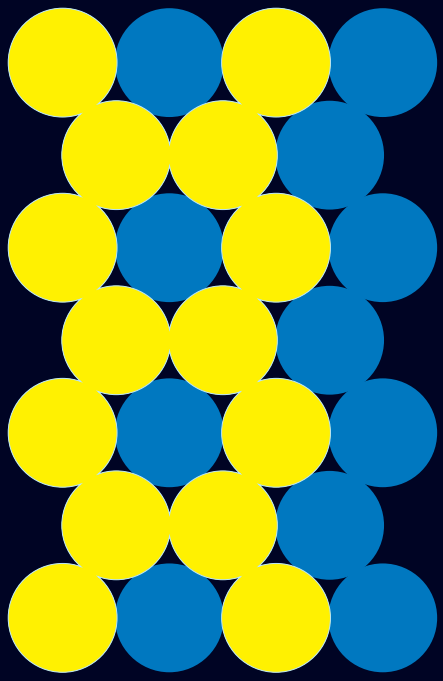


NIMS WEEK 2019

Abstracts

Day 2

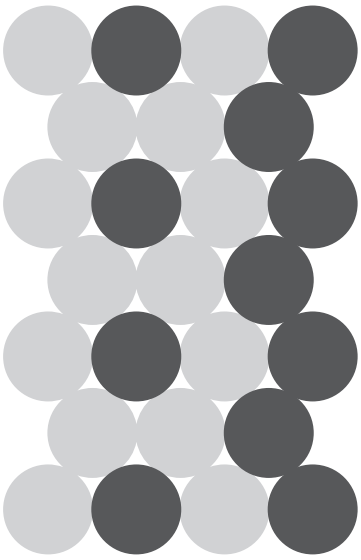
NIMS Award 2019

Academic Symposium

— Materials Innovations Driven by AI + DATA! —

October 30, 2019 Tokyo International Forum, Japan

Organized by National Institute for Materials Science (NIMS)
Supported by Ministry of Education, Culture, Sports, Science and Technology (MEXT)



NIMS WEEK 2019

MEGA EVOLUTION of MATERIALS

NIMS Award Symposium

Contents

MaDIS: Research and Services Division of Materials Data and Integrated System

Greetings from the President

The National Institute for Materials Science (NIMS) is one of the three designated national research and development agencies in Japan. One of the missions of NIMS is to carry out fundamental research on materials science and nanotechnology, thereby developing human resources in the area. As a core national institute, NIMS is also expected to contribute to strengthening Japan's industrial competitiveness toward the realization of Society 5.0 (Super Smart Society), which proposed in the 5th Science and Technology Basic Plan of Japan.

NIMS WEEK is the largest and most important event that NIMS organizes every year. This year, NIMS WEEK is comprised of ”Open House”, “NIMS Award and Academic Symposium”, “NIMS Technology Transfer” and “STAM 20th Anniversary Symposium.” Through this event we introduce NIMS and our research activities in various forms.

The theme of this year’s “NIMS Award and Academic Symposium” is “Materials Innovations Driven by AI + DATA!”. NIMS Award is an international award, which is given to distinguished researchers who have conducted innovative research in materials science. NIMS wishes to honor the distinguished achievements in the field of “Data-Driven Materials Research and Data Infrastructure” by selecting the following two winners: Prof. Gerbrand Ceder (University of California Berkeley) and Dr. Pierre Villars (Director and Owner, Material Phases Data System). The research results of both award winners have made a profound impact on society. Their comprehensive studies have pioneered new avenues in the utilization of data in materials research. We also invite world-class researchers in the field and introduce the latest academic achievements from the perspective of materials science. We have scheduled a poster session for young researchers who will present their research results in the award winners’ relevant area.

I would like you to see the front line of evolving materials research throughout this NIMS WEEK.

Kazuhito Hashimoto
President, National Institute for Materials Science (NIMS)

Aim and Scope

Materials Innovation Driven by AI + DATA!

In the field of materials R&D—which has relied on trial and error for years—"materials informatics" (MI), a scientific approach that utilizes artificial intelligence (AI) technologies to predict structures and production methods of materials with desired performance from enormous research data, is now sweeping the world. Results exceeding previous expectations are now being reported one after the other, and concrete new material development is being made through MI rapidly. What is the key to data-driven materials R&D that differs in essence from conventional simulation technologies?

In addition to construction of computational data infrastructure under intense competition, AI technologies and high-quality materials databases for analyzing big data are essential. The precision of machine learning using massive quantities of research data hangs on the quality and quantity of data.

At this year's NIMS Academic Symposium, NIMS Award will be presented to researchers who have achieved remarkable results in data-driven materials design and database development on a global scale. Furthermore, the lectures presented by researchers at the forefront of the field are sure to provide a bird's eye view of the most recent advances in and future outlook for materials research utilizing AI and data.

Speakers have been requested to make their presentations understandable to researchers, engineers, and students who are not specialists in the relevant fields. Simultaneous Japanese-English interpretation will be provided for all lectures.

We welcome participation by researchers, professionals, and students from a broad range of fields.

NIMS WEEK2019 Academic Symposium Program

10:00~18:00, October 30 (Wed), 2019

9:30~10:00	Registration	
10:00~10:05	Opening Remarks	President Kazuhito Hashimoto
10:05~10:20	NIMS Award Ceremony (Chair: Dr. Kazuhiro Hono)	
10:20~11:05	**NIMS Award Winning-lecture (1)** **Prof. Gerbrand Ceder** (University of California, Berkeley (USA)) Synthesis and AI as the next frontier for Computationally Driven Materials Development	
11:05~11:50	**NIMS Award Winning-lecture (2)** **Dr. Pierre Villars** (Material Phases Data System (Switzerland)) Principal Concept of Database Creation Aiming Holistic Views on the Fundamentals of Materials Science	
11:50~13:30	Lunch and Poster Session	
	Chair: Dr. Keitaro Sodeyama	
13:30~14:00	**[Invited Talk 1]** **Prof. Koji Tsuda** (NIMS/the University of Tokyo) Materials Discovery with Machine Learning: New Directions	
14:00~14:30	**[Invited Talk 2]** **Prof. Brian E Hayden** (University of Southampton (UK)) Materials Development in the Energy and Electronics Sectors through Combinatorial Synthesis, High-Throughput Screening and Machine Learning	
14:30~14:45	**[NIMS Talk 1]** **Dr. Randy Jalem** (NIMS) Smart and Data-efficient Exploration of Novel Solid Electrolytes by DFT and Machine Learning	
	Chair: Dr. Yasuyuki Nakamura	
14:45〜15:15	**[Invited Talk 3]** **Prof. Yaroslava Yingling** (North Carolina State University (USA)) Challenges and Solutions in Soft Materials Informatics	
15:15~15:30	**[NIMS Talk 2]** **Dr. Masanobu Naito** (NIMS) Practical Application of Machine Learning for Soft Matters	
15:30~16:15	Coffee Break and Poster Session	
	Chair: Dr.Satoshi Minamoto	
16:15〜16:45	**[Invited Talk 4]** **Prof. Surya R. Kalidindi** (Georgia Institute of Technology (USA)) Materials Innovation Driven by Data and Knowledge Systems	
16:45〜17:00	**[NIMS Talk 3]** **Dr. Masahiko Demura** (NIMS) Data Scientific Approaches in Materials Integration	
	Chair: Dr. Guillaume Lambard	
17:00~17:30	**[Invited Talk 5]** **Prof. Alan Aspuru Guzik** (University of Toronto (Canada)) From the Harvard Clean Energy Project to Self-Driving Laboratories: A Journey in Materials Discovery	
17:30~17:45	**[NIMS Talk 4]** **Dr. Masashi Ishii** (NIMS) From Data Extraction to Data Utilization: Techniques for Practical Use of NIMS Materials Database	
17:45~18:00	Poster Award Ceremony and Closing (Closing Remarks: Ms. Yuko Nagano, Executive Vice President/Director of MaDIS)	

NIMS WEEK Day2 Poster Presentation List

I. Data-driven Research in Functional Materials (I-01~23)

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
I-01	Dr	Ryo	Tamura	NIMS	Efficient recommendation tool of materials on Windows computers
I-02	Dr	Jiwon	Park	Materials Data Center, Korea Institute of Materials Science, Republic of Korea	Data-Driven Materials Discovery of Indirect Band-Gap Semiconductors for Photovoltaics
I-03	Mr	Jun	Miyamoto	Laboratory for Materials and Structures, Institute of Innovative Research, Tokyo Institute of Technology	Machine Learning Model for Predicting Dielectric Constants of Oxides
I-04	Mr	Taruto	Atsumi	Nagoya Institute of Technology	Compositional descriptor-based prediction for the chemical compound stability
I-05	Ms	Maho	Harada	Nagoya Institute of Technology	Experimental search for NASICON-type solid electrolytes with high Li-ion conductivity guided by Bayesian Optimization
I-06	Ms	Yu	Kitamura	Graduate School of Science and Technology, Kwansei Gakuin University	Machine–Learning–Assisted for Exploration of Synthesis Condition for Metastable Novel Lanthanide Metal–Organic Frameworks Using Failed Experiments
I-07	Mr	Takuma	Wakiya	Graduate School of Science and Technology, Kwansei Gakuin University	Machine–Learning–Assisted Synthesis of Silver Thiolate Metal Organic Frameworks
I-08	Mr	Jaekyun	Hwang	The University of Tokyo	Predicting Chemical and Electronic Properties Using a Novel Descriptor “Elemental Fingerprints set” with Neural Networks
I-09	Mr	Sirawit	Pruksawan	NIMS, Program in Materials Science and Engineering, University of Tsukuba	Design and Optimization of Epoxy Adhesives through Active Learning from a Small Dataset
I-10	Mr	Luca	Foppiano	NIMS	Automatic Extraction Framework of Superconductors Related Information from Scientific Literature
I-11	Dr	Masaya	Kumagai	Center for Advanced Intelligence Project, RIKEN	Data-Driven Design of Thermoelectric Materials with Experimental Data on Starrydata
I-12	Dr	Yukari	Katsura	The University of Tokyo	Starrydata: a web system for experimental data extracted from published plot images
I-13	Dr	Guillaume	Lambard	NIMS	Active learning: A Booster for Discovering New Materials from Small Datasets
I-14	Mr	Koki	Kitai	Graduate School of Frontier Sciences, The University of Tokyo	Accelerating metamaterials design by quantum annealing
I-15	Dr	Hiori	Kino	NIMS	Automation of the first-principles calculation and machine learning to search functional materials of high entropy alloys
I-16	Dr	Takashi	Miyake	AIST	Orbital Field Matrix: A New Descriptor for Materials
I-17	Dr	Takashi	Miyake	AIST	Subgroup Relevance Analysis: A Scheme for Selecting Important Descriptor Groups
I-18	Dr	Ryo	Kobayashi	Nagoya Institute of Technology, NIMS (CMI2, MaDIS)	High-throughput production of force-fields for Li-ion battery materials
I-19	Mr	Haein	Lee	Nagoya Institute of Technology	Data-driven Exploration of Ion Conductive Alkali Metal Oxide for Batteries Using Materials Simulation
I-20	Dr	Yu	Inatsu	RIKEN Center for Advanced Intelligence Project	Active learning for level set estimation under input uncertainty
I-21	Dr	Kazuto	Akagi	AIMR, Tohoku University	Topological Data Analysis toward Design of Functional Materials

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
I-22	Ms	Xiaolin	Sun	The university of Tokyo	Leveraging Legacy Data in Materials Science via Preference Learning
I-23	Mr	Jinzhe	Zhang	Tsuda Lab, Computational Biology and Medical Sciences, Graduate School of Frontier Sciences, Utokyo	Metabolite Identification with de novo Molecule Generation

II. Data-driven Research in Structural Materials (II-01~28)

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
II-01	Dr	Kimiyoshi	Naito	NIMS	Data Driven Research for Composite Materials (Structural and Mechanical Properties of PAN- and Pitch-based Carbon Fibers)
II-02	Dr	Hiroyuki	Oguma	NIMS	Experimental evaluation on the environment resistance and fracture characteristics of multi-functional CFRP
II-03	Dr	Keiichi	Shirasu	NIMS	Structure and mechanical properties of carbon fibers and polymers: Nanoindentation tests and molecular dynamics simulation study
II-04	Dr	Yinbo	Zhao	Department of Aerospace Engineering, Tohoku University	Constructing crosslinked epoxy resins and investigation of mechanical properties with molecular dynamics simulations
II-05	Dr	Yutaka	Oya	Department of aerospace engineering, Tohoku University	Field theoretical approach to polymer phase separation and its mechanical properties
II-06	Prof	Yoshifumi	Amamoto	Kyushu University	Complex Network Representation for Describing Structure-Property Relationships of Rubber Materials
II-07	Dr	Houichi	Kitano	NIMS	Search for Prevention Condition of Solidification Cracking of Parts Made by Selecting Laser Melting Process by Bayesian Optimization Approach
II-08	Mr	Lei	Yuchao	Department of Materials Processing, Tohoku University	Optimization and verification of electron beam melting process of non-weldable superalloy Inconel 713ELC23
II-09	Mr	Takuma	Kohata	NIMS	Optimization of gas atomization process parameters for Ni-based superalloys
II-10	Dr	Masahiro	Kusano	NIMS	Prediction of Tensile Properties of Ti-6Al-4V Fabricated by Selective Laser Melting Based on Microstructural Features
II-11	Dr	Yujie	Cui	Institute for Materials Research, Tohoku University	Influences of plasma rotating electrode process parameters on the particle size distribution and microstructure of Ti-6Al-4V powder
II-12	Dr	Shi-Hai	Sun	Division of Materials and Manufacturing Science, Osaka University	Effect of scanning strategy on the crystallographic texture and Young's modulus of β-type biomedical Ti–15Mo–5Zr–3Al alloy fabricated by selective laser melting
II-13	Dr	Yoshiaki	Toda	NIMS	Prediction of Precipitation Sequences in Practical High-temperature Alloys with Energetics
II-14	Dr	Yufan	Zhao	Chiba Laboratory, Institute for Materials Research, Tohoku University	Influence Factors on Grain Morphology in a CoCrMo Alloy Fabricated by Electron Beam Powder-bed Additive Manufacturing
II-15	Mr	Katsuya	Yokota	Department of Mechanical Engineering, Graduate School of Osaka University	Prediction and Mechanism of Tensile Strengthening in Single β-phase Ti-Ta Alloys with Oxygen Solutes
II-16	Mr	Yuta	Ohigashi	Division of Materials and Manufacturing Science, Graduate School of Eng. Osaka University	Phase-field simulation of crystal growth under solidification condition for Additive Manufacturing
II-17	Dr	Hoheok	Kim	Graduate School of Materials Engineering, The University of Tokyo	Automatic deconvolution of a dilatometric curve in continuous cooling transformations of steels using machine learning
II-18	Prof	Shiro	Torizuka	University of Hyogo	True stress - true strain curves up to large strain extent at elevated temperatures in Ti alloys with image analysis tensile test method
II-19	Mr	Junya	Sakurai	The University of Tokyo	Prediction of Creep Rupture Time for Ferritic Steels Using Machine Learning

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
II-20	Dr	Yoh-ichi	Mototake	Institute of Statistical Mathematics	Universal Framework of Bayesian Creep Model Selection for Steel
II-21	Dr	Takayuki	Shiraiwa	Department of Materials Engineering, The University of Tokyo	Fatigue Performance Prediction of Steel Welded Joints by Materials Integration
II-22	Mr	Shoya	Kato	The University of Tokyo	Microstructure Prediction of Dual Phase Steel with Optimal Strength-Elongation Balance
II-23	Dr	Kishan	Habib	NIMS	Estimation of fatigue lives from the short fatigue crack growth data of a Ni-Co base superalloy
II-24	Dr	Dmitry S.	Bulgarevich	NIMS	Automatic Sorting of Metallurgical Microscopy Images with Machine Learning Tools
II-25	Prof	Naohiro	Shichijo	Tokyo University of Technology	CMC Virtual Test: Material Integration for designing high temperature parts used in turbine engines
II-26	Dr	Shin-ichi	Ito	The University of Tokyo	Bayesian inference of grain growth prediction via multi-phase-field models
II-27	Dr	Hiroshi	Wakameda	ITOCHU Techno-Solutions Corporation	Application of neural network for thermodynamic data of non-equilibrium multiphase field model
II-28	Dr	Kazuto	Akagi	AIMR, Tohoku University	Mathematical Approach to High-dimensional Structural Materials Data

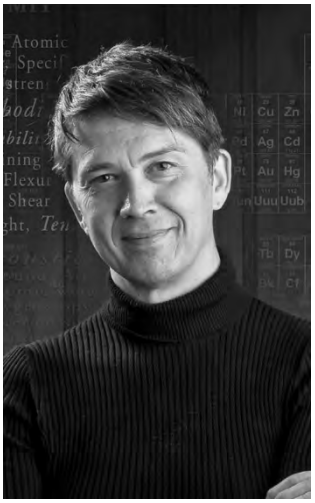
III. Materials Data Infrastructure Including Measurements (III-01~26)

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
III-01	Dr	Mineharu	Suzuki	NIMS	M-DaC: Materials Data Conversion Tools Published to Recreate Interoperative and Reusable Measurement Data Files
III-02	Dr	Kou	Amano	NIMS	tq : A Comprehensive Disciplinary Language for Materials Science
III-03	Mr	Yasuhiro	Takada	NIMS	FigResourceMiner: A search text in images, and graph visualization platform for academic articles
III-04	Ms	Junko	Hosoya	NIMS	Materials Data Platform Infrastructure System: Construction of hardware infrastructure to support subsystem development
III-05	Dr	Yoshitomo	Harada	NIMS	Effective use of outdated experimental apparatus by electronic laboratory notebook (ELN) and IoT data transfer systems
III-06	Dr	Asahiko	Matsuda	NIMS	Vocabulary Management System for the Materials Data Platform using Wikibase for Peer Collaboration
III-07	Dr	Bo	Da	NIMS	Data-driven spectral analysis method in electron-beam based techniques
III-08	Dr	Bo	Da	NIMS	A universal method to determine material-parameter-dependent empirical formula for a given experimental data
III-09	Dr	Shinji	Kikuchi	NIMS	API-FWK: Software Adapter Component for DPFC Integration
III-10	Mr	Masaomi	Takahashi	NIMS	Text Data Mining Platform System to Support Mining and Machine Learning of Scientific Literatures
III-11	Dr	Thaer	Dieb	NIMS	Automatic Construction of Superconducting Materials Database from Tables in related Research Papers
III-12	Dr	Takuya	Kadohira	NIMS	Implementation of FAIR data principles with Materials Data Platform System

Presen No.	Title	First name	Last name	Affiliation	Presentation Title
III-13	Dr	Takuya	Kadohira	NIMS	A proposal of standardized model for data exchange among systems on MDPF
III-14	Mr	Toshiki	Ishida	Metallurgical Research Laboratory, Hitachi Metals, LTD.	Method for calculating the conversion of plastic work into heat"
III-15	Dr	Kosuke	Tanabe	NIMS	Materials Data Repository (MDR)
III-16	Dr	Hiroshi	Shinotsuka	NIMS	Fully automatic peak and background analysis of XPS spectral data -- Sparse modeling of XPS spectra
III-17	Dr	Noriko	Yamashita	RIKEN Center for Advanced Photonics, RIKEN	Large-Scale 3D Observation of Steel Microstructures Using a desktop-sized 3D Internal Structure Microscope
III-18	Mr	Hiroyuki	Naito	NIMS	CAS: Central Authentication and Authorization Service H.Naito
III-19	Dr	Hiroyuki	Shindo	Nara Institute of Science and Technology	Information Extraction of Polymer Names and Properties from Tables in Scientific Papers
III-20	Mr	Isao	Kuwajima	NIMS	NIMS Materials Database, "MatNavi"
III-21	Dr	Kei	Wakabayashi	Universty of Tsukuba	Reducing Annotation Cost for Automatic Named Entity Extraction by using Domain-Specific Dictionary
III-22	Dr	Taichi	Abe	NIMS	Thermodynamic Database for Open Science
III-23	Dr	Jun	Fujima	NIMS	Exploratory Visual Analytics Platform with Multiple Coordinated Views for Materials Informatics
III-24	Dr	Tetsuya	Baba	NIMS	Thermophysical property database of solids for materials informatics
III-25	Dr	Kentaro	Kudo	Department of Mechanical Engineering, Kyushu University	Development of materials database for sintering analysis of Ni-based superalloy
III-26	Dr	Fumiko	Ogushi	NIMS	Study of Grain Boundary Structures using Topological Data Analysis and Simple Evaluation with Local Energy
III-27	Dr	Shigeyuki	Matsunami	NIMS	High-throughput Data Collection and Automatically Data Analysis Using IoT Device

NIMS Award

NIMS Award Winner 1



Prof. Gerbrand Ceder

(University of California, Berkeley (USA))

Research Field Data-driven materials research

History

1988	M.S. Metallurgy and Applied Materials Science, University of Leuven, Belgium
1991	Ph.D. Materials Science and Engineering, University of California, Berkeley
1989	Teaching Assistant, University of California, Berkeley
1991～1995	Assistant Professor, Massachusetts Institute of Technology
1995～2000	Associate Professor, Massachusetts Institute of Technology
2000～2015	Professor, Massachusetts Institute of Technology
2015～Present	Faculty Seminar Scientist, Lawrence Berkeley National Laboratory
2015～2018	Chancellor's Professor, University of California, Berkeley
2018～Present	Daniel M. Tellep Distinguished Professor in Engineering, University of California, Berkeley

Major Awards

2003	Best Graduate Teaching Award, Massachusetts Institute of Technology
2004	Research Award, Battery Division, Electrochemical Society
2006	Best Paper Award, CALPHAD
2006	Graduate Council Teaching Award, Massachusetts Institute of Technology
2007	Graduate Teaching Award, School of Engineering, Massachusetts Institute of Technology
2009	Gold Medal, Materials Research Society
2015	Class of 2015 Fellow, Materials Research Society

Major Publications

1) A. Jain, K. Persson, G. Ceder, Research Update: The materials genome initiative: Data sharing and the impact of collaborative ab initio databases, APL MATERIALS 4, 053102 (2016).
2) K. Kang, Y.S. Meng, J. Bréger, C.P. Grey, and G. Ceder, Electrodes with high power and high capacity for rechargeable lithium batteries, Science 311 (2006) 977-980.
3) Wang, W. D. Richards, S. P. Ong, L. J. Miara, J. C. Kim, Y. Mo, and G. Ceder. Design Principles for Lithium Superionic Conductors. Nat. Mater. 14, 1026–1031 (2015).

Research Achievement Title

Pioneering data-driven materials research based on the first-principles calculations

Research Summary

Prof. Ceder has opened a new era of computational materials science by realizing the idea of linking the first-principles calculation data with statistical thermodynamics. He has demonstrated the power of materials design based on a large amount of computational data and pioneered data-driven materials research. Prof. Ceder has achieved outstanding results in the design and development of various functional materials, including lithium ion battery cathode materials, solid electrolytes, and thermoelectric conversion materials.

Impact on the Academic and Industrial Sectors

Prof. Ceder's idea on materials design based on a large amount of first-principles calculation data had great impacts on academia and industry. His work has led to the development of present computer data infrastructures dedicated to materials design. Prof. Ceder created a recent trend in materials development using data science.

Synthesis and AI as the next frontier for Computationally Driven Materials Development

Gerbrand Ceder
Department of Materials Science and Engineering
University of California at Berkeley, USA

Abstract

The ab-initio prediction of properties has made tremendous progress in the last three decades, making it now possible to predict many functional properties of compounds with high reliability. This has led to many examples of computer-designed materials and the development of high-throughput computing, which can now make many properties of compounds available on demand. Building on this success, computational materials science needs to start addressing new challenges: 1) As computational property prediction continues to extend its reach, we are becoming increasingly limited by the time required needed to synthesize new materials in a predictive and controlled manner. Hence, further acceleration of materials development will require quantifiable and predictive models for the synthesis of materials. Can we for example, predict synthesis pathways, and predict which metastable phases can exist ? 2) Some materials behavior is so complex that no quantified models exist yet that can be used to build a quantifiable relation between a materials description, and its properties. While a data-driven approach may be more useful this can be difficult due to the lack of large and consistent datasets from which machine learning can be attempted. I will show some of our recent work on using machine learning and natural language processing to extract basic scientific ideas and information from text.

NIMS Award Winner 2

Pierre Villars

Director
Material Phases Data System MPDS, Switzerland

Research Field

Fundamental research supporting data-driven materials research

History

1981	PhD, Institute for Crystallography, Swiss Federal Institute of Technology ETH-Zurich, Switzerland
1983～1985	Research scientist, Institute of Solid State Physics, ETH-Zurich, Switzerland
1984	Establishment of Material Phases Data System (MPDS), Director
1988～1995	Editor of CRYSTMET, CISTI, NRCC, Canada
1995～present	Editor-in-chief of the PAULING FILE database

Major Publications

(1) Inorganic Substances Bibliography by P. Villars, K. Cenzual and M. Penzo, vols. 12, DeGruyter, Berlin, Germany, 2012-2017 (all together about 24’000 pages)
(2) Pearson’s Handbook of Crystallographic Data for Intermetallic Phases, Second Edition by P. Villars and L.D. Calvert, vols. 1-4, ASM International, Materials Park, OH, USA, 1991 (5’366 pages)
(3) Crystal Structure Data in PDF-4+ by. P. Villars and K. Cenzual (15 releases), International Centre for Diffraction Data (ICDD), Newtown Square, PE, USA, 2005-2019
(4) NIMS Inorganic Materials Database (AtomWork-Adv.) P. Villars, K. Cenzual, K. Osaki, H. Okamoto and F. Hulliger (1 release), NIMS, Tsukuba, Japan, 2017-2019 (www.atomwork-adv.nims.go.jp)

Research Achievement Title

Development of Pauling File, inorganic materials database

Research Summary

Dr. Villars advocated the concept of a database that organically links crystal structures, phase diagrams and properties of inorganic materials, and developed “Pauling File”, a high quality and comprehensive world's largest inorganic materials database, from more than 180,000 documents published in over 1,000 scientific journals after year 1900 with unique curation method. As of July 2019, about 335,000 crystal structures, 44,000 state diagrams, and 400,000 properties have been recorded, and updates are ongoing.

Impact on the Academic and Industrial Sectors

8 database products such as AtomWork and AtomWork Adv. provided by NIMS and Crystal Structure Data in PDF-4 + by ICDD, as well as 8 handbooks such as Landolt-Börnstein Handbook of Inorganic Substances (Springer) and Inorganic Substances Bibliography (DeGruyter) have been published based on the constructed inorganic materials database and are widely used throughout the world. In recent years, "data-driven materials research" using this database has been activated, and it is recognized as an important data resource to support the area.

Principal Concept of Database Creation Aiming Holistic Views on the Fundamentals of Materials Science

Pierre Villars
Material Phases Data System (MPDS), Unterschwanden 6, Vitznau, CH-6354 Luzern, Switzerland
E-mail: villars.mpds@bluewin.ch

Abstract

The atomic number (AN) of the elements together with their periodic number (PN_{MD} Mendeleev) were found to form an efficient pair for the discussion of metallurgical and structural experimental facts. The periodic number PN_{MD} represents a different enumeration of the elements, emphasizing the role of the valence electrons. In contrast to the atomic number, PN_{MD} depends in details on the underlying Periodic Table of the elements. As a first result we describe the elemental-property parameters 'atomic size SZ_a' and 'atomic reactivity RE_a', derived from fits to various experimental and theoretical data sets. These two parameters can be approximated as simple functions of AN and PN_{MD}. We argue that all elemental-property parameter patterns are derived from AN and PN_{MD}, which are independent from each other.

On the example of compound formers/non-formers in binary, ternary and quaternary chemical systems we demonstrate that a quantitative link exists between material properties (experimental metallurgical facts) and AN, PN_{MD} (or simple functions of both) of the constituent elements.

Crystallographic structures (structural experimental facts) can be classified within the prototype classification (based on symmetry), as well as within the atomic environment types (AET) classification (based on the coordination polyhedron of each atom). We analyzed all binary compounds at the equi-atomic composition based on a comprehensive set of literature data using the PAULING FILE. The periodic number (PN_{MD}) was successfully used to classify all AB binary compounds by developing prototype structure maps, as well as atomic environment type maps, both leading to clear stability domains within such maps. These maps also show clear separation between chemical systems where binary AB compounds form and those where no compounds form. These maps make it possible to predict the existence of compounds that have not yet been investigated (prototype/atomic environment).

The PAULING FILE is a relational database for materials scientists, grouping crystallographic data, phase diagrams, and physical properties of inorganic crystalline substances under the same frame. Focus is on experimental observations and the data are processed from the original publications, covering world literature from 1900 to present date, further details see www.paulingfile.com. Its recently developed platforms called AtomWork-

adv (NIMS) and Materials Platform for Data Science (MPDS) (see www.crystbd.nims.go.jp and www.mpds.io), aim to give easy access to large amounts of different kinds of critically analyzed experimental data (over 1 mio. data), and by this propose giving a general overview on crystalline inorganic substances (also distinct phases called), offering possibilities to reveal yet undiscovered patterns among data and facilitate a sensible and efficient search for new materials with tailored properties. In combination with different data mining and simulation (CHALPHAD, DFT, USPEX) techniques, it provides guidelines for **Materials Design and Accelerated Development** by giving holistic views on inorganic crystalline substances, confirming that *"the whole is greater than the sum of its parts"*.

Oral Presentations

1. The Latest Trends in Data-Driven Materials Research
2. Data Infrastructure to Materials Innovation

Materials Discovery with Machine Learning: New Directions

Koji Tsuda[a,b,c]
a: GSFS, The University of Tokyo, Japan, b: NIMS, Japan, c: RIKEN AIP, Japan
Email: tsuda@k.u-tokyo.ac.jp

Abstract

It is increasingly common that machine learning is used together with experiments and simulations to discover new materials. The search problem is mathematically formulated as a black-box optimization problem. Given a large number of candidate materials, one is required to find the one with best target property with a minimum number of observations. According to the study design, the observation may be done with experiments or simulation. Machine learning methods such as Bayesian optimization, heuristic search, and deep learning have been successfully applied so far. Still, new technological developments are required to make material informatics truly useful for users. To consider possible research directions, it is necessary to classify the materials design problems into four different domains according to hardness of data acquisition and the size of search space (Table 1). In this talk, I first focus on the domain of hard data acquisition and small space, and present our strategy based on preference learning to leverage legacy data to accelerate materials search. The second topic is about the domain of easy data acquisition and large, combinatorial search space. I present how quantum annealing is employed to design complicated metamaterials.

Table 1: Four domains of materials informatics and possible research directions.

		Search Space	
		Small	Large
Data Acquisition	Hard	Data collection and integration	Search space reduction via domain knowledge
	Easy	Already addressed	Better surrogate models, global optimizers

Koji Tsuda received B.E., M.E., and Ph.D degrees from Kyoto University, Japan, in 1994, 1995, and 1998, respectively. Subsequently, he joined former Electrotechnical Laboratory (ETL), Tsukuba, Japan, as Research Scientist. When ETL was reorganized as AIST in 2001, he joined newly established Computational Biology Research Center, Tokyo, Japan. In 2000–2001, he worked at GMD FIRST (currently Fraunhofer FIRST) in Berlin, Germany, as Visiting Scientist. In 2003–2004 and 2006–2008, he worked at Max Planck Institute for Biological Cybernetics, Tübingen, Germany, first as Research Scientist and later as Project Leader. Currently, he is Professor at Department of Computational Biology and Medical Sciences, Graduate School of Frontier Sciences, the University of Tokyo. He is also affiliated with National Institute of Material Science (NIMS) and RIKEN Center for Advanced Intelligence Projec

Materials Development in the Energy and Electronics Sectors through Combinatorial Synthesis, High-Throughput Screening and Machine Learning

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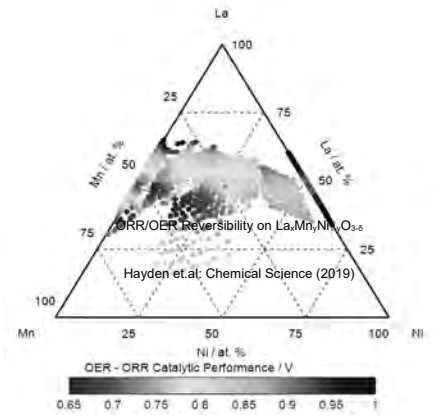
University of Southampton, UK

Abstract

The combinatorial synthesis of solid-state materials combined with high-throughput characterization and screening provides an opportunity to develop increasingly large materials data-bases, with the ultimate goal of understanding the function/composition/structure relationship, and ultimately to predict and confirm the function of new materials. There have been several approaches taken centred on combinatorial thin film synthesis of materials, however a step change in the development of new functional materials has taken place with the introduction of combinatorial evaporative PVD (ePVD) synthesis. The advantages of the approach are exemplified in combinatorial studies of solid solution in perovskite oxides, and in metal alloys. Imbedded in the associated informatics, machine learning approaches are crucial in aspects of the building, interpretation and exploitation of such data-bases, which can ultimately include physical and chemical descriptors from, for example, ab-initio calculation. The challenge is to ensure an audited content and consistent format of the experimental data. Examples of how machine learning is being developed in the interpretation of raw data sets is presented using data from high throughput investigations of perovskite electrocatalysts mediating the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) for the development of reversible fuel cells and rechargeable metal-air batteries. The use of neural-networks in the interpretation of perovskite lithium ion conductors for solid state batteries is also presented. The results provide an insight into the potential opportunities of machine learning in the future in the predictive development of functional materials.



Brian Hayden FRSC FIoP is Professor of Chemistry at the University of Southampton and director of the Advanced Composite Materials Facility dedicated to combinatorial materials discovery and their incorporation into devices, through evaporative PVD methods on a 150mm wafer scale. He is a founder (2004), an executive director and Chief Scientific Officer of Ilika plc, a £50M spin-out company involved in materials discovery and development for the electronics and energy sectors, and with strong partnerships with multinational corporations. His present research interests include the development of fuel cell electrocatalysts, materials in solid state lithium ion batteries, optoelectronic and metamaterials and tunable dielectric materials for 5G applications. He is author of over 150 refereed papers {h-index 39} and over 30 active patent families including catalysts for PEMFC and materials for solid state Li-ion batteries.
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Smart and Data-efficient Exploration of Novel Solid Electrolytes by DFT and Machine Learning

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Battery Materials Group, MaDIS, NIMS, Japan

Abstract

All-solid-state batteries with high energy density are strongly sought nowadays because of their promise of high safety and reliability during operation, these features are especially desirable in applications such as portable electronic devices, electrical stationary power and storage, and electric vehicles. One critical component of such energy devices is the solid electrolyte component which is required to be of high ionic conductivity and high chemical/electrochemical stability. Meanwhile, material screening via combined high-throughput materials simulations based on density functional theory (DFT) and machine learning techniques has now become widespread in the battery field, aiding experimentalists by identifying promising candidate materials for experimental testing. In this presentation, recent efforts of our group related to the development of smart and data-efficient computational workflows for finding novel fast ionic conductors for battery applications will be presented. Specifically, a developed workflow based on the Bayesian optimization framework will be highlighted, which employs computation-intensive battery properties (by DFT methods) as the objective functions (e.g., ion migration energy barrier, ionic conductivity, etc.) in order to efficiently screen target chemical spaces that are mainly generated *in silico*.

Randy Jalem is a senior researcher staff of the GREEN center and member researcher of the MaDIS center at the National Institute for Materials Science (NIMS), Japan. He received his MS and PhD degrees in materials science and engineering from Nagoya Institute of Technology, Japan in 2011 and 2014, respectively. After completing postdoctoral research at Kyoto University - ESICB in 2014-2015, he moved to NIMS as a postdoctoral researcher in 2015-2016, JST PRESTO researcher and open-lab researcher in 2016-2017, researcher staff in 2017, and senior researcher staff in 2018. He also joined the Kyoto University - ESICB as a project assistant professor in 2017. His research interests include battery materials design and development, in particular, using computational modeling and materials informatics. Email: JALEM.Randy@nims.go.jp.

Challenges and Solutions in Soft Materials Informatics

Yaroslava G. Yingling
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North Carolina State University, USA

Abstract

The number of applications of data-driven materials discovery is rapidly growing. The large amount of available materials characterization and computational data, combined with high-level statistical algorithms, is proving to be extremely useful in developing complex predictive models. However, in the field of soft matter, which includes complex materials such as polymers, liquids, emulsions, colloids, and gels, there is a slower adoption of informatics strategies than in adjacent fields mainly due to complexity of underlying processes and plethora of processing components that dictates the properties. In this talk, I will discuss the examples of using materials informatics for the design of ligand functionalized nanoparticles (NPs). Such NPs can be used as transfection vectors for efficient wrapping or packaging of DNA and RNA which is a critical part enabling gene delivery. Because DNA/RNA transfection is dependent on the size, shape, and surface properties of the DNA/RNA-vector complex, control over assembly structure is critical for creating effective transfection agents. Evolving nanomaterials to the clinic requires optimization, which is prohibitively expensive, and a mechanistic understanding of carriers-NA interactions, which remains unknown. We attempt to advance tailored materials for gene delivery by a multiscale optimization employing all-atom simulations techniques and machine learning algorithms. We were able to design novel nanoparticle ligands capable of controlled wrapping of NA around NP. Our methods can significantly speed up the search for a new ligand design based on experimental, in silico and available literature data for ligand-stabilized NPs.

Yaroslava G. Yingling is Professor and Director of Undergraduate Program at Materials Science and Engineering at North Carolina State University. She received her University Diploma in Computer Science and Engineering from St. Petersburg State Technical University of Russia in 1996 and her PhD in Materials Engineering and High Performance Computing from the Pennsylvania State University in 2002. She carried out postdoctoral research at Penn State University Chemistry Department and at the National Institutes of Health National Cancer Institute prior to joining North Carolina State University in 2007. She received the National Science Foundation CAREER award (2012), American Chemical Society Open Eye Young Investigator Award (2012) and was named a NCSU University Faculty Scholar in 2014. Research interests in Prof. Yingling's group are focused on the development of soft materials informatics, advanced computational models and novel algorithms for multiscale molecular modeling of soft and biological materials. She has published more than 80 papers, gave 100 invited talks and seminars, organized 10 professional symposiums and workshops and has been serving as an Editor for Journal of Materials Science and as an Editorial Board Member of ACS Biomaterials Science and Engineering and ACS Applied Materials and Interfaces.

Practical Application of Machine Learning for Soft Matters

Masanobu Naito
Group Leader, Research and Services Division of Materials Data and Integrated System (MaDIS), NIMS

Abstract

Development times for new materials generally takes 10–20 years, despite the ever-growing materials literature. In order to reduce both the time-to-market and development cost of new products, machine learning techniques began to play an important role in the discovery of novel functional materials with high performance. Typically, machine learning trains its algorithms on large databases, in order to identify unrecognized trends or patterns, and even propose new candidate materials. However, experimental datasets in the materials science field are often expensive to build or involves missing and sparse data with certain amount of unintentional errors.

In this talk, we will introduce our attempt on the prediction and optimization of adhesive materials, for which datasets are very limited, by combining the design of experiment techniques, an active learning pipeline, and a Bayesian optimization. This study demonstrates the promising use of an active learning pipeline in the construction of an accurate machine learning model using initially a very small or no existing dataset, and then cyclically use it to accelerate the design and development of extremely strong structural adhesive from a massive combination of candidate materials and reaction condition.

Masanobu Naito completed his PhD studies in biotechnology at the Tokyo Institute of Technology in 2001. Afterwards, he took a JSPS postdoctoral position at University of California, Irvine. In 2002, he joined the Graduate School of Materials Science, Nara Institute of Science and Technology, as an assistant professor. Since April 2010, he has become a principal investigator. In 2011, he promoted to be an associate professor. During this time, he joined PRESTO-JST project.
In 2012, he joined the National Institute for Materials Science (NIMS) Japan as a principal researcher. In 2016, he became a group leader, and now he conducts the data-driven polymer design group in research and services division of materials data and integrated system (MaDIS). Concurrently, he joined the university of Tokyo and Tsukuba university as an associate professor and a full professor, respectively. Since this October, he joined CREST-JST on Revolutional Materials Development as a research director. His research interests include surface chemistry, adhesive, coating, and functional polymeric materials.

Materials Innovation Driven by Data and Knowledge Systems

Surya R. Kalidindi
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School of Computational Science and Engineering
School of Materials Science and Engineering
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Abstract

Emerging concepts and toolsets in Data science and Cyberinfrastructure can be strong enablers for systematic mining and automated capture of Materials Knowledge and its dissemination to distributed cross-disciplinary teams engaged in materials innovation efforts. A data-driven framework is also foundational to the development and implementation of autonomous explorations of the unimaginably large materials and process design spaces while synergistically leveraging all available experimental and simulation data. Although tremendous progress has been made in the development and validation of a wide range of simulation toolsets capturing the multiscale phenomena controlling the material properties and performance characteristics of interest to advanced technologies, their systematic insertion into the materials innovation efforts has encountered several hurdles. The ongoing efforts in my research group are aimed at accelerating materials innovation through the development of (i) a new mathematical framework that allows a systematic and consistent parametrization of the extremely large spaces in the representations of the material hierarchical structure (spanning multiple length/structure scales) and governing physics across a broad range of materials classes and phenomena, (ii) a new formalism that evaluates all available next steps in a given materials innovation effort (i.e., various multiscale experiments and simulations) and rank-orders them based on their likelihood to produce the desired knowledge (expressed as PSP linkages), and (iii) novel higher-throughput experimental assays that are specifically designed to produce the critically needed fundamental materials data for calibrating the numerous parameters typically present in multiscale materials models. I will present and discuss ongoing research activities in my group.

Surya Kalidindi is a Regents Professor, and Rae S. and Frank H. Neely Chair Professor in the Woodruff School of Mechanical Engineering at Georgia Institute of Technology, Georgia, USA with joint appointments in the School of Materials Science and Engineering as well as the School of Computational Science and Engineering. Surya earned a Ph.D. in Mechanical Engineering from Massachusetts Institute of Technology in 1992, and joined the Department of Materials Science and Engineering at Drexel University as an Assistant Professor. After twenty years at Drexel University, Surya moved into his current position at Georgia Tech. Surya's research efforts have made seminal contributions to the fields of crystal plasticity, microstructure design, and materials informatics. Surya has been elected a Fellow of ASM International, TMS, and ASME. In 2016, he and his group members have been awarded the top prize as well as one of the runner-up prizes in the national Materials Science and Engineering Data Challenge sponsored by the Air Force Research Lab in partnership with the National Institute of Standards and Technology and the U.S. National Science Foundation. He has also been awarded the Alexander von Humboldt Research Award, the Vannever Bush Faculty Fellow, the Government of India's Vajra Faculty Award, and the Khan International Award.

Data Scientific Approaches in Materials Integration

Masahiko Demura
Research & Services Division of Materials Data and Integrated System (MaDIS)
National Institute for Materials Science (NIMS), Tsukuba, Japan

Abstract

Processing, structure, property, and performance are the basic elements in materials science and engineering. Materials Integration is a concept to computationally link among the four elements for predicting performance from processing. We have intensely applied data scientific approaches in Materials Integration and obtained higher accuracy of predictions or more flexibility in use of experimental data. In this talk, we will introduce how we have used them particularly in the field of structural materials through a couple of application examples. Firstly, we have applied the Bayesian inference framework of model selection to the prediction of creep behavior in high Cr heat resistant steels. Our model selection analysis revealed that the experimental data of creep strain vs. time curves support the existence of a steady state in the creep deformation of a Gr. 91 steel. The same model selection method made it possible to identify what alloying elements dominate long-term creep rupture time in low carbon steels. Secondly, we have applied machine learning algorithms to build an accurate prediction model of creep rupture time, which model is applicable for a wide range of ferritic steels. Our work clearly demonstrates that the accumulation over 40 years in the NIMS creep data sheet has a great potential to extract the prediction of creep rupture time within a factor of two at least. Besides, we will shortly present the application of pattern recognition to the quantification of metallic microstructures.

This work was supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Materials Integration for Revolutionary Design System of Structural Materials” (Funding agency: JST).

Dr. Masahiko Demura, Deputy Director of Research & Services Division of Materials Data and Integrated System at National Institute for Materials Science (NIMS), Japan. He received his B. Eng. in Metallurgy in 1993 and M. Eng. in Material Science and Engineering in 1995 at The University of Tokyo (U. Tokyo). He started working at National Research Institute for Metals (current National Institute for Materials Science, NIMS). He received his Dr. Eng. in Material Science and Engineering from U. Tokyo in 2003. In 2015 he became Project Professor at U. Tokyo, where he remained until he moved back to NIMS in April, 2017. His recent research interests include the digital transformation in materials research, particularly in the field of structural materials. Demura can be reached by email at DEMURA.Masahiko@nims.go.jp.

From the Harvard Clean Energy Project to Self-Driving Laboratories: A journey in Materials Discovery.

Alan Aspuru-Guzik
Professor of Chemistry and Computer Science
Canada 150 Research Chair in Quantum Chemistry
Canada CIFAR AI Chair | Vector Institute | CIFAR Senior Fellow
University of Toronto, Canada

Abstract

In this talk, I will discuss my group's trajectory in the field of the accelerated discovery of organic materials. We began in 2006 planning what became the Harvard Clean Energy Project. It was, at the time, the largest quantum chemistry set of calculations that I am aware of. Since then, our research group has been developing tools to accelerate the discovery of materials such as organic photovoltaics, organic light-emitting diodes and organic flow batteries. We recently came to the realization that high-throughput screening is not enough to close the loop in materials discovery, and that materials acceleration platforms, or self-driving aboratories, comprising robotics, high-performance computing and automation can lead to a mode of "autonomous" materials discovery. I try to describe the trajectory from 2006 to thirteen years later and will end describing our current efforts in the autonomous discovery of thin-film organic conductive materials, organic photovoltaics and the beginning of a multiple-PI project on self-driving organic laser discovery.

Alán Aspuru-Guzik*'s research lies at the interface of computer science with chemistry and physics. He works in the integration of robotics, machine learning and high-throughput quantum chemistry for the development of materials acceleration platforms. These "self-driving laboratories¨ promise to accelerate the rate of scientific discovery, with applications to clean energy and optoelectronic materials. Alán also develops quantum computer algorithms for quantum machine learning and has pioneered quantum algorithms for the simulation of matter. He is jointly appointed as a Professor of Chemistry and Computer Science at the University of Toronto. Alán is a faculty member of the Vector Institute for Artificial
Intelligence. Previously, Alán was a full professor at Harvard University where he started his career in 2006. Alán is currently the Canada 150 Research Chair in Quantum Chemistry as well as a CIFAR AI Chair at the Vector Institute. Amongst other awards, Alán is a recipient of the Google Focused Award in Quantum Computing, the MIT Technology Review 35 under 35, and the Sloan and Camille and Henry Dreyfus Fellowships. Alán is a fellow of the American Association of the Advancement of Science and the American Physical Society. He is a co-founder of Zapata Computing and Kebotix, two early-stage ventures in quantum computing and self-driving laboratories respectively.

NIMS Talk 4

From Data Extraction to Data Utilization: Techniques for Practical Use of NIMS Materials Database

Masashi Ishii
Research and Services Division of Materials Data and Integrated System (MaDIS)
National Institute for Materials Science (NIMS), Tsukuba, Japan

Abstract

NIMS materials databases known as "MatNavi" have been widely used by organic and inorganic scientists. Recent data-driven science typically known as materials informatics (MI) requires information gigantism in the database service. The enormous service is designed with advanced but practical techniques of (1) rapid data mining techniques and (2) big data integration service.

(1) Rapid data mining techniques

Data curation policy in NIMS is "Management of Quality and Quantity (MQ^2)". The Quality data curation in MQ^2 is based on the know-how which was established by steady trials in NIMS. Even for MI, the quality data may provide a reasonable prediction model. On the other hand, for the Quantity data curation in MQ^2, we rely on an originally developed data mining system, in which artificial intelligence (AI) is act as a core technology. Despite popular expectation for AI, we complementally use a rule-based target-data extraction. The complementally use is caused by that AI-based extraction decreases precision because of false positive (FP), while rule-based extraction decreases recall on account of false negative (FN). The developed system successfully satisfied the competitive requirements for bigdata and unerring data, and 85 kinds of polymer properties, 86,415 points of data were automatically extracted as of May 29, 2019. The data points are increasing at this moment.

The combination of AI- and rule-based techniques was also applied to make "Materials recipe". Process conditions to be used for machine learning of process optimization or prediction of possible chemical reaction paths were systematically extracted by AI that studied grammatic modification structures. It was confirmed that a rule-base preprocessing well cover sentence variety in writings.

(2) Big data integration service

For the data-driven scientific applications by users, we are constructing data providing services using Application Programming Interface (API) and resource description framework (RDF). Although RDF was developed as an international protocol for metadata description, we recognize compatibility of the protocol with data-driven science. RDF can integrate various public data and makes a hierarchy of the integrated data. A protocol and RDF query language (SPARQL) can create a subclass according to demands for MI. We have partly made RDF of a NIMS database and demonstrated integration with Nikkaji and PubChem public databases made by other organizations, Japan Science and Technology Agency (JST) and National Institute of Health (NIH).

Masashi Ishii is a group leader of the Matrials Database Group of MaDIS at the National Institute for Materials Science (NIMS). He received his PhD degree in engineering from Osaka University in 1995. After completing postdoctoral research at RIKEN, and as a beamline scientist at SPring-8, he moved to NIMS as a scientist in 2003. His research interests include metrological informatics in spectroscopies, database construction in semantic frameworks. Ishii can be reached by email at ISHII.Masashi@nims.go.jp.

Poster Presentations

I. Data-driven Research in Functional Materials

II. Data-driven Research in Structural Materials

III. Materials Data Infrastructure Including Measurements

I-01

Efficient recommendation tool of materials on Windows computers

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[1]International Center for Materials Nanoarchitectonics, National Institute for Materials Science
[2]Research and Services Division of Materials Data and Integrated System, National Institute for Materials Science
[3]Graduate School of Frontier Sciences, University of Tokyo
[4]Center for Advanced Intelligence Project, RIKEN
[5]Graduate School of Medicine, Kyoto University

To accelerate the discoveries of novel materials, an easy-to-use materials informatics tool is essential. We developed materials informatics applications, which can be executed on a Windows computer without any special settings[1]. Our applications are composed of two executable files: COMBO.exe and PDC.exe. These are available from our project page[2]. COMBO.exe is a Bayesian optimization tool based on the COMmon Bayesian Optimization library (COMBO)[3]. This selects candidate materials, which may have the desired properties, for syntheses or simulations by machine learning. On the other hand, the selection of a candidate point to efficiently complete a phase diagram can be performed by PDC.exe based on the uncertainty sampling for the phase diagram construction (PDC)[4].

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I-02

Data-Driven Materials Discovery of Indirect Band-Gap Semiconductors for Photovoltaics

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Owing to long lifetime of band-to-band recombination, indirect band-gap semiconductors would be applicable to high-performance solar cells if processing the adequate direct band gap to absorb visible light efficiently. In this study high-throughput computational screening was conducted to discover interesting indirect-gap semiconductors for photovoltaics by exploring the Materials Project [1] database. The screening procedure is as follows: i) search for the chemically stable, indirect band-gap semiconductors with favorable E_g^{dir} then ii) find candidates with optimal values of $E_g^{dir} - E_g^{ind}$ and finally iii) choose materials with small effective masses of electron and hole. Among the final 31 candidates, we investigated the optical and defect properties affecting power conversion efficiencies of $SiAs_2$, $GeAs_2$, and $NaSbS_2$ that have advantages over other candidates in terms of cost and abundancy of constituting elements. The results show that the absorption coefficients of the materials look promising. Our defect calculations provided guidelines to optimize growth conditions for these materials.

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I-03

Machine Learning Model for Predicting Dielectric Constants of Oxides

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Dielectric oxides are technologically important as to their applications to electronic devices. To find novel dielectric oxides, high-throughput *ab initio* calculations are effective,[1)] but the search space is severely limited by the computational cost. In this work, we construct an efficient prediction model of both electronic and ionic dielectric constants in oxides from a combination of high-throughput calculations and machine learning techniques.

The construction of machine learning models includes the following steps: (i) density functional perturbation theory calculations[2,3)] of dielectric constants; (ii) representation of oxides with descriptors[4,5)]; (iii) training of random forest regression models[6)] for reciprocal dielectric constants; and (iv) verification with RMSEs. The resultant RMSE for reciprocal ionic dielectric constants is 0.037, which implies that the model is accurate enough to predict the order of the dielectric constants.

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I-04

Compositional descriptor-based prediction for the chemical compound stability

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A very active area of materials research is to devise methods that use machine learning to extract predictive models from existing materials data, *i.e.* descriptors to featurize materials. There are two types of descriptors: crystal structural descriptor and compositional descriptors for inorganic solid-state compounds. In general, obtaining a structure descriptor is more costly than compositional descriptors. Therefore, prediction of materials properties only by compositional descriptors are attractive idea and useful tools for screening desirable materials as reported[1].

Recently, we suggested general descriptors, usable for materials datasets containing various compositions and crystal structures. The basic idea of the descriptor is binning and the frequency of occurrence for material-related features, i.e., "histograms of features"[2]. The obtained histogram is smeared by the Gaussian function with appropriate smoothing factors, since each neighboring bin is independent to follow machine-learning-based regression. In this study, we predicted chemical compound stability with only histograms of compositional features. Details of results and discussion will be given in the presentation on the day.

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I-05

Experimental search for NASICON-type solid electrolytes with high Li-ion conductivity guided by Bayesian Optimization

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[2] ESICB, Kyoto University
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Li-ion batteries (LIB) are widely used for electric vehicle, and demand for high energy density and further safety of Li-ion batteries is growing. Replacing the liquid electrolyte in conventional Li-ion batteries with solid electrolytes is advantage of not only inflammability but also increasing energy density. Recently, NASICON-type solid electrolyte $LiZr_2(PO_4)_3$ (LZP) has attracted as an oxide-based solid electrolyte, and be reported high Li-ion conductivity [1-3] and stable charge-discharge cycling as all solid-state LIB[4].In this study, we focused on the CaO and Y_2O_3 co-doped Li-rich NASICON-type LZP solid electrolytes. It was reported that Li-ion conductivity was improved by doping small amount of Ca or Y is reported [1,2]. We evaluate Li-ion conductivity for 49 composition of $Li_{1+x+2y}Zr_{2-x-y}Y_xCa_y(PO_4)_3$ ($0 \leqq x \leqq 0.376$, $0 \leqq y \leqq 0.376$), and demonstrate Bayesian Optimization approach[5] to search for optimal composition with high Li-ion conductivity efficiently.

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I-06

Machine–Learning–Assisted for Exploration of Synthesis Condition for Metastable Novel Lanthanide Metal–Organic Frameworks Using Failed Experiments

Yu Kitamura [1], Emi Terado [1] and Daisuke Tanaka [1, 2]
[1] Graduate School of Science and Technology, Kwansei Gakuin University, Japan
[2] JST PRESTO

Lanthanide Metal–Organic Frameworks (Ln–MOFs) have been widely studied for luminescence and sensor application. It is well known that the synthesis of Ln–MOFs has been suffered from many crystal polymorphisms because various reaction intermediates exist. Moreover, Ln–MOFs generally provide many crystal polymorphisms because lanthanide ions show many flexible coordination geometry, resulting in isostructural crystal structure regardless of different metal ions. Therefore, it is difficult to synthesize crystal polymorphs of Ln–MOFs selectively, and synthesis guidelines have not been established. In this study, we tried to extract the dominate factors of the synthesis by using machine learning techniques; cluster analysis and decision tree. As a result, it was suggested that the reaction condition to synthesize novel phase showed strong dependency on reagent company and a few impurities in the reagent affects the crystallization.

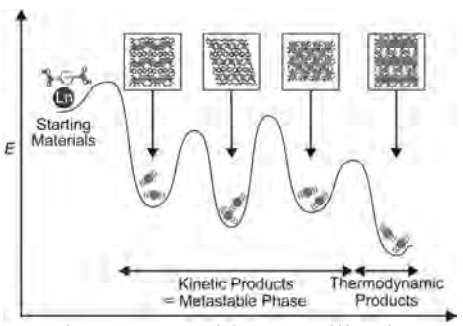

Fig 1. Metastable crystallization process

Machine–Learning–Assisted Synthesis of Silver Thiolate Metal Organic Frameworks

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[1] Graduate School of Science and Technology, Kwansei Gakuin University, Japan
[2] JST PRESTO

Metal Organic Frameworks (MOFs) exhibit promising various functionalities by utilizing their uniform framework structures. In this work, we explored the synthesis conditions of MOFs containing Ag-S bonds by high throughput screening systems. We tried to synthesize MOFs composed of trithiocyanuric acid (H_3ttc) as a sulfide containing ligand and Ag^I as a center metal ion. We implemented cluster analysis to categorize their powder X-ray diffraction (PXRD) patterns into several different types. By evaluating the correlation between synthesis conditions and PXRD patterns with decision tree, unknown PXRD patterns appeared under specific synthesis conditions (Fig. 1). We have demonstrated that decision tree analysis is useful to predict the reaction mechanism and explore synthesis condition for the novel MOFs. In addition, we have succeeded in determining crystal structures of the novel MOFs, $Ag(H_2ttc)$ and $Ag_2(Httc)$.

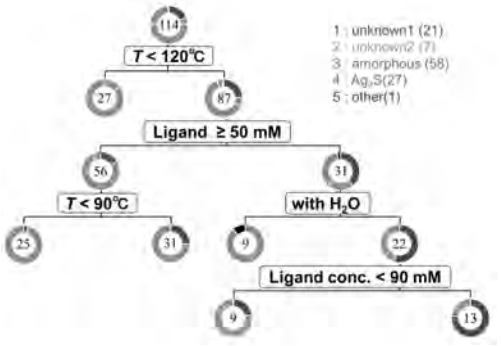

Fig 1. Decision tree derived from a series of synthesis conditions

Predicting Chemical and Electronic Properties Using a Novel Descriptor "Elemental Fingerprints set" with Neural Networks

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Rapid growth of machine learning (ML) techniques enables to predict various material properties, screen promising candidate materials, etc. In many cases, however, a model for ML is applicable only to a specific family of materials or requires information difficult to obtain in real experiments. We propose a novel descriptor set named "elemental fingerprints set" for situations where only limited information, concentration of raw materials or chemical formula, is available for ML.

The elemental fingerprints set is made from the frequency distribution of properties of the elements in the target material. This feature fits well with the situations where actual atomic arrangements are unknown and only the experimental conditions and target materials are controllable. To demonstrate the effectiveness of the elemental fingerprints set, we tried to predict the standard formation energy and band gap energy by ML using data taken from Open Quantum Materials Database (OQMD). The models for ML were constructed using the fully connected neural network ensemble with adversarial training.

We found that the elemental fingerprints set can predict these quantities better than two other descriptor sets suggested previously. Moreover, we found that the combination of these three descriptor sets gives better prediction performance: The standard formation energy and the bandgap energy are predicted with the mean absolute error of 31 meV/atom and 38 meV respectively.

I-09

Design and Optimization of Epoxy Adhesives through Active Learning from a Small Dataset

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Machine learning has begun to play an important role in design and development of novel high-performance functional materials. However, experimental datasets in the polymer-science field are typically limited and they are expensive to construct. Their size (< 100 samples) limits the development of chemical intuition from experimentalists, as it constrains the use of machine-learning algorithms for extracting relevant information. We tackle this issue to predict and optimize adhesive materials by combining laboratory experimental design, an active learning pipeline and Bayesian optimization. We start from an initial dataset of 32 adhesive samples that were prepared from various molecular-weight bisphenol A-based epoxy resins and polyetheramine curing agents, mixing ratios and curing temperatures. Our data-driven method allows us to propose an optimal preparation of an adhesive material with a very high adhesive joint strength measured at 35.8 ± 1.1 MPa after three active learning cycles. A Gradient boosting machine learning model was used for the successive prediction of the adhesive joint strength in the active learning pipeline, and the model achieved a respectable accuracy with a coefficient of determination, root mean square error and mean absolute error of 0.85, 4.0 MPa and 3.0 MPa, respectively. This study demonstrates the important impact of active learning to accelerate the design and development of tailored highly functional materials from very small datasets.

I-10

Automatic Extraction Framework of Superconductors Related Information from Scientific Literature

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The automatic collection of materials information from research papers is highly required for rapid materials development using big data, namely materials informatics (MI). Unfortunately, the development of such tools is made difficult by the variability of expressions in technical writing. We present an interdisciplinary work [1] to construct a robust system for the automatic collection of superconductor-related information from scientific literature using text mining techniques.
We focus on the identification of superconducting material names and their key property critical temperature (Tc). The system achieved convincing results with minimal training data.
We are working on improving the initial prototype with better algorithms and collaborating with domain experts to create a bulk dataset for the superconductors properties extraction.

[1] L. Foppiano, T. M. Dieb, A. Suzuki, and M. Ishii. Proposal for Automatic Extraction Framework of Superconductors Related Information from Scientific Literature. Letters and Technology News, vol. 119, no. 66, SC2019-1 (no.66), volume 119, pages 1–5, Tsukuba, May 2019. ISSN: 2432-6380.

Data-Driven Design of Thermoelectric Materials with Experimental Data on Starrydata

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The experimental data accumulated by materials researchers are the seeds for the Materials Informatics (MI). However, most of the published experimental data are embedded in plot images, and digitization of such data is difficult by automatic programs. Therefore, we developed an open web application named *Starrydata*, in which persons can efficiently collect and share experimental data on published papers. We have currently succeeded in collecting thermoelectric properties of over 19,000 samples extracted from over 3,700 papers. Each experimental data is associated with sample information including chemical composition.

In this study, we developed machine learning models to predict experimental thermoelectric properties directly from chemical compositions. We attempted to search for candidate thermoelectric materials with high *ZT* and optimization of complex compositions to increase the *ZT*. We predicted *ZT* of over 7000 stable semiconductors obtained from *Materials Project*, at different temperatures. We also predicted *ZT* of arbitrarily generated 10,000 compositions composed of up to 5 elements, to visualize the composition dependences of *ZT* on the ternary maps with 3 free parameters.

Starrydata: a web system for experimental data extracted from published plot images

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We developed an open web system named *Starrydata* (https://www.starrydata2.org)[1], which shares the links to the papers, their bibliographic information (title, authors, journal names etc.), and the numerical data extracted from the plot images in the papers. *Starrydata* allows worldwide users to browse, add, edit and download the data, free of charge. The data on *Starrydata* can be collectively downloaded as data files or automatically retrieved through an API. Two types of datafiles: raw data and interpolated data are available. The datafiles can be displayed in our interactive visualizer. *Thermoelectric Materials* database is our prototype database in *Starrydata,* which contains temperature (*T*) dependences of Seebeck coefficient *S*, electrical conductivity σ, electrical resistivity ρ, total thermal conductivity κ, power factor $P=S^2\sigma$ and dimensionless figure of merit $ZT=PT/\kappa=S^2\sigma T/\kappa$ of 19,000+ samples extracted from reported in 3,700+ papers. Databases on other functional materials are on development. [1] Y. Katsura, M. Kumagai et al., *Sci. Technol. Adv. Mater*. **20** (2019) 511-520.

I-13

Active learning: A Booster for Discovering New Materials from Small Datasets

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The size of the experimental and/or computational datasets available in materials science and related fields is usually small (<< 1,000 samples). This strongly constrains the use of machine learning (ML) algorithms for accelerating the search and discovery of novel functional materials. Furthermore, ML recent developments are usually focused on huge datasets (>> 1M samples) because of the primary goals from companies like Google, Microsoft or Amazon to deliver services driven by a mass-consumption. However, it actually exists a branch of ML called active learning (AL), also known as optimal experimental design, which is underrepresented in the present literature. AL is a kind of on-line supervised learning algorithm which query new experiments to be taken according to an internal score which balance the trade-off between exploitation and exploration of a free parameters space. The results from the queried experiments are then fed back to the supervised learner component of the AL pipeline to be fine-tuned and express new queries. This AL cycle: "supervised training"–"queries"–"experiments" can guide the search for an optimal design of a material and this by starting from a fairly small dataset (several tens of samples). Therefore, one doesn't need to randomly grow a huge database from scratch to luckily make a breakthrough but can smartly direct the growth of experimental data according to a final goal. Thus, I will present an overview of the AL principle and illustrate it through the successful design of an epoxy resin with the highest adhesive strength on the market. An AL pipeline is field-, data- and goal-agnostic, and it can therefore be applied to any kind of materials optimization.

I-14

Accelerating metamaterials design by quantum annealing

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Materials design is often a try-and-error process, because we seldom have a priori knowledge about how the targeted property responds to the complex structure of materials. The problem is classified as a black-box optimization. We proposed a new black-box optimization method combining factorization machines (FM) and D-Wave 2000Q, a quantum annealing (QA) machine, in Ref. [1]. QA is used to guide through the enormous search space based on a regression model of FM.

We coupled the new method with an atomistic simulation to design complex radiative cooling metamaterials composed of SiO_2, SiC, and Poly(methyl methacrylate), to demonstrate an example of automated materials design.

[1] K. Kitai et al., arXiv:1902.06573 (2019).

I-15

Automation of the first-principles calculation and machine learning to search functional materials of high entropy alloys

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The high entropy alloys attract much attention originally because of strength/hardness. They are potentially also useful as functional materials, such as high Curie temperature and high magnetic moment, and large spin-orbit coupling. However, the difficulty of the research of the high entropy alloys is that there exist too huge number of possibilities for humans to handle. Therefore, it is wise and inevitable to screen materials that have high functionality in the first-principles before executing experiments.

We already have basic technologies to massively calculate periodic structures in the first-principles automatically without any human resources. However, we didn't have it for random structures in the first-principles calculation. We first introduce a newly developed workflow to converge the electric structure self-consistently and to estimate physical properties of random alloys automatically in the first-principles. We also introduce some of the first-principles results, and explain key features for high Curie temperatures and high magnetic moment.

I-16

Orbital Field Matrix: A New Descriptor for Materials

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We propose a novel representation of materials called Orbital Field Matrix (OFM) [1,2]. In the OFM, the local structure of a material, defined by the Voronoi partition, is expressed by a matrix using the information of electron configuration of the central atom and adjacent atoms. We apply the OFM to construct Kernel-ridge regression model for transition-metal rare-earth compounds. We find that the model can reproduce the formation energies and local magnetic moments, obtained by first-principles calculation, with the mean absolute error of 0.10 eV/atom and 0.03 μ_B, respectively.

[1] T.-L. Pham et al., STAM **18**, 756 (2017).
[2] T.-L. Pham et al., J. Chem. Phys. **148**, 204106 (2018).

I-17

Subgroup Relevance Analysis: A Scheme for Selecting Important Descriptor Groups

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We propose an interactive scheme for selecting important descriptors and descriptor groups. In this scheme, we adopt hierarchical clustering in the descriptor space, and execute relevance analysis. It helps us choose the combination of good descriptors and understand the meaning of the selected combination of descriptors. As a demonstration, we analyze the Curie temperatures of rare-earth transition-metal binary alloys. By comparing subgroup relevance analysis (SRA) with the exhaustive search, we show that SRA successfully selects important descriptors and descriptor groups.

[1] H.-C. Dam et al., J. Phys. Soc. Jpn. **87**, 113801 (2018).

I-18

High-throughput production of force-fields for Li-ion battery materials

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There are a lot of possible candidates for solid-state electrode materials in Li-ion battery and thus computational approaches of screening are employed to reduce the search space instead of producing and testing all those candidate materials. Usually, ab-initio methods such as density functional theory (DFT) are used to compute some properties of candidate materials. However, computational cost of ab-initio methods is high and it is not feasible to perform large supercell systems or dynamic simulation to assess the properties of all the candidates. Thus the classical force-fields (FF) are employed to achieve high-throughput screening, but the FF is not always available and sometime its accuracy is unsatisfactory. We have developed a program (Nagoya atomistic-simulation package; nap) for the production of classical FFs efficiently with a satisfactory accuracy by learning from small amount of DFT calculations. We will show some example of FFs for Li-ion battery materials produced using nap and show dynamical properties of the FF produced via semi-automatic manner.

Data-driven Exploration of Ion Conductive Alkali Metal Oxide for Batteries Using Materials Simulation

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In this study, efficient high-throughput computational approaches for exploration of alkali ion conductive materials by exhaustive and informatics-aided calculations are discussed. The alkali metal oxide, ~1000 compounds total, are targeted. Fast force field (FF) calculations and automation of the computational scheme enable exhaustive search for ion migration in the compound lattices. Using more general descriptors, usable for materials datasets containing various compositions and crystal structures, machine-learning-based regression is performed to build a prediction function of the evaluated diffusion coefficient D_{ion}. Accordingly, we demonstrated an improved efficiency by the materials informatics approach for identifying ion-conducting ceramics.

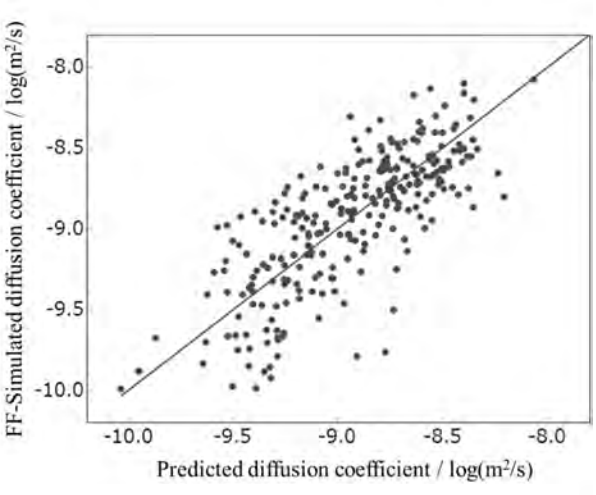

Figure 1. Diagnostic plots of the predicted and FF-simulated diffusion coefficient

Active learning for level set estimation under input uncertainty

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In this study, we consider the level set estimation (LSE) which identifies whether values of an objective function are above or below a certain threshold under input uncertainty (IU). We study two types of LSE with different IU and objective function settings. We first consider LSE for a black-box function whose evaluation is expensive under cost-dependent IU. We second consider LSE for a probability function where the black-box function exceeds the threshold under IU. We extend a MILE acquisition function which is based on expected improvement strategy proposed in a previous study to situations with IU and propose a new active learning method for LSE under IU. We give several theoretical guarantee for our proposed method. In addition, we confirm that the proposed method has same or better performance than other previous methods through numerical experiments.

I-21

Topological Data Analysis toward Design of Functional Materials

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Understanding relationship between structure and functional property is one of the essential subjects in materials science, and data driven approach such as machine-learning has recently made a remarkable progress in this problem based on the combination of computational simulations and advanced measurements. Once we think of treating disordered or complex systems (glass, composite materials, ...), however, there still remains difficulty in how to translate such structural information into quantitative and useful descriptors.

Topological data analysis, especially persistent homology is a powerful mathematical tool to compute and describe the "shape" of discrete objects such as atomic configurations and pixel/voxel data. In this framework, geometrical information is extracted and summarized as a two-dimensional map called persistence diagram (PD), in which birth and death of n-dimensional holes in data are recorded. Once PD is appropriately converted to vector data, any machine-learning techniques become applicable to solve inverse problems. In this poster presentation, we introduce the outline of our activities and a few of scientific achievements supported by "Materials research by Information Integration" Initiative (MI^2I) project of the Support Program for Starting Up Innovation Hub from Japan Science and Technology Agency (JST).

I-22

Leveraging Legacy Data in Materials Science via Preference Learning

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Machine learning applications in materials science are often hampered by lack of experimental data. Integrating legacy data from past experiments is a viable way to solve the problem. Even if an additional dataset about the physical quantity of interest is available in literature or databases, naive data mixing leads to poor results, because of different measurement conditions or assumptions. In this paper, we present a novel strategy to enhance the performance of Bayesian optimization with preference learning.

The learning process is solely based on pairwise relations of data in the same dataset, avoiding comparison of quantities in different datasets. Main framework consists of Gaussian process preference learning and Bayesian optimization. In benchmarking our method, we consider two types of problems. One is searching for organic molecules with longer absorption wavelength and the other is searching for the largest bandgap from an inorganic oxide dataset. Overall, preference learning was effective in exploiting information in legacy data. The performance of integration depends on the overlap between candidate materials and examples in legacy data. We demonstrate that Bayesian optimization is significantly enhanced via addition of legacy data. This approach could be a new tool of data integration in a wide range of materials science problems.

Metabolite Identification with de novo Molecule Generation

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NMR spectroscopy is a powerful tool to identify molecules in a sample. Previously observed NMR spectra are accumulated in public databases, but they cover only a tiny fraction of chemical space. Molecule identification with database search is often unsatisfactory and requires *ad hoc* modification by experts. We propose NMR-TS, a machine-learning-based algorithm that aims to identify *any* molecule automatically. Given a target spectrum, NMR-TS employ deep learning and DFT-based spectrum prediction to discover novel molecules whose predicted spectrum matches the target. We conducted a proof-of-concept study of identifying prototypical metabolites from their predicted spectrum.

II-01

Data Driven Research for Composite Materials (Structural and Mechanical Properties of PAN- and Pitch-based Carbon Fibers)

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Polyacrylonitrile (PAN)-based and pitch-based carbon fibers are widely used as reinforcements in composite materials owing their high specific strength and specific modulus. These composites are dominant materials in several industries. The trends in the development of carbon fibers are characterized as follows; high tensile strength, a fairly high strain to failure (approximately 2%) and a high specific modulus with high thermal conductivity. Several high strength (exceeding 5 GPa) PAN-based and high modulus (more than 900 GPa) pitch-based carbon fibers are commercially available at present. However, the mechanical properties of the high strength and high modulus PAN- and pitch-based carbon fibers have not yet been characterized well. In this study, structural and mechanical were evaluated for commercially available high strength PAN-based, high modulus PAN-based, high modulus pitch-based, and high ductility pitch-based carbon fibers. I would like to clarify the anisotoropic properties and fracture mechanics, and to build the database for structural and mechanical properties of PAN- and pitch-based carbon fibers in order to use multiscale analysis and optimum design of composite materials.

This work was supported by Council for Science, Technology and Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Materials Integration for revolutionary design system of structural materials”(Funding agency:JST).

II-02

Experimental evaluation on the environment resistance and fracture characteristics of multi-functional CFRP

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The application of carbon fiber reinforced plastic (CFRP) as a structural material has been actively pursued for the purpose of reducing weight via its attractive mechanical properties, such as high-specific strength. Further weight-reduction in machine structure and cost-cutting of the material by adding functionalities (e.g. flame retardant, thermal conductivity or vibration-damping etc.) have received a lot of attention in recent years. Against such a background, a novel CFRP with functional domain(s) is going to be developed to provide required functionalities in the next-gen aircraft and vehicles. In this presentation, the following research topics conducted as a part of the “Cross-ministerial Strategic Innovation Promotion Program (SIP)” are introduced:

- Multi-scale investigations on the fracture mechanism and influential factors (e.g. high-temperature environment) on the static/fatigue strength properties of the novel CFRP;
- Construction of the database of mechanical and functional properties of CFRPs (incl. fibres and polymer matrices);
- Quantification/formulation of correlation between functional domain(s) and strength properties.

II-03

Structure and mechanical properties of carbon fibers and polymers: Nanoindentation tests and molecular dynamics simulation study

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Carbon fiber reinforced plastic composites (CFRPs) have been extensively used in various industrial applications, such as aerospace, energy, automotive, and sports. The mechanical and physical properties of carbon fibers and polymer matrix determine the reliability and performance of the mechanical structures made of CFRPs. Thus, determination and prediction of the mechanical properties of carbon fibers and polymers are of practical importance for the design and analysis of CFRPs. In this study, the indentation behavior of single carbon fibers embedded in the epoxy matrix has been investigated on longitudinal and transversal cross-sections of carbon fibers. The carbon fibers used in the study include high strength PAN-based (T700SC) and high modulus pitch-based (K13D) carbon fibers. To determine the elastic constants of individual carbon fibers, nanoindentation tests are carried out. The indentation results reveal that the contact modulus of the transverse section of the carbon fibers is approximately twice of that of the longitudinal section of the carbon fibers Furthermore, we have conducted molecular dynamics (MD) simulation to evaluate the mechanical properties such as density and Young's modulus of the two kinds of epoxy resin with different curing conversion. We have found that the density decreases but Young's modulus increases as the curing conversion increases, which is may be due to the growth of crosslinked network structure and free volume.

II-04

Constructing crosslinked epoxy resins and investigation of mechanical properties with molecular dynamics simulations

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Epoxy thermoset resin is widely used due to its thermomechanical properties, which are closely related to the crosslinking structure. Molecular dynamics simulations are an effective tool to investigate the mechanism of deformation of epoxy thermoset resin with large atomic system. In this work, various kinds of base resins and curing agents are adopted to simulate the curing reaction. Then, influence of each different combination on curing characteristics is analyzed as well. Finally, we compare the mechanical properties of these epoxy thermoset resins under tension to uncover different deformation mechanisms.

II-05

Field theoretical approach to polymer phase separation and its mechanical properties

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A multi-component polymer system, such as a polymer blend and a block co-polymer melt, exhibits inhomogeneous structure of segment density. This structure is called phase separation. In past few decades, phase separations have been used as a matrix of a composite in order to realize higher stiffness and toughness. However, there have been few simulations that accurately consider the complex spatial shape of a composite material. This is because traditional computational methods such as self-consistent field theory (SCFT) are based on finite different method, which is difficult to consider the effect of a reinforcement on the phase separation. Therefore, in this study, a new simulation procedure is developed by combining SCFT with finite element method (FEM).

In the result of the system of block-copolymer melt, we found that phase transition point between lamella phase and cylinder phase is strongly influenced by the volume fraction of a reinforcement. Furthermore, we show the results of periodic unite cell analysis in FEM. This simulation enables us to obtain mechanical characteristics depending on a pattern of phase separation.

II-06

Complex Network Representation for Describing Structure-Property Relationships of Rubber Materials

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The network heterogeneity of rubber materials is significant for the mechanical properties. However, the heterogeneity in terms of connectivity has not been quantitatively calculated due to a lack of the method to evaluate it. In this presentation, we represent an estimation of network centrality of rubber materials based on closeness centrality, which is one of the indicators utilized in complex network science. In addition, the effect of the centrality for the mechanical properties is introduced.

Rubber materials with homogeneous and heterogeneous network structures were constructed using molecular dynamics simulations. The closeness centrality was evaluated by considering cross-linking points and connected polymer chains as nodes and links, respectively (Fig. 1). The rubber materials were uniaxially elongated, and the effect of the centrality for the stress was evaluated. We found cross-linking points with higher centrality contributed to the stresses than lower ones.

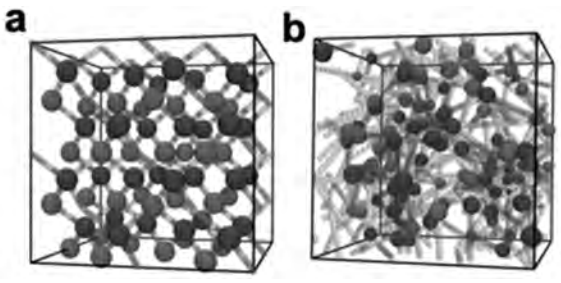

Fig. 1. Network centrality of (a) homogeneous and (b) heterogeneous elastomers. The sizes of cross-linking points correspond to the centrality.

Search for Prevention Condition of Solidification Cracking of Parts Made by Selecting Laser Melting Process by Bayesian Optimization Approach

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The selective laser melting (SLM) process is attracting attention as a next-generation metal processing technology for manufacturing complicated shape parts. However, there is a problem that cracks may occur in the solidification process of the metal powder. When cracks occur, the characteristics of the parts are affected. Therefore, it is important to establish a process parameter search method that can prevent cracks.

This study focuses on prevention of solidification cracks that occur at solid-liquid coexistence temperature range. We constructed a method to analyze the high-temperature plastic strain behavior in the solid-liquid coexistence temperature range, which was the main factor of occurrence of solidification cracks, by the thermoelastic-plastic finite element method. Then, the maximum laser power condition, which was the most efficient condition, without causing solidification cracking and porosity was searched using Bayesian optimization and thermoelastic-plastic finite element analysis.

Optimization and verification of electron beam melting process of non-weldable superalloy Inconel 713ELC

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Process optimization of additive manufacturing (AM) is challenging because of the complex combined effect of high-dimensional governing process parameters. Furthermore, manufacturing non-weldable superalloys with AM is more difficult since severe cracking occurs during AM process. And such cracks are generally considered to lead to brittle mechanical properties.

We have used an efficient method for optimizing process parameters based on support vector machine (SVM) [1] to manufacture a non-weldable nickel base superalloy Inconel 713ELC with selective electron beam melting (SEBM).

Despite the existence of grain boundary cracks along building direction, SEBM built Inconel 713ELC showed remarkable tensile property at room temperature and creep resistance at 980 ˚C, which is superior to those mechanical properties of traditional cast Inconel 713LC alloys.

These results suggest that the current approach is very effective to optimize process parameters of SEBM process.

[1] K. Aoyagi, H. Wang, H. Sudo, A. Chiba, Additive Manufacturing 27 (2019) 353-362.

II-09

Optimization of gas atomization process parameters for Ni-based superalloys

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Due to increase of the number of plane passengers and alternative demand of aircraft, the demand of high quality Ni-based super alloy powders are rapidly rising. The powders are fabricated by gas atomization, then, these are processed by sintering and forging to turbine discs or by additive manufacturing to turbine blades, combustor and so on. The distribution of grain size, grain shape and oxygen concentration are important factors as quality of the powder. These strongly depend on process parameters of gas atomization. During the gas atomization process, the stream of molten metal from upper crucible is disrupted to fine droplets by high velocity gas from inert gas nozzle. Then, these are cooled down during their fall down in the atomizing tower. In this work, we investigated relation between process parameters and distribution of grain size, grain shape and oxygen contents. The main process parameters are temperature of molten metal, Ar gas pressure for inert gas jets, geometry of inert gas nozzle and inert molten metal nozzle and so on. We found that higher molten metal temperature and higher gas pressure give finer grain size and, fewer number of satellites, which are very fine particles attached larger grains, or of void in the grains. By applying Bayesian optimization algorithm to the obtained parameter-data sets, the number of experiments was successfully minimized.

II-10

Prediction of Tensile Properties of Ti-6Al-4V Fabricated by Selective Laser Melting Based on Microstructural Features

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Selective laser melting (SLM), which is one of additive manufacturing methods, is advantageous for the fabrication of near-net shape metal by melting metal raw powder, and it can be applied to difficult-to-process materials. In the process, laser beam scanning on the metal powder layer causes the fast and cyclic temperature rise and fall. As a result, the SLMed samples have characteristic microstructures. In the case of Ti-6Al-4V, the as-fabricated microstructure is usually improved by prescribing post heat treatment so as to obtain optimum mechanical properties.

In this study, the microstructural features of Ti-6Al-4V alloy with different heat treatment conditions were quantified with analyzing the scanning electron microscope images. Based on the microstructural features (such as the fraction of alpha phase, the width of alpha grain, circularity, and so on), the tensile properties of the Ti-6Al-4V alloy were predicted with multivariable regression analyses. While the ultimate tensile strength and the yield stress were successfully found to be correlated with the microstructural features, it was cleared that the prediction of elongation was still difficult owing to lack of other features, such as minute defects, composition in each phase, three dimensional structures, and so on.

II-11

Influences of plasma rotating electrode process parameters on the particle size distribution and microstructure of Ti-6Al-4V powder

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Plasma rotating electrode process (PREP) is one centrifugal atomization method, which is currently a leading candidate for titanium powder production. The arc electric current, electrode diameter and the electrode rotating speed are closely related to the particle size distribution of the powder produced by PREP. However, there is a lack of systematic research how these parameters in PREP affect the particle size distribution and microstructure of Ti-6Al-4V powder. We investigated the influences of plasma rotating electrode process parameters on the particle size distribution and microstructure of Ti-6Al-4V powder using PREP equipment (Fuji Electronic Industrial Co., Ltd). The variation of arc electric current ranging from 70 to 90 A has little influence on the average particle size of Ti-6Al-4V powder. The average particle size was decreased by increasing electrode rotating speed or electrode diameter. In addition, the martensite size of Ti-6Al-4V powder was decreased with the increasing electrode rotating speed.

II-12

Effect of scanning strategy on the crystallographic texture and Young's modulus of β-type biomedical Ti–15Mo–5Zr–3Al alloy fabricated by selective laser melting

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Two types of distinct crystallographic textures in biomedical β-type Ti-15Mo-5Zr-3Al alloy were achieved using selective laser melting with controlling the scanning strategy at a suitable power, pitch and scanning speed. Bidirectional scanning with and without a rotation of 90° between the layers gave rise to single-crystalline-like texture with preferential orientations of 〈001〉 and 〈011〉 along the build direction, respectively. The origin of the variation in texture was ascribed to the change in the extending direction of the columnar cells in the melt pools, depending on the scanning strategies. It is found that the epitaxial growth governs the growth of columnar cells in the melt pools. The obtained material exhibited a low Young's modulus of 68.7± 0.9 GPa, which potentially allows for the development of implants that can suppress stress shielding. These results demonstrate that controlling the scanning strategy can be an important approach in the development of materials with superior mechanical properties through additive manufacturing.

II-13

Prediction of Precipitation Sequences in Practical High-temperature Alloys with Energetics

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Inverse problems analyses, that predict optimized material compositions and/or processes from information of desired performances, are expected as an innovation of materials development techniques. I believe that one of the strategy for inverse problems analyses is to predict microstructures and performances by means of comprehensive forward direction calculations, to build materials databases listed relationships among compositions, processes, microstructures and performances, and to find a desired alloy from the database. Because it is generally effective to use precipitation strengthening effect for improvement in performances of high-temperature alloys, precipitation models are important for inverse problems analyses of high-temperature alloys. Many input parameters and long times are necessary to analyze precipitation behaviors in practical multicomponent alloys with the conventional precipitation models. Then, the conventional models are not suitable to explore a new alloy comprehensively. In this study, I proposed a new model, which predicts precipitation behaviors of practical multicomponent high-temperature alloys quickly from a few already-known basic parameters using energetics (and simple kinetics). I could predict the precipitate of second (and third) phase from supersaturated matrix in some heat-resistant nickel-based, titanium-based alloys and steels, and could make calculated time-temperature-precipitation diagrams successfully.

II-14

Influence Factors on Grain Morphology in a CoCrMo Alloy Fabricated by Electron Beam Powder-bed Additive Manufacturing

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As an advanced additive manufacturing technology, powder-bed fusion with electron beam (PBF-EB) has been increasingly attracting attention from material engineers. For extensively practical applications, flexible control of not only the shape but also the microstructures are highly demanded. The interaction between high-energy beam and material causes strong fluid flow in the molten pool. Solidification behavior within a dynamic molten pool controls grain morphology. For microstructure control, process parameters (i.e., power and scan speed) and solidification conditions (i.e., constitutional undercooling and convective fluid flow) that can overcome prevalent columnar growth are worthy of attention.

Single-track melting on CoCrMo (CCM) alloy substrate was carried out in PBF-EB apparatus. Computational thermal-fluid dynamics (CtFD) simulation was conducted to get the data of fluid flow and solidification parameters. The key elements, including temperature gradient (G), solidification rate (R), and fluid velocity (U), were obtained from each mesh block of the computational domain. They were corresponded to solidification structure experimentally by microscopy with image analysis of grain morphology. In addition, an artificial neural network (ANN) was performed to figure out the determination of each process parameter and solidification condition for grain morphology evolution in as-built CCM alloy.

Prediction and Mechanism of Tensile Strengthening in Single β-phase Ti-Ta Alloys with Oxygen Solutes

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Homogeneous solid solution with O is one of the methods to strengthen Ti alloys. For elucidating the strengthening mechanism, computational science is a powerful tool. In this study, single β phase Ti-Ta-O alloys were synthesized and investigated by powder metallurgy and first-principles calculations.

The alloy samples were synthesized using powder metallurgy. The crystal structures were characterized by XRD and first-principles calculations. The tensile strength was also measured.

The first-principles calculations suggest that the solute O is most stable at the interstitial octahedral site. The computational lattice parameters were in good agreement with those of experiments as shown in Fig.1, which indicates that the alloy samples form a solid solution with O at the octahedral site.

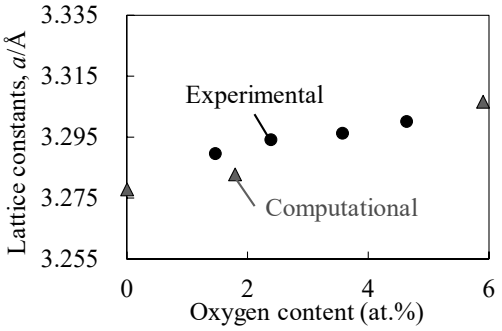

Fig.1 Experimental and theoretical changes of lattice parameters by O solid solution.

Phase-field simulation of crystal growth under solidification condition for Additive Manufacturing

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Additive manufacturing (AM) technologies are attracting attention since it can build 3-D parts even with very complicated geometry. Moreover, AM process can control material property significantly via the control of solidification conditions such as power, diameter, etc. The cooling rate and temperature gradient (G) in AM process is much higher than those in conventional casting processes. In this study, we applied the phase-field method to simulate the microstructure evolution in Al alloy and Ni alloy during solidification to reveal the influences of the solidification condition on the solidification structure with special focus on the effect of the extremely high cooling rate in powder bed fusion type additive manufacturing process. It turns out that the solidification microstructure strongly depends on solidification condition, i.e. G, solidification rate (R) and cooling rate ($G \cdot R$). The interface morphology strongly depends on cooling rate whereas is independent of morphology factor (G/R). High cooling rate leads to the generation of finer dendrites, and more secondary dendrite arms at higher R. However, no secondary arm is formed in the case with extremely high cooling rate. This is consistent with experimental observation.

II-17

Automatic deconvolution of a dilatometric curve in continuous cooling transformations of steels using machine learning

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Continuous cooling transformation diagrams are used to identify the transformation kinetics of steels during cooling processes. To obtain the diagrams, a dilatometric experiment which measures the volume change of a sample are often conducted. The experiment, however, always contains uncertainty induced during the manual analysis of the experimentally measured change in physical properties. In addition, several different phases such as ferrite, pearlite, and bainite develop competitively from austenite, making a dilation curve complex. Therefore, an indication of nucleation of a new phase, which is identified by a slope change in a dilatometric curve, is often smeared out. Thus, the fundamental difficulty in analyzing a dilatometric curve is to detect the starting temperature of the nucleation process manually. In this study, the exchange Markov chain Monte Carlo (MCMC) method, which is widely used in computational physics, is applied to the dilatometric curve with the Johnson–Mehl–Avrami–Kolmogorov transformation model of a phase, for automatic deconvolution. As a result, a dilatometric curve is decomposed into one or more curves of the physical model by explicitly incorporating several different transformation kinetics of each phase. By doing so, the transformation start temperatures and physical parameters of each phase can be predicted accurately from a individually decomposed curve.

II-18

True stress - true strain curves up to large strain extent at elevated temperatures in Ti alloys with image analysis tensile test method

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For large deformation in forging, forgeability should be evaluated by accurate stress – strain curve up to large strain. A new tensile test method to obtain a true stress - true strain curve at elevated temperature was established. A CCD camera and an image analysis device were equipped with thermomechanical treatment simulator to enable the in-situ measuring of the change in the necking geometry and load simultaneously during a tensile test. In near-β Ti alloy, Ti-17, true stress –true strain curves at elevated temperature up to large strain are obtained with this image analysis tensile test method, and their accuracy are evaluated. At 850 ℃, resultant true stress decreased slightly at the strain rate of 0.01 s^{-1} and increased at the strain rate of 0.2 s^{-1} after yielding up to fracture, while true stress in compression test decreased largely. Big difference was obtained between the two methods. In compression test, geometrical change and non-uniform strain distribution in a specimen rather than metallurgical structural change inside largely affect true stress – strain curve, resulting in the inaccuracy in the curve. This image analysis tensile test method can obtain accurate true stress – strain curve which is directly attributed to metallurgical structural change. Image analysis tensile test method is a powerful tool to obtain accurate true stress – true strain curves to large strain extent at elevated temperatures attributing to establish MI system.

II-19

Prediction of Creep Rupture Time for Ferritic Steels Using Machine Learning

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The creep test costs long time and is expensive. It is desired to predict the creep rupture time from experimental database. NIMS Creep database contains materials compositions, creep test conditions and rupture time, and the other related properties such as 0.2% proof- and tensile- stresses. This multidimensional variable space is expected to consist of many regions differing in mechanisms, which complexity leads to the difficulty in prediction. In the previous study, we applied XGBoost, which is an implementation for gradient tree boosting, to make a prediction model for wide space of ferrite-base heat-resistant steels. The resultant predictor showed an excellent performance that the predicted value is within 0.5-2 times of experimental one for test data that were not used for learning. In this study, we applied several other non-linear machine-learning methods to attempt to achieve better predictive performance. Gradient tree boosting, random forest, neural network regression and support vector regression were listed as candidates and were compared each other. As a result, better predictive performance was obtained by support vector regression than that of previous result. Almost datasheets were predicted with high precision by using compositions, test stress and test temperature as descriptors except for CDS53 consisted of 2 heats which have same compositions while different heat treatments. Addition of 0.2% proof stress within descriptors enabled prediction for both heats.

II-20

Universal Framework of Bayesian Creep Model Selection for Steel

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Evaluating the long-term creep deformation process is important for improving the energy efficiency of power plants by increasing the operating temperature. There is an analysis framework that estimates the rupture time of this process by regressing the strain-time relationship of the creep process using a regression model called the “creep constitutive equation”. Because many creep constitutive equations have been proposed, it is important to construct a framework to determine which one is best for the creep processes of different steel types at various temperatures and stresses. Bayesian model selection is one of the best frameworks for evaluating creep constitutive equations. In previous studies, approximation approaches such as the Laplace approximation were used to realize the Bayesian model-selection method. Such methods cannot be applied to creep constitutive equations that violate the assumption of approximation. In this study, we propose a universal Bayesian model-selection framework that can be applied to various types of creep constitutive equations. Using the exchange Monte Carlo method, we propose a Bayesian model-selection framework without approximation. To evaluate the effectiveness of this proposed framework, we applied it to the evaluation problem of a creep constitutive equation called the Kimura model, which is difficult to evaluate by existing methods. Through a model evaluation using the creep measurement data of Gr.91 steel, we confirmed that our proposed method realized a more reasonable evaluation of the Kimura model than existing methods. Through this evaluation, a model candidate that could improve the Kimura model were also obtained.

II-21

Fatigue Performance Prediction of Steel Welded Joints by Materials Integration

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The fatigue performance of welded joints is affected by various factors such as joint shape, surface treatment, residual stress and microstructure. The purpose of this study is to develop a numerical framework that predicts the fatigue life by combining several computational techniques based on the concept of materials integration. In the proposed framework, temperature field and residual stress generated during a welding process was calculated by thermo-mechanical finite element method (FEM). The hardness distribution was predicted from the temperature history and chemical composition in consideration of the phase transformation. The macroscopic stress field under cyclic loading condition was calculated by the macroscopic finite element model considering the hardness distribution. To calculate the fatigue crack initiation life, the microstructural models were reconstructed by a tessellation method with the grain size distribution, and the stress field analysis was carried out by crystal plasticity finite element method (CPFEM). The crack initiation life was calculated based on the Tanaka-Mura model which considers the local plastic shear strain amplitude over potential crack paths. The initial crack was introduced to the macroscopic model and the cycles for fatigue crack propagation were analyzed by extended finite element method (X-FEM). The total number of cycles to failure was eventually obtained by the sum of initiation and propagation. The prediction results for crack initiation and total fatigue life were compared with experimental data. Also, the sensitivities of various factors on fatigue life will be discussed through the uncertainty propagation analysis using the developed framework.

II-22

Microstructure Prediction of Dual Phase Steel with Optimal Strength-Elongation Balance

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Dual phase (DP) steels consisting of hard martensite and soft ferrite phase offer a good combination of strength and elongation. However, present day industrial applications require steels with higher strength and deformability. In general, the tensile properties of DP steels strongly depend on microstructural parameters such as volume fraction, grain size and spatial phase distribution. Many researchers pay attention to data driven approach to predict these structure-property linkages. This study is aimed at proposing a new method to predict optimal microstructures corresponding to desirable properties by bayesian optimization (BO). DP steels with different microstructures were produced, and the microstructural observations and tensile tests were conducted. To calculate the tensile properties of synthetic microstructures, 2D representative volume elements (RVE) with varied microstructural parameters were generated by anisotropic voronoi tessellation, and stress-strain curves of RVEs were calculated by crystal plasticity finite element method (CPFEM) with damage parameter. Stress-strain curves were calibrated by the experimental results. CPFEM calculation for RVE is done to obtain tensile property as output function of microstructural parameters as input variables. By applying BO to this function, maximum tensile property and optimal microstructural parameters were estimated. The predicted results were compared with experimental result of other literatures and discussed.

II-23

Estimation of fatigue lives from the short fatigue crack growth data of a Ni-Co base superalloy

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In this study, the data obtained from the experimental fatigue tests, were analyzed to predict the fatigue lives of the Ni-Co base superalloys. Specifically, tension-compression fatigue tests were conducted at room temperature, and a stress ratio of -1. The continuous short fatigue crack growth data was recorded by an automatic in-situ observation system in combination with digital image correlation technique (DIC). Subsequently, DIC analysis was performed from the fatigue crack growth images, and the fatigue crack opening point was determined to be under the tensile stress. In addition, the fatigue crack growth rate curve showed a linear behavior, and the fatigue crack growth was almost similar to the fatigue crack growth evaluated by fracture mechanics. Three-dimensional (3-D) crack growth behavior was also observed at the short fatigue crack tip by using 3-D scanning electron microscope, to evaluate the microstructure effect on the crack growth.

II-24

Automatic Sorting of Metallurgical Microscopy Images with Machine Learning Tools

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The microstructures of steels from optical/SEM images reflect steel chemical composition and processing history as well as greatly determine its mechanical properties and performance. Consequently, the quantitative microstructure phase analysis is one of the primary interests for metallurgy. So far, however, it is very time consuming due to manual processing by experts. In this work, the optical microscopy images of steel materials were effectively categorized into classes on preset ferrite/perlite, ferrite/perlite/bainite, and bainite/martensite type microstructures with image pre-processing and statistical analysis including the machine learning techniques. Though several popular classifiers were able to get the reasonable class-labelling accuracy, the random forest one was virtually the best choice in terms of overall performance/usability. Such categorizing classifier [D. S. Bulgarevich, et al. STAM 2019 20:1, p. 532] could assist in choosing of suitable pattern recognition method from our recently reported library for various steel microstructures [D. S. Bulgarevich, et al. Scientific Reports 2018 8:1, p. 2078]. That is, the combination of the categorizing and pattern-recognizing methods provides a total solution for automatic accurate quantification of a wide range of steel microstructures. *This work was supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), 'Structural Materials for Innovation' and 'Materials Integration for Revolutionary Design System of Structural Materials' (Funding agency: JST).*

II-25

CMC Virtual Test: Material Integration for designing high temperature parts used in turbine engines

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Simulating degradation of Ceramic Matrix Composite's (CMCs) is one of the biggest challenges in computational material science due to its complicated microstructure and constitutive phenomena, especially in their working conditions. Nevertheless, the need for simulating CMCs is ever increasing due to increased usage as airplane turbine engines parts and remaining high cost for fabrication and testing. To cope with this, we introduce a new concept "Augmented virtual testing", a hybrid assessment approach of CMC degradation using both virtual testing and physical testing. By controlling conditions of physical testing dynamically, parameters in degradation model of each constitutive elements are precisely obtained. By using those parameters simulation would be accelerated compared to pure virtual testing. As our first report in augmented virtual testing, basic concept and theoretical backgrounds are presented. *This work was supported by Council for Science, Technology and Innovation(CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), Material Integration for Revolutionary Design System of Structural Materials (Funding Agency: JST).*

II-26

Bayesian inference of grain growth prediction via multi-phase-field models

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We propose a Bayesian inference methodology to evaluate unobservable parameters involved in multi-phase-field models to accurately predict the observed grain growth, such as in metals and alloys. This approach integrates models and a set of observational image data of grain structures. Because the image data set is not a time series, directly applying conventional inference techniques that require time series as the input data is difficult. The key idea in our methodology to overcome this difficulty is to construct a time series with an appropriate statistic that characterizes static image data of grain structures. Our methodology implements the empirical Bayes method. It can estimate not only a probability density function of the parameters but also an initial phase field, which is generally unobservable in real experiments. After validating the proposed method through numerical tests using synthetic data, we apply it to real experimental images of grain structures in a steel alloy. The proposed method properly estimates unobservable parameters along with their uncertainties and successfully selects the initial phase field that best explains the experimental data from among candidate initial phase fields.

Application of neural network for thermodynamic data of non-equilibrium multiphase field model

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A multi-phase field method using the finite interface dissipation model is applied to simulate the solidification microstructure evolution of a stainless-steel composition including the delta-ferrite to gamma austenite peritectic transformation. The calculation is performed for a quinary system of engineering steel in a two-dimensional field. Thermodynamics calculations using the CALPHAD database in this multi-phase field method is replaced by machine learning prediction to reduce the numerical time. Neural network methodology is introduced for machine learning in this study. The Gibbs free energy and chemical potential values estimated from the CALPHAD database coupling results are inputted in to the neural network learning procedure together with the composition and temperature values. The microstructure evaluated using the obtained neural network parameter is in good agreement with that directly coupled with the CALPHAD database. This calculation is approximately five times faster than direct CALPHAD calculation.

Mathematical Approach to High-dimensional Structural Materials Data

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Finding and understanding relationship between microscopic structure and mechanical property is one of the essential subjects to design high-performance structural materials. Convolutional neural network (CNN) type machine-learning approach has made a remarkable success also in the treatment of observed images, but once we want to quantify them, store in a database and/or extract its scientific meaning, there still remain serious difficulties.

Topological data analysis, especially persistent homology, is a powerful mathematical tool to compute and describe the “shape” of discrete objects such as atomic configurations and pixel/voxel imaging data. In this framework, geometrical information is extracted and summarized as a two-dimensional map called persistence diagram (PD), in which birth and death of n-dimensional holes in data are recorded. By converting PD into vector data, any machine-learning techniques become applicable to solve inverse problems keeping the clues to scientific understandings. It is also available as a way to generate descriptors for advanced materials database.

In this poster presentation, we introduce our strategy and a few of achievements supported by Council for Science, Technology and Innovation (CSTI), Cross-ministerial Strategic Innovation Promotion Program (SIP), “Materials Integration for revolutionary design system of structural materials” (Funding agency:JST).

III-01

M-DaC: Materials Data Conversion Tools Published to Recreate Interoperative and Reusable Measurement Data Files

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The conversion of measurement data from raw data to machine-readable data package is one of the key preparation techniques prior to informatics analysis. Our conversion flow consists of (1) to convert binary or binary-text mixed raw data to plain text data, (2) to retrieve measurement parameters and to create metadata set, (3) to exchange primary parameter terms to general vocabularies, and (4) to reconstruct numerical value array to machine readable one. Metadata gives us a capability of electronic quick search of the data of interest among huge data bank. Primary parameters ensure a repeatable/reproducible measurement. Metadata and formatted numerical data are utilized for statistical data analysis and sustains a long life time for interoperability and reusability with the parser software. We are publishing sets of data conversion tools in M-DaC on our web site [1]. Using by these tools, one can generate XML files of raw and primary parameter sets, human-legible/machine-readable csv numerical file, and visualized image file. The conversion tools under MIT license are applicable for raw data of XPS spectrum and powder XRD data generated by ULVAC-PHI SmartSoft-XPS and Rigaku SmatLab software. [Ref. 1: https://www.nims.go.jp/MaDIS/about/M-DaC.html]

III-02

tq : A Comprehensive Disciplinary Language for Materials Science

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Materials science is based on multiscale and multiphysical disciplines (scientific discipline); therefore, in this field, there are many types of data, models, and terms with various meanings. Although data-driven science have many prospects, it is difficult to operate data on unified discipline (data discipline). However, a well-defined uni-language that treats multimodal forms can help operations. Therefore, we are developing a language that can parse tree or graph structures, enabling the operation of several data formats, models, and dictionaries for materials science. The language is neither a solver nor an analyzer; it is a format converter and a dictionary (syntax) parser, which is connected to solvers and analyzers.

The developed language, named “tq,” should satisfy the following: parsing tree structure, parsing graph structure, searching dictionary, matching terms using dictionary, reforming unstructured data to structured data, and conversion to other well-known formats such as JSON. Its challenges are matching or searching tree or graph structures, rewriting of term or phrase (sub-tree) in tree or graph structures based on the similarity (Term Rewriting by Network Similarity (TRNS); pronounced “trans”), daemonizing dictionary system, and parallelizing.

As a next step, we are restructuring the data structure of tq for parallelizing. In the current structure, the tree structure and node property are strongly related; therefore, parallelizing is difficult. We are attempting to divide the data structure into tree structure and node table.

III-03

FigResourceMiner: A search text in images, and graph visualization platform for academic articles

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A platform, called FigResourceMiner, was designed to realize the following two objectives: The first is to accumulate a large amount of material data from images in papers based on material study; to this end, the images in the papers were subjected to optical character recognition and the texts in the images were extracted to form a database. Thus, materials focusing on physical quantities and units could be identified, which could not be realized by conventional paper search services. The second objective is to increase the discoverability of material research data; to achieve this, the connection of each element of the paper (paper, chapter, drawing, and image) was visualized in the form of a graph, which helps us identify data in a short duration, confirming the relationships among these elements.

III-04

Materials Data Platform Infrastructure System: Construction of hardware infrastructure to support subsystem development

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To support subsystem development, we constructed “Materials Data platform Infrastructure System (MPDF)” consisting of the analysis cluster computing system, virtualization infrastructure system, MDPF-FW (Firewall), MDPF-VPN (Virtual Private Network), MDPF-WAF (Web Application Firewall) and various auxiliary servers of the aforementioned systems. MPDF has a maximum theoretical performance level of 0.5 PFLOPS, and a data storage capacity of 10 PBytes.

MDPF can mainly provide the following two services. The first one is to provide high performance computing resources using the analysis cluster system, which contains 4x NVIDIA Volta (V100) GPUs and 4x 18 core CPUs in one node, and a large amount of high throughput storage that can store 1.5 PBytes. The second one is to supply virtual machines (VM) to the developers of various services provided by DPFC such as Materials Data Repository. This virtualization infrastructure system consists of 25 servers, VMware, NSX and so on. We are able to provide over 120 VMs with irreducible minimum resources.

This flexible and highly usable system was designed after interviewing MaDIS researchers and developers. The basic and specific designs, system construction and various tests in were completed in about five months. We consequently launched the services to the MaDIS members in June 2019, so that MDPF services will be deployed on this infrastructure.

III-05

Effective use of outdated experimental apparatus by electronic laboratory notebook (ELN) and IoT data transfer systems

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An outdated experimental apparatus occasionally still generates much valuable data in the materials science fields. There may be an issue of insufficient signal capture from the control system, which should be recorded in a raw digital data as key parameters. The protocol of data storage and transfer is, furthermore, not following the evolution of PC and communication networking architecture. Due to these reasons, it is difficult to perform effective data collection and sharing. Thus, to solve the former problem of digital recording of important experimental parameters, we are introducing (A) the electrical laboratory notebook (ELN) system. We are also installing (B) the secure IoT data transfer system via Wi-Fi network for the latter problem of transferring data from data acquisition PC to data manipulation PC. By linking metadata, specimen information, and experimental parameters with measured raw data, it is possible to carry out reproducible experiments and to create interoperative data. As the typical example, we can show the only one apparatus in the world to acquire absolute Auger signals to estimate chemical compositions in topmost regions of solid materials. We have retrofitted (A) and (B) to this Absolute Auger Electron Spectrometer passing more than 20 years since the first instrumentation and it is anew producing globally valuable materials data every day. We are expecting that a large amount of integrated data will be statistically analyzed using MI techniques to extract feature quantities that contribute to new material development in near future.

III-06

Vocabulary Management System for the Materials Data Platform using Wikibase for Peer Collaboration

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In handling a wide variety of materials research data, it is highly beneficial to have a centrally-managed service for materials vocabulary management, to be referenced in metadata management of research data, assist concept identification in text/data mining, and ultimately to assist new discoveries. There have been efforts to build standard materials vocabularies and ontologies, but we need a scheme to adopt them as one of the services in a wider data platform. Such a service should also allow building on top of aforementioned efforts, to expand them and keep up with the latest progress in the fields.

To address this, we are developing a wiki-powered vocabulary management service, to allow for peer collaboration in developing the vocabulary. Our system adopts a dockerized version of Wikibase, the software behind the Wikidata project. Concepts can be edited either by humans through a web browser or by bots using the system's API. User edits are constantly imported into a SPARQL query service, and allows for highly flexible querying. Additional developments have been made to the Docker container to allow centralized user authentication, setup enhancements, and increased portability. Further efforts are ongoing to allow such query results to be delivered to other systems. The vocabulary being developed on this platform is based on NIST's Materials Data Vocabulary, IUPAC Gold Book etc., and since has been expanding by limited peer collaboration. The system is scheduled to launch in autumn 2019 as part of the NIMS Materials Data Platform, to serve as the hub for vocabulary data.

III-07

Data-driven spectral analysis method in electron-beam based techniques

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There are a lot of electron-beam based techniques in surface analysis, and each of them has its own characteristics, but they also have, at least, one characteristics in common, the information about the target sample is obtained through the analysis of identified signal data. These techniques generally are inefficient for quantitative purpose because only the signal data contribute to the conclusions, while other detected data, the overwhelming majority of measured data, have been completely disregarded as undesirable background data. Therefore, there is a need for a universal method that could extract meaningful information from background data. In this paper, we proposed a data-driven analysis method to extract meaningful information from the background signal and to propose an important breakthrough for the next generation surface analysis. The unique feature of this method is to use the combinations of a large number of spectral groups measured by intentionally changing a plurality of experimental conditions, to describe the background data, instead of interpreting individual spectrum in terms of physically meaningful parameters. Some combinations provided an “intermediate level” between “background signals” and “understandable information,” which enabled a better understanding of measured backgrounds.

III-08

A universal method to determine material-parameter-dependent empirical formula for a given experimental data

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The robust TPP-2M formula is the most popular empirical formula for the prediction of electron inelastic mean free paths from simple material parameters. However, the TPP-2M formula poorly describes several materials because it adopts traditional least-squares analysis. Herein, we propose a new framework based on machine learning. This framework allows a selection from an enormous number of combined terms (descriptors) to build a new formula that describes the electron inelastic mean free path. The number of terms in the new formula can be automatically adjusted according to the importance of the terms in the particular application scenario. The obtained framework not only provides higher average accuracy and stability but also reveals the physical meanings of several newly found descriptors; for example, it reveals the important role of the atomic number (Z) and provides data-driven evidence of the importance of the existing term of the free-electron plasmon energy (Ep). Our findings suggest that machine learning is powerful and efficient and has great potential in building a regression framework for data-driven problems. Our method can be used in the development of the simplest empirical formulas, showing the deeply buried meanings of terms.

III-09

API-FWK: Software Adapter Component for MDPF Integration

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Hitherto, owing to the many fields of materials science, various research data have been produced and acquired through various experimental procedures, methods, principles, facilities, and systematized utilities. Accordingly, various legacy databases and systems have been developed, such as Research Data Management (RDM) accumulating sample data from various distributed measurement devices, vast amounts of libraries for simulation and obtained calculation results, and sets of specialized databases. As each of them has been implemented and deployed according to diverse requirements from academia and industry in those eras, they generally possess a strong heterogeneity with poor standardization and weak coherence of their implemented computational environments. To exchange these data between one another with shareability and reusability, there are certain demands for standardization in communicational procedures, linkages among subsystems, and their semantics. A software adapter component called API-FWK for MDPF integration is dedicated to supporting the standardized communications and procedures among these systems. The role and concept for this is drawn from conventional Enterprise Application Integration (EAI) for handling seamless communications between diverse distributed applications and the central hub channel with mediation and translation from “localized communication protocol and message format" into the standardized format. The major purpose of developing this API-FWK is to reduce effort for developing and integrating communication functions by supplying a common customizable software component.

III-10

Text Data Mining Platform System to Support Mining and Machine Learning of Scientific Literatures

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As one of the research support functions of the material data platform, a text data mining platform system was developed to collect literature data, arrange it in a uniform data format, and extract knowledge from the collected data.

The purpose of this system is to mine physical property values and the like, contained in the text of the body of the paper, figures, and tables, and extract them as knowledge data contributing to substance search and material development.

Therefore, the TDM system has a machine learning function for mining. The system aims to improve extraction accuracy by registering a corpus by a user and enable various materials to be mining targets.

This system has a function of accumulating a paper file (body, chart, etc.) produced by a publisher in a research server, extracting papers and data closely related to technical terms (vocabulary data) uploaded by a user, and visualizing and exporting this information as a search result.

Automatic Construction of Superconducting Materials Database from Tables in related Research Papers

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There is a growing need for automatic construction of materials databases. In this study, we propose an approach for automatic collection of superconducting materials and their critical temperature (Tc) from tables in related research papers using a rule-based approach and a chemical data extractor [1]. Figure 1 illustrates the outline of the system.

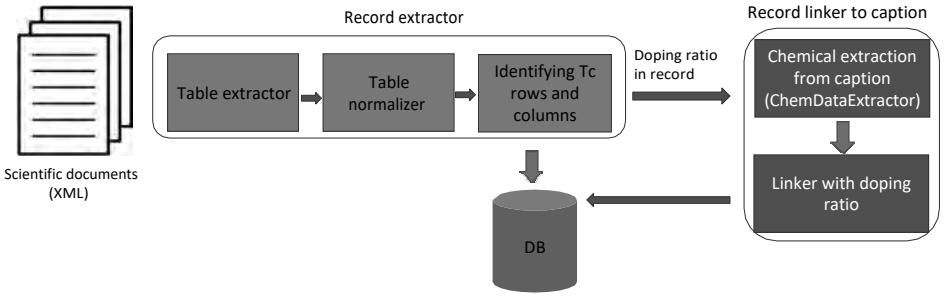

Figure 1. Automatic collection of superconducting materials and their critical temperature from tables in related research papers.

[1] Swain, M. & Cole, J. M. ChemDataExtractor: A toolkit for automated extraction of chemical Information from the scientific literature. Chem. Inf. Model 56, 1894–1904 (2016).

Implementation of FAIR data principles with Materials Data Platform System

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Materials Data Platform (MDPF) aims to support researchers in the field of Materials Science and Engineering (MSE) by providing functions for management of data along with four stages of data life cycle, creation, storing, utilization and disclosure. We designed MDPF as a set of independent systems and orchestrate them to provide the functions in line with the data life cycle by the following four linkages; (1) Authentication linkage by which users can access all of the authorized systems in MDPF once he/she login, (2) Master data sharing that enables the systems commonly to identify vital concepts and/or objects such as measurement method, classes of substances, types of target properties, etc., (3) Data relay service among the systems, which allows us to handle data expressed in a common structure along the data life cycle, and (4) Metadata integration of relayed data. As we implement all the types of linkages, the relayed data can be findable, accessible, interoperable and reusable with the integrated metadata, i.e., it can satisfy the FAIR data principles.

III-13

A proposal of standardized model for data exchange among systems on MDPF

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We propose a common model of data on Materials Data Platform (MDPF) which aims to support researchers in the field of Materials Science and Engineering (MSE) by providing functions for management of data along with data life cycle, i.e. creation, storing, utilization and disclosure. Structured metadata is adopted to describe not only basic information for archiving digital data, but also several mandatory items to manage data in MSE field, for example, specimen details, method of measurement or calculation, and research targets such as structures and/or various kinds of materials properties. In addition, controlled vocabulary is used to describe metadata with persistent identifiers given in a management system for vocabulary. Using this system, users can collectively give various relationships among managed words as well as define some properties of each word such as names, description etc., so that it helps all the users to understand each data in the same way. All the metadata on MDPF will be converted to a description using Resource Description Framework, which allows us to integrate metadata and search that in a semantic way.

III-14

Method for calculating the conversion of plastic work into heat”

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In hot forging simulation using Finite Element Method (FEM), the material properties and the boundary condition are very important input parameters to the accurate prediction of forging condition. For example, high strain-rate deformation of metal generates a significant amount of heat, and this heat can result in spectacular local temperature rise and affect the microstructure of metal. The ratio of plastic work converted into heat is called Taylor-Quinney coefficient (TQC), and depends on material. TQC is one of important parameter for high accurate simulation, but there is not sufficient information about measurement method and result of TQC.

We found that our unique uniform compression test for measuring flow stress of metal can also apply to measuring TQC. Our compression test enables us to measure TQC conveniently and precisely, because the effects of heat transfer from the specimen to the test grip, emissivity from specimen, and friction between the specimen and test grip can be neglectable. We applied this measurement method of TQC to Alloy 718 used in aircraft and land-based gas turbine engines, and got the result that TQC depends on strain and is smaller than general used value (0.9).

III-15

Materials Data Repository (MDR)

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This poster describes "Material Data Repository" (MDR), which is being developed by the National Institute for Materials Science and scheduled to be launched on December 2019. MDR is designed to inherit and extend the roles of our former institutional repositories, and offers public access to materials science datasets as well as publications. In this poster, we will focus on the complex metadata requirements for a data repository in the domain of materials science, and will describe the approaches to managing sophisticated metadata from a variety of sources including automated tools for laboratory equipment and standard controlled vocabulary created from external knowledge bases and peer collaboration. We will also focus on data retrieval APIs which enables integration with a number of other systems in Materials Data Platform in order to provide functions to help management of data along its life cycle.

III-16

Fully automatic peak and background analysis of XPS spectral data -- Sparse modeling of XPS spectra

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[3] Scienta Omicron Inc.

High-throughput measurement has become increasingly important for the efficient development of science and technology. Even in X-ray photoelectron spectroscopy (XPS), which is a time-consuming characterization technique, the use of high-intensity synchrotron radiation and a high sensitivity detector enables us to obtain a large amount of spectral data over a short time period. Therefore, high throughput of data processing is also required for efficient spectral data analysis.

We have developed and implemented a fully automated method to perform XPS spectral analysis based on the active Shirley method and the information criteria. Our method searched a lot of initial fitting models by changing a degree of smoothing, and then optimized the peak parameters and the background parameters to get a lot of fitting results. The goodness of those optimized models was ranked by information criteria. As a result of applying this algorithm to measured XPS spectra, we found that using the Bayesian information criterion (BIC), a simple model with reasonably good agreement and a moderate number of peaks was selected. The model selected by BIC is close to the result of peak fitting performed by XPS analysis experts.

III-17

Large-Scale 3D Observation of Steel Microstructures Using a desktop-sized 3D Internal Structure Microscope

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Large-scale three-dimensional (3D) observation of microstructures in ferrous materials was conducted using a desktop-sized three-dimensional internal structure microscope. Our system uses a serial sectioning method performed by automatic precision cutting, etching, and observation of the cross-sections. The precision cutting can create a mirror-like cross-section within a minute at depth intervals of 1 μm. Etching time can be controlled precisely using numerical control. The cross-sections were captured using an optical microscope with a digital camera. It demonstrated an automatic 3D observation for 0.15C-1.5Mn steel. The 3D model offered a range of 867×645×1500 μm^3, which had 1000 cross-sections at 1.5-μm intervals and a resolution of 0.066×0.066×1.5 μm^3. The total voxel size became 13196×9824×1000 voxels. It took an observation time of 3.5 min per section and about 60 h in total. The 3D image had sufficient quality for recognizing clear microstructures even in the reconstructed side surfaces.

III-18

CAS: Central Authentication and Authorization Service

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Materials Data Platform (MDPF) is currently being built as a system that can loosely link different types of services according to the stages of a data lifecycle, which include generation, storage, utilization, and disclosure. The MDPF should be sufficiently flexible to allow new services to be delivered as required. To realize an MDPF with these features, we adopted a protocol termed "Central Authentication Service (CAS)", which enables us to unify the control of authentications and authorizations for users.

CAS can provide single sign-on services to users, which means users do not need to log in to additional systems once they have logged in to any one system. In addition, CAS can also provide administrative rights to manage users and authorization information in a unified manner for all services linked on the MDPF, in cooperation with the human resource management system. For example, the National Institute for Materials Science (NIMS) can provide services to users outside the NIMS by expanding trusted-ID providers in the CAS server while controlling the authorization levels.

Information Extraction of Polymer Names and Properties from Tables in Scientific Papers

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Data curation of polymer names and properties are fundamental process for data-driven polymeric material design. However, manual collection of such information from academic literature requires huge amount of time and effort. In this work, we present a machine-learning approach for automatic extraction of polymer names and properties. More specifically, our method first detects the regions of tables in scientific papers with the computer vision method, then analyzes the table structures and detects polymer information with natural language processing. We evaluate the performance of our method by using the Polymer Database PoLyInfo, and show that our method successfully extracts polymer information accurately.

NIMS Materials Database, “MatNavi”

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Since the National Institute for Materials Science (NIMS) launched the NIMS Materials Database, named MatNavi, one of the world's most-extensive online databases for materials, in 2003, it has boosted material-based R&D and innovation. Use of MatNavi is free. All you need to do is register. MatNavi is an integrated database (DB) system comprising 14 materials databases, including the Inorganic Material DB (crystal structures, phase diagrams, physical properties…), Polymer DB (chemical structures, physical properties, NMR spectra,…), Metallic Material DB (density, elastic constants, creep characteristics,…) and Computational Electronic Structure DB (band structures obtained by first-principles calculations…). Currently, there are over 140,000 registered users.

Also, MatNavi data is using as the basic data for data-driven research such as materials informatics (MI) at the Japan Science and Technology Agency (JST) project called the “Materials research by Information Integration” Initiative (MI^2I). Currently, we are renewing MatNavi for link the Materials Data Platform (MDPF) under development with MatNavi data.
This poster introduces the recorded data and functions of a typical MatNavi database.

- Polymer Database (PoLyInfo)
- Inorganic Material Database (AtomWork)
- Computational Electronic Structure Database (CompES-X)
- Diffusion Database (Kakusan)
- Superconducting Material Database (SuperCon)
- Metallic Material Database (Kinzoku)

III-21

Reducing Annotation Cost for Automatic Named Entity Extraction by using Domain-Specific Dictionary

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In recent years, the number of publications that report the physical properties of materials is rapidly growing. Developing a database of the physical properties by collecting the reported results from these papers is useful for exploration of new materials. Since the amount of papers is too large to check by human experts, automatic extraction of the information by using text mining technology based on machine learning is attractive and desired. However, for applying machine learning methods, we need a substantial amount of training data that consists of sentences that are annotated to indicate which part should be extracted. Development of training data is not an easy task in this case because the annotation work requires an expertized knowledge so that the worker must be a domain expert who is usually busy, and the workers need to receive and understand instructions to correctly put annotations.

This study addresses the issue of the high annotation cost and explores a computational method to reduce it by "distant supervision" strategy leveraging domain-specific dictionaries. In this strategy, we first put incomplete annotations to the texts using the domain-specific dictionaries that contain names of entities to be extracted, e.g., names of materials, names of physical properties, etc. Then we attempt to recover the incompleteness of the extraction by applying a machine learning method extended to allow partial training data. We report some experimental results that show the proposed method improves the coverage of extraction compared to the simple rule-based dictionary matching.

III-22

Thermodynamic Database for Open Science

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Center for Materials Research by Information Integration, National Institute for Materials Science (NIMS)

Phase diagrams and related thermodynamic quantities are foundations of materials science, which is expanding its application area into wide scientific subjects with data science as known as ICME (Integrated Computational Materials Engineering). Of many key factors for both statistics and dynamics implemented in ICME, Gibbs free energy database and defect property database are highly important, and are being constructed in this study under the project of "Materials research by Information Integration Initiative (MI^2I)". Such fundamental databases are necessary to be opened for the public to accelerate ICME methodology.

Our database, CPDDB (Computational Phase Diagram Database shown in the right figure), which includes Gibbs energy functions of phase in mainly binary and higher order systems, and Gibbs energy with vacancies in pure elements of stable and metastable structures. Currently, it includes about 500 systems. In this presentation, focusing on our future activities, thermodynamic data on CPDDB will be presented. Please find me with the word "CPDDB".

III-23

Exploratory Visual Analytics Platform with Multiple Coordinated Views for Materials Informatics

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Materials research by Information Integration Initiative (MI^2 I),
Research and Services Division of Materials Data and Integrated System (MaDIS),
National Institute for Materials Science (NIMS)

There are numerous resources for materials informatics in an uncoordinated fashion. This presentation introduces an web-based integrated materials informatics platform, Material Acquisition by Data Science (MADS). The platform provides three main functionalities, a repository for data sharing and publishing, an analytic workspaces for exploratory visual analysis, and catalyst property prediction tool with pretrained machine learning models. With the support of the platform, researchers in materials science can enter into materials informatics to collect their data and apply different analytic and visualization methods to them. Uploaded data as well as their analysis results can be published on the platform for collaboration with other users. Thus, the introduced platform contributes towards the advancement of materials informatics for both specialists and non-specialists.

III-24

Thermophysical property database of solids for materials informatics

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A thermophysical property database which contains thermal conductivity, electric conductivity, heat capacity and thermal diffusivity of solid materials has been developed. When we develop specific heat capacity database, more than 50,000 points of temperature dependent specific heat capacity data were systematically collected and digitized. Specific heat capacity per kilogram scatters considerably, clear tendency is observed by converting specific capacity per kilogram to specific heat capacity per atom・mole by counting atomic number. This is known as known as Dulong-Petit law.

We can accelerate materials informatics based on the information below.

1. Prediction of specific heat capacity from Debye temperature.
2. Recognizing “Debye temperature” as one of the major descriptor, investigate correlation with other descriptors.
3. “Deviation from Debye temperature” especially at high temperatures can be interpreted as descriptor.

Data of thermal conductivity and electrical conductivity of metals were also surveyed, digitized and accumulated. Correlation between thermal conductivity and electrical resistivity was analyzed and discussed based on Wiedemann-Franz-Lorenz law.
It is well-known that electrical resistivity of metals can be expressed by Bloch-Grüneisen formula using Debye temperature.

III-25

Development of materials database for sintering analysis of Ni-based superalloy

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In sintering process of powder compacts, distortion or non-uniformity of microstructure in sintered body are problematic. In order to predict the problems, numerical methods for simulating sintering behavior have been developed. However, materials database of the material properties, that is, the longitudinal viscosity, the viscous Poisson's ratio, and the sintering stress, is required to put the numerical methods into practical use. There is no standardized system for measuring the material properties of metal powders at elevated temperatures, that require atmosphere control during testing. In this study, we will develop a measurement system with atmosphere-controlled, sinter-forging testing machine for metal powders, and aim to establish a database for sintering simulation.

For the first step of the study, we consider the densification and the microstructural evolutions of Ni-based alloys TMP-5002 powder, as a target material. After the powder compacts are formed, pre-sintering tests are performed without pressure, and the specimens with relative density in the range from 60% to 80% and grain size of 30 μm to 50 μm are obtained. These specimens will be used in the sinter-forging tests to measure the material properties and microstructural parameters in wide range of sintering temperature and time.

III-26

Study of Grain Boundary Structures using Topological Data Analysis and Simple Evaluation with Local Energy

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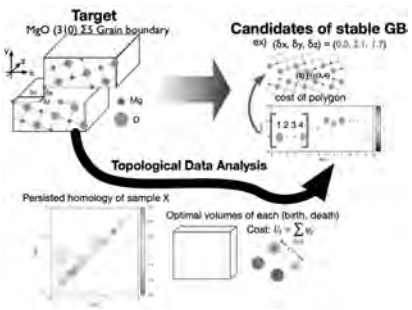
[1] Center for Materials Research by Information Integration (NIMS)
[2] Japan Science and Technology Agency, PRESTO
[3] Kyoto University Institute for Advanced Study, Kyoto University
[4] Advanced Institute for Materials Research, Tohoku University

Local heterogeneity has crucial influence on physical properties of the entire system. To evaluate the geometrical features of the heterogenous system, we adopt topological analysis bases on persistent homology. The target structure can be identified with a set of polyhedra. As a test case, we investigate the grain boundary that is a geometric mismatch region between two crystals. On a basis of the geometrical cost of the constituent polyhedra, mechanical stability of the boundary structure is roughly but effectively evaluated.



High-throughput Data Collection and Automatically Data Analysis Using IoT Device

S. Matsunami[1], Y. Harada[1], M. Suzuki[1], H. Shinotsuka[1], H. Nagao[1], A. Matsuda[1], K. Nagata[1], and H. Yoshikawa[1]

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DPFC is developing a high-throughput data collection and data analysis system for measurement informatics by using IoT devices. The data transfer systems from instruments utilize IoT technologies which can transfer raw data automatically and safely to a data server by wireless communication, Wi-Fi SD, even if computer (PC) is not connected to a network to ensure information security and fully stabilize the instrument control by PC. This Wi-Fi SD enables efficient collection of large amounts of data transferred from instruments or process equipment. Next step, meta data extraction and vocabulary conversion from the measurement data files are performed in order to improve machine readability. By extracting meta data, it is possible to easily search for a specific data file from a huge number of measurement data groups, even if the data format is different depending on the measuring instruments or manufacturer. For X-ray photoelectron spectroscopy measurement, an algorithm that automatically spectral peak separation and spectral analysis based on the Bayesian information criterion (BIC) is currently implemented in the data server. Thus, by simply attaching Wi-Fi SD device to the equipment and when the raw data is dragged and dropped to this device, it is possible to realize the high-throughput data collection, data accumulation, and data analysis. By developing this system, research efficiency can be significantly improved and materials informatics can be advanced.

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