yet insufficient, it is required to vary the data acquisition conditions such as those for composition of the material. As this procedure increases the probability that the results will be influenced by completely unexpected factors, the deductive approach does not function satisfactorily, unless preceded by a huge number of verification experiments. In such a situation, there may be cases in which an inductive approach initiative led by data analysis can be more efficient in advancing the accumulation of meaningful information.

Whether or not challenging a topic under the initiative of data analysis is possible is greatly dependent on the type and quantity of the collected data. Therefore, NEC decided to build an innovative sample preparation/evaluation system that acquires data efficiently by using a combinatorial type experimentation technology in the search for new thermoelectric conversion materials. The combinatorial technique performs exhaustive batch data acquisition from the expected search domains and combinations, and has been developed for the fields of chemical synthesis, thin film synthesis and physical properties evaluations.

Fig. 1 (a) shows a scheme used by NEC to prepare the composition gradient of samples using the oblique-angle sputter deposition technique. The deposition sources are installed obliquely so that a difference in the film deposition rate can be given between the area close to the substrate and that far from it. It is according to this difference that a distribution composition is produced inside the substrate. In each deposition source, three sputtering sources capable of film deposition on various materials including a metal, semiconductor and oxide are installed in mutually opposed positions so that the multicomponent compound thin film in which the composition varies successively over the entire substrate can be fabricated as a single process.

Fig. 1 (b) is an experimental method to evaluate a material's properties. Hundreds or more of thin film sample pieces are fabricated on a single substrate and the physical property data of each of them is acquired automatically. The evaluation using a probe system measures the electric and thermoelectric properties. Other evaluated properties include the composition evaluation using x-ray analysis, the crystal structure evaluation using X-ray diffraction and, as required, the optical and magnetization property evaluations using ellipsometry.

The measured composition and crystal structure data are referenced to obtain an exhaustive prediction of the physical properties presented by actually fabricated samples. For example, band structures obtained by first principles simulation can provide detailed data, including predictions of physical properties and information on the atomic orbitals with the potential of affecting the physical properties.

3.2 Materials data analysis utilizing informatics

NEC is positively advancing the auto processing of data acquired by experimentation and simulation. Advanced informatics technology is here being actively applied.

Fig. 2 shows an overall image of the materials development cycle adopted by NEC. Data is acquired by varying the material compositions and fabrication conditions of a series of combinatorial experiments and combinatorial physical property calculations. It is then fed to the data processing AI that employs the technology for auto extraction of feature quantities from the massive amount of spectral data, including the X-ray diffraction data[3]. Automation of data processing utilizing the AI tool has a very wide range of application and can accurately and quickly process the work that previously used to need much expertise and time. The acquired data is used as information reflecting the actual features of the material from a first principles simulation to ensure accuracy of the results.

The data to be used in analyzing change trends is then selected as the dependent variable y and the physical property parameters obtained by other experimentations and simulations is selected as independent variable x_i, and it is subjected to a regression analysis, or "fitting". Function f is the physical model expressing the mechanism, and the variables strongly reflected in the regression can be regarded as the parameters that have high correlations with the analysis target data.

The model building AI that performs the regression analysis employs NEC's heterogeneous mixture learning technology as the analysis engine. One of the most significant features of heterogeneous mixture learning is the high readability of the analysis results (white box property). It turns the obtained physical property model into the information on the parameters with high correlations for the analysis target data, in a form that is easy to understand by the persons concerned. It thereby allows them to easily evaluate the purpose of the physical property model.

Even in a case when the mechanism existing in the background of a physical property is not understood, the data correlations derived by the AI can provide extremely useful information sources for various checks; whether or not the planned hypothesis is appropriate, we need new hypotheses, any errors exist in experiments and measurements. As a result, as the types and quantities of data are increased, the work for building a physical property mode/mechanism that narrows down the property parameters "descriptors" to be referenced for optimizing the target properties, may then be advanced more efficiently.

Once the descriptors are defined, new knowledge can be accumulated in the next step of the development cycle, which is the narrowing down of new material candidates by means of screening and utilizing physical property simulations[5]. Alternatively, in some cases, the new material candidates are chosen based on the knowledge of the developer and then the next stage of the material development cycle is performed, which is the verification of new material candidates by experiment.

3.3 Search for spin-current thermoelectric materials

One of the biggest issues in the utilization of MI for the spin-current thermoelectric materials, has been the

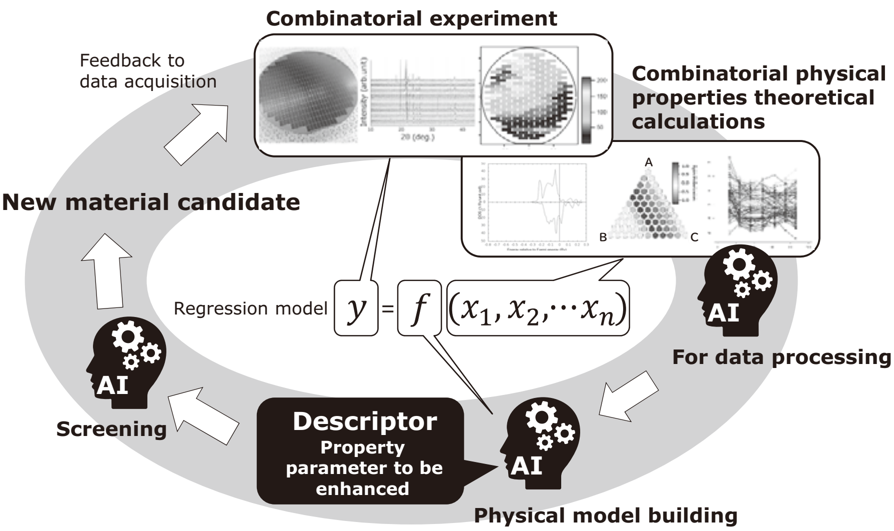

Fig. 2 Materials development cycle utilizing MI.

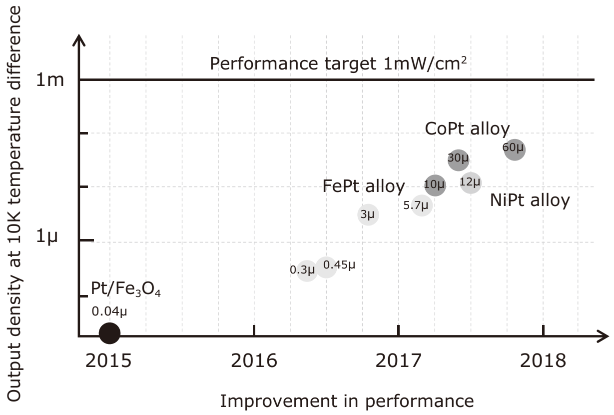

Fig. 3 Improvement in the performance of spin-current thermoelectric conversion materials.

acquisition of thermoelectric conversion coefficient data. Previously, data of a few conditions were accumulated per day by depositing the material, fabricating elements and measuring them. This process has recently been changed resulting in the generation of much experimental data per day due to the batch generation of samples and the creation of new measurement processes. The speed of materials development has thereby been accelerated considerably.

Fig. 3 plots the recent improvement in the performance of spin-current thermoelectric conversion materials. The target performance of 1 mW/cm² (temperature difference 10K) is defined by setting that of the commercially available semiconductor thermoelectric conversion modules as the benchmark. The current performance has now reached about 1/30th of the target performance, which is expected to be reached in a year or two[6].

4. Applications of Spin-Current Thermoelectric Conversion Technology

The commercially available thermoelectric conversion modules made of semiconductor materials such as BiTe that have been used hitherto are based on the physical phenomena of conversion between the charge and heat current such as the Seebeck effect and Peltier effect that were discovered in the 1800's. The basis of the recently adopted materials and modularization technologies were developed in the 1960's aiming at use in the radioisotope thermoelectric generator of artificial satellites and space probes.

Recently, however, the thermoelectric conversion technology is used in high-power electronic devices and compact refrigerator cooling systems as a technology for cooling that features small size and low noise, often called electronic cooling. In addition, it is also put to practical use as a thermal flow sensor making use of the function that outputs the thermal flow that passes through the element as a voltage. On the other hand, although it is actively embedded for the purpose of power generation in aerospace and defense products, it is not so readily available in the manufacture of consumer products. The market scale remains small compared to that of the cooling and sensor applications.

The principal factor causing a delay in expansion in the power generation market is that the value of generated power is below the expected level in most cases, considering the cost of introduction and the durability of the technology. To resolve this issue, improvement in the overall performance of the device component is obviously necessary. It is also important to continue to search for applications that can provide high added values.

The development of the spin-current thermoelectric conversion technology was started by aiming at achieving a breakthrough in the device cost as a result of noticing that it is based on new principles, and that it is expected to be unquestionably advantageous in the cost and durability of the component although the conversion efficiency is not as yet optimized.

One of the exemplary candidates of high added-value applications is the compact energy harvesting type power source for use in generating power at the scale of the button battery. The Internet of Things (IoT) is going to be implemented, which optimizes the whole of society by applying advanced data analyses to a huge amount of information collected from an infinite number of information device components that are randomly located worldwide. In the realization of the IoT, it is expected that the means of power supply to each individual device will be one of the most critical issues. Innovation of thermoelectric conversion technology is expected to be the key technology in enabling the creation of great value, which evolves the technology to the next stage that converts the real world into data.

5. Conclusion

The MI targeting unknown new materials, which is a system complicated by various factors, can be regarded as an attempt to understand and optimize systems under the initiative of data. The results of spin-current thermoelectric conversion materials development achieved using MI up to the present, show clearly the effectiveness both of data-driven and of an informatics-based approach in the field of materials science developments. Although there is a need to resolve the issue of how to acquire data sets individually from each materials field, an increase in the number of use cases can be expected in the future.

The utilization of MI is advancing improvements in the performance of the spin-current thermoelectric conversion technology. The overall performance, including the cost and durability that tend to produce issues in the thermoelectric conversion technology, has already been improved and its practical use is expected soon. Especially, for applications in power generation that have been delayed, verification experiments are underway to open new areas, such as for autonomous power supplies that can contribute to the coming of the IoT society.

6. Acknowledgement

The present research has been achieved with the support of the exploratory Research for advanced Technology (ERATO) "Saitoh Spin Quantum Rectification Project" and the project entitled "Development of Basic Technologies for Advanced Materials Informatics through Comprehensive Integration among the Theoretical, Experimental, Computational and Data-Centric Sciences" of the Japan Science and Technology Agency (JST).

Reference

1) Ken-ichi Uchida et al.: Thermoelectric generation based on spin Seebeck effects, Proceedings of the IEEE, Volume 104, Issue 10, pp.1946-1973, October 2016
2) Masahiko Ishida: Development of a spin-current driven thermoelectric conversion device, OYO BUTURI, Vol.87 No.1, 2018
3) Yuma Iwasaki et al.: Comparison of dissimilarity measures for cluster analysis of X-ray diffraction data from combinatorial libraries, npj Computational Materials 3, Article number 4, 2017
4) Yuma Iwasaki et al.: Machine-learning guided discovery of a high-performance spin-driven thermoelectric material, Cornell University Library, May 2018 https://arxiv.org/abs/1805.02303
5) Ryohto Sawada et al.: Boosting Material Modeling Using Game Tree Search, Phys. Rev. Materials 2, 103802, August 2018
6) NEC Press Release: NEC and Tohoku University Succeed in AI-Based New Material Development, February 2018 https://www.nec.com/en/press/201802/global_20180209_04.html

Authors' Profiles

ISHIDA Masahiko
Senior Principal Researcher
System Platform Research Laboratories

IWASAKI Yuma
Assistant Manager
System Platform Research Laboratories

SAWADA Ryohto
System Platform Research Laboratories

KIRIHARA Akihiro
Principal Researcher
System Platform Research Laboratories

SHIRANE Masayuki
Senior Manager
System Platform Research Laboratories

Information about the NEC Technical Journal

Thank you for reading the paper.
If you are interested in the NEC Technical Journal, you can also read other papers on our website.

Link to NEC Technical Journal website

Japanese

English

Vol.13 No.1 Sustainable Data-driven City Management

Vol.13 No.1

November 2018

Special Issue TOP

Remarks for Special Issue on Sustainable Data-driven City Management
Start-up of Data Utilization-type Smart Cities

Papers for Special Issue

Vision for Data-driven City Management
Global Perspective for Data-Leveraged Smart City Initiatives
A Paradigm Shift in City Management Practices Targets the Sustainable Society

Demonstration and Implementation Examples of Data-driven Smart Cities
Case Study of Data-driven City Management in Cities Abroad
Building a Common Smart City Platform Utilizing FIWARE (Case Study of Takamatsu City)
Initiatives to revitalize regional economies by advancing "*OMOTENASHI*"
— Hospitality offered to foreign visitors to Japan
Case Studies of Data Utilization by Municipal Governments:
Applying Data in Various Fields Such as Financial Affairs, Childcare, and Community Revitalization

City Management Technologies
FIWARE, Information Platform for Implementing Data Utilization Based City Management
FogFlow: Orchestrating IoT Services over Cloud and Edges
Security Requirements and Technologies for Smart City IoT
European Trends in Standardization for Smart Cities and Society 5.0
City Evaluation Index Standards and their Use Cases

Co-creation with Local Communities
An Introduction to "Partnership for Smart City Takamatsu" as a Platform to Engage in Local Co-creation Activities
Launch of Setouchi DMO — A Co-Creation Venture That Goes beyond the Conventional ICT Framework
Community Co-creation Based on a Comprehensive Cooperation Agreement
A Common-Sense Approach to the Future — Study Group for Co-creation of New Municipal Services

General Papers

Spin-Current Thermoelectric Conversion — Informatics-Based Materials Development and Scope of Applications
Reducing the Power Consumption and Increasing the Performance of IoT Devices by Using NanoBridge-FPGA
Development of Nano-carbon Materials for IoT Device Applications
Proof of Concept of Blockchain Technology in the Field of Finance Using Hyperledger Fabric 1.0

NEC Information

NEWS
2017 C&C Prize Ceremony