

# Development of Materials Integration System

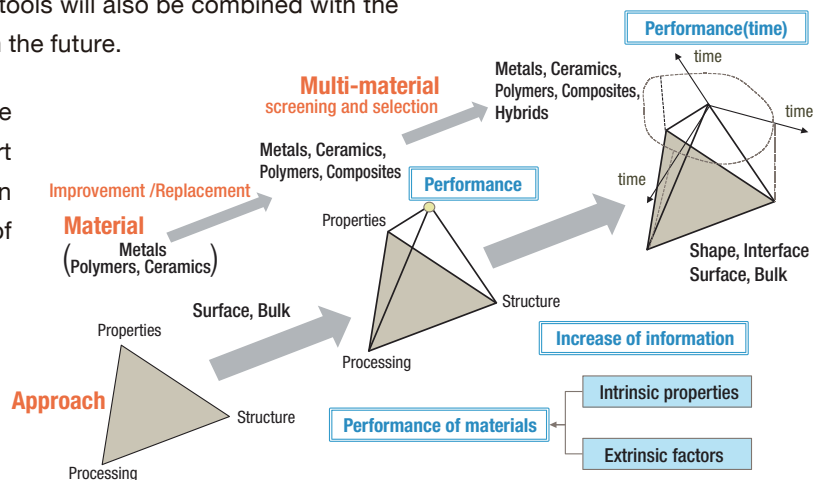
Theories, experiments, simulations, and data analyses are integrated to support research and development of materials.



Research and development of materials has seen the expansion of material types and the advancement of approaches. For practical materials, it is useful to quickly ascertain their performance and its time dependency. These tools will also be combined with the Internet of Things (IoT) or artificial intelligence (AI) in the future.

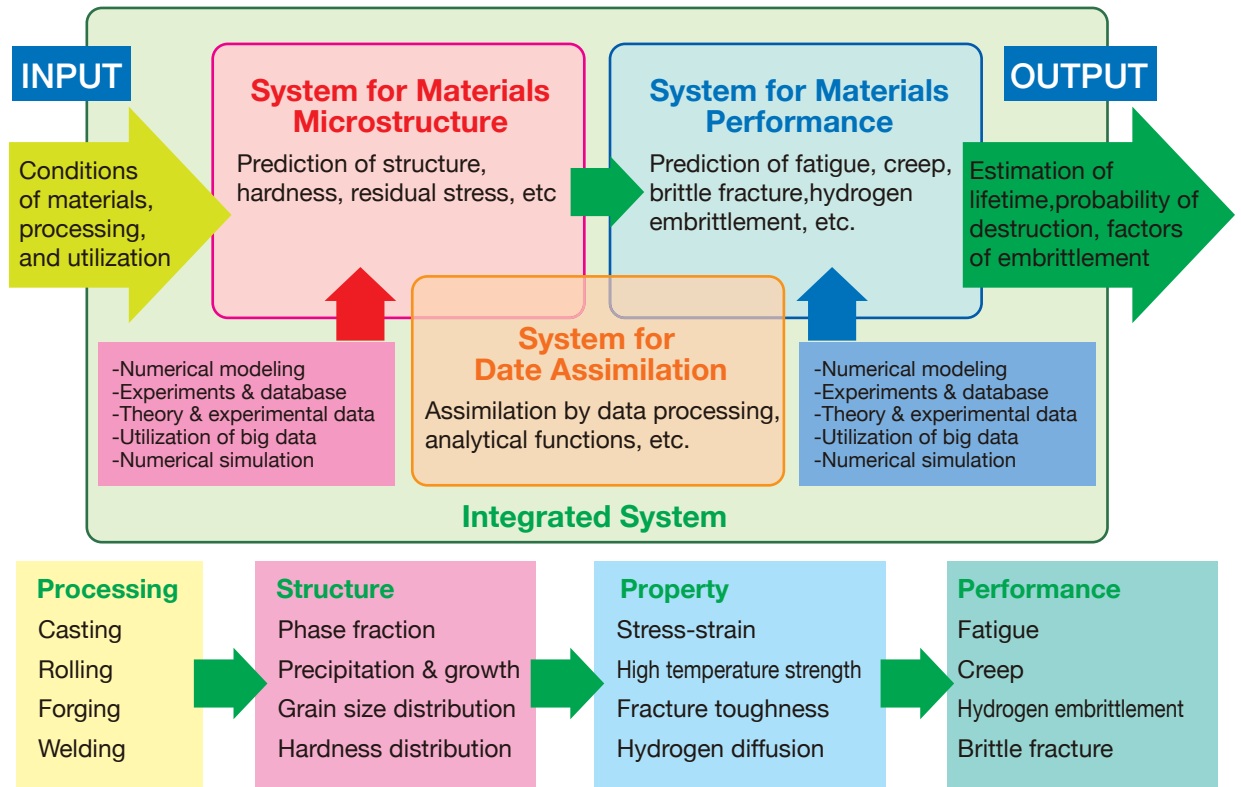
Materials integration is defined as a comprehensive material technological tool aiming to support research and development of materials from an engineering viewpoint by integrating all areas of science and technology (such as theories, experiments, analyses, simulations, databases, and experiences) in order to use the findings of material science and leading-edge ideas.

This tool aims to help shorten the time required for research and development of materials.



## Concept and Approach

### Materials Integration (MI) System (for metals)



We are developing systems for predicting the performance and life-time of structures made of combinations of various materials and processes by integrating theories, empirical rules, computational simulations, databases, and other tools. We aim to realize systems that help greatly shorten the material development time, develop materials efficiently, cut costs, optimize processes for material selection, manufacture, use, and processing, predict the reliability of structures, improve maintainability, establish centers of materials research and development and centers of personnel training, and build international networks, etc.

## Research Themes and Participating Laboratories

### Development of Microstructure Prediction System

#### Development of microstructure prediction system and modules

##### Tokyo University

- Microstructure prediction system
- Analytic engines based on the phase-field method
- Microstructure formation data
- Microstructure prediction modules based on theory and empirical rules

##### National Institute for Materials Science

- Combined system between the phase-field method and CALPHAD method

##### Hokkaido University

- Modules for predicting microstructure formation by solidification

##### Tokyo University of Agriculture and Technology

- Diffusive phase transformation modules

##### Nagoya University

- Displacive phase transformation modules

##### JFE Steel, Kobe Steel, IHI, UACJ

- Development and verification of modules for predicting welded structures

### Development of performance prediction system

#### Development of performance prediction system and modules

##### Tokyo University

- Performance prediction system
- Computational modules for high precision fatigue performance
- Computational modules for brittle fracture
- Fast computational modules for fatigue performance
- Performance prediction database tools

##### National Institute for Materials Science

- Computational modules for creep performance
- Fatigue database modules

##### Teikyo University

- Computational modules for hydrogen embrittlement

##### JFE Steel, Kobe Steel, IHI, UACJ

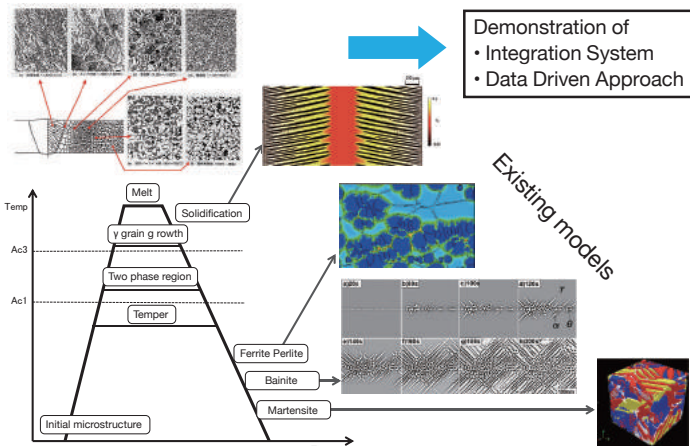
- Development and verification of modules for performance prediction

# Research and development in materials integration systems

## Development of Microstructure Prediction System

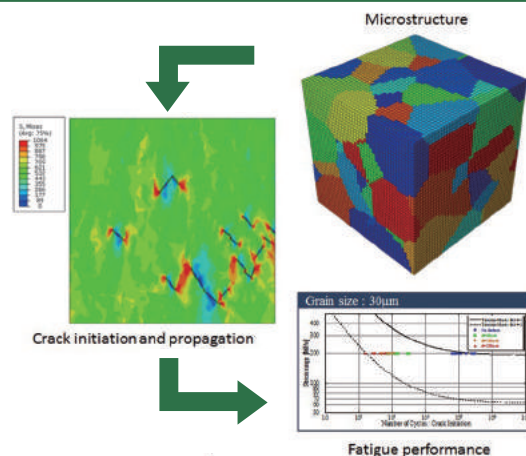
Microstructure of materials changes drastically due to the thermal cycles during welding, often resulting in the deterioration of mechanical properties. Precisely predicting the microstructural change in this heat-affected zone (HAZ) is therefore important for the safety of welded structures. Among the numerical simulation techniques proposed so far are the experimental and theoretical equations such as the estimation equation for HAZ hardness, the carbon equivalent equation and the evaluation equation of hardenability, as well as the computational simulation technologies such as phase-field method, cellular automata method, and Monte Carlo method. We reevaluate these conventional theoretical equations and numerical simulation techniques, while developing new modules for improving the prediction accuracy of numerical modeling. Moreover, the microstructure during multiple heat cycles, for which an experimental equation has not yet been adequately established, and the microstructure of welded metal will also be modeled by prediction equations through previously accumulated data.

Prediction of microstructure evolution in steels during welding thermal cycle



## Development of Performance Prediction System

Prediction of fatigue strength, creep strength, hydrogen embrittlement and brittle fracture. The system for time-dependent performance prediction of structural materials such as fatigue strength, creep strength, hydrogen embrittlement and brittle fracture is developed based on microstructural information which is predicted by the microstructure prediction system. This performance prediction system consists of two module groups. One is the simulation module group based on theoretical physical model and forward analysis, and the other is the database module group utilizing huge accumulated performance data. Validation of system is ensured by comparing the predicted results with experimental data. Also the module to predict the time-dependent performance under a certain condition due materials, welding conditions and structures is developed without microstructural information



## Development of Data Assimilation System

Development of data assimilation system for supporting microstructure and performance prediction systems by using data processing and analysis

### Tokyo University

- Data Assimilation System
- Multidimensional data-driven prediction techniques based on statistical mechanics
- Data assimilation of materials mechanical properties
- Probabilistic performance prediction techniques

### National Institute for Materials Science

- Multidimensional data-driven prediction techniques based on information theory and statistical mechanics

### Kagoshima University

- Microstructure databases
- Establishment of property prediction techniques based on information theory and statistical mechanics

### Riken

- Techniques for grasping a material property space
- Microstructure databases

### Nagoya University

- Optimization of parameters for the phase-field method by data assimilation

## Development of Materials Integration System

Development of the basic structure and external interface of a Materials Integration system that links and controls the various systems

### National Institute for Materials Science

- Materials Integration system
- Establishment of a base for integrating various databases and modules

### Tokyo University

- Implementation of performance prediction database tools

### Toyo University

- Data and knowledge representation for materials

### Aoyama Gakuin University

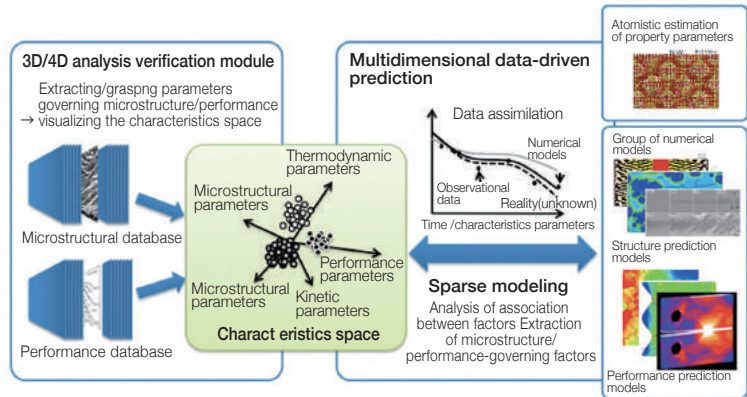
- Web user interface for MI system

### Nagoya University

- Visualization systems

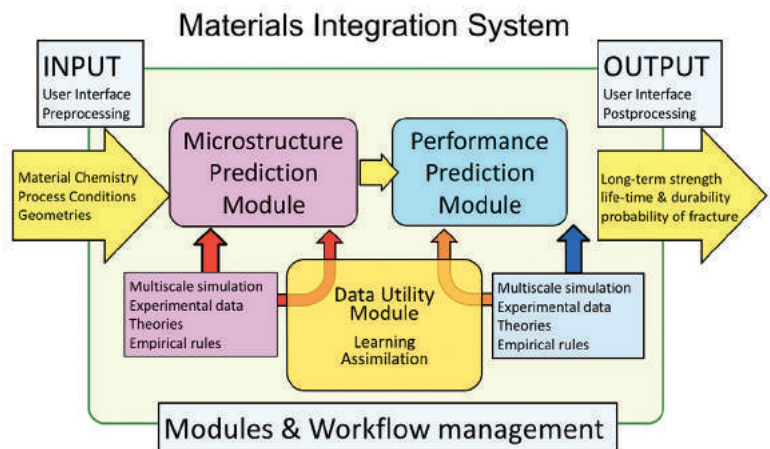
### Development of System for Data Assimilation

By applying information theory and statistical mechanics, we are attempting to establish a method for grasping a characteristics space consisting of descriptors that determine performance and microstructure. More specifically, we are applying sparse modeling (which involves extracting useful findings from various descriptors and models from databases) and data assimilation (which estimates various parameters and their uncertainties based on databases) to prediction modules developed in microstructure prediction and performance prediction systems. At the same time, we are developing modules for automatically extracting geometrical factors designed to describe the microstructure of materials and analyzing the correlation between parameters and various input conditions used in various prediction modules.



### Development of Materials Integration System

The Materials Integration (MI) system, Integrated R&D Support system for materials engineering, will be developed, in which various modules for prediction of microstructure and mechanical properties are integrated in order to support R&D of structural materials. Long term mechanical performance such as fatigue and creep life can be estimated from chemical compositions, process conditions, and geometries. It also contains data driven analysis modules. In future, the system will be come more powerful tool to accelerate materials development by incorporating data and modules from users.



## Members of Research Domain D: Development of Materials Integration System

### Hopes for materials integration

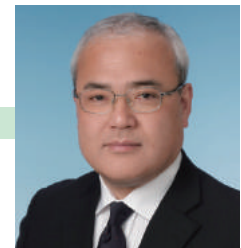
**TERUO KISHI**  
Program Director



The major purpose of materials integration is to take full advantage of computational material science, databases, informatics, and other sciences, to help in shortening the time required for research and development of structural materials. Our technology provides a new type of tool that is not an extension of established infrastructural technology for material development. An integrated system has not yet been developed for linking the four elements of structural materials (i.e. process, structure, characteristics, and performance) for predicting the life and other characteristics of the materials as components. Our SIP research aims to establish an internationally recognized cutting-edge system, resulting in the successive delivery of innovative structural materials.

### Materials Integration System

**TOSHIHIKO KOSEKI**  
Director, Materials Integration System Center



The Materials Integration System is a system to support and accelerate the development of advanced materials. The system enables the prediction of materials structure, properties, and performance by combining knowledge, accumulated experimental data, and numerical simulations for materials. Eight universities, two national institutes, and four companies are participating in the development of the system. We are developing various kinds of modules and databases, and the integration system that combines them to realize the consistent prediction of material structure and performance. In this project, the system has been developed for structural metallic materials, but is a platform that can be applied to various kinds of materials.

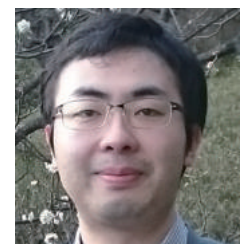
## Prediction of fatigue performance by physical models and data-driven methods

Keywords : Fatigue, Finite element method, Crystal plasticity, Machine learning

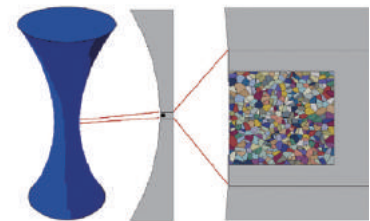
**MANABU ENOKI**  
School of Engineering,  
The University of Tokyo



**TAKAYUKI SHIRAIWA**  
School of Engineering,  
The University of Tokyo



In the development of structural materials, it often takes significant time and cost to evaluate their properties. In the case of fatigue properties, several fatigue tests need to be conducted to validate statistical behavior of fatigue failure. Accordingly, the evaluation of fatigue properties in shorter time becomes essential. We are developing new fatigue prediction methods for a wide range of structural materials by utilizing physical model and data-driven methods. In the first approach, several simulation methods for predicting the behavior of the fatigue crack initiation based on crystal plasticity finite element analysis are developed. The second approach is to use the fatigue database accumulated over the years. Empirical equations are derived by applying machine learning techniques to the database. These fatigue predictions will reduce the time and cost required for the development of new materials.

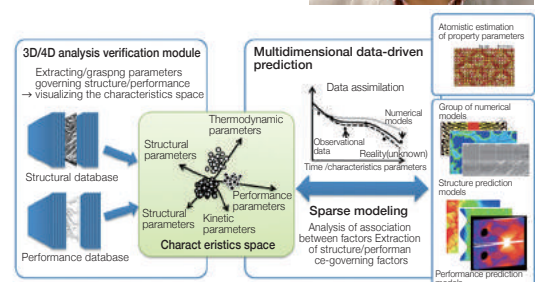


## Development of Performance Prediction System Considering Uncertainty

Keywords : knowledge, database, uncertainty, data-driven approach, prediction module

**JUNYA INOUE**  
RCAST.U.Tokyo

The advantage in the field of the development of structural materials for Japanese industries resides in the tremendous amount of knowledge amassed during the course of the development of various advanced materials. Thus, it is extremely important to take all this knowledge into account in the performance prediction system for structural materials to be used in the future. Above all, gaining an understanding of uncertainty originating from many sources, such as complexity of the mechanisms and inhomogeneity of the microstructures, is particularly important. Accordingly, our group aims to develop a system that will enable us to quantify uncertainty in the prediction modules developed in the project by introducing many data-driven approaches based on the database stored in society.

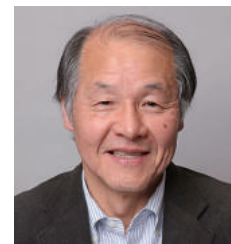


# Systems for Materials Microstructure / Experiments • Database

Keywords : Steel, Phase transformation, Microstructures

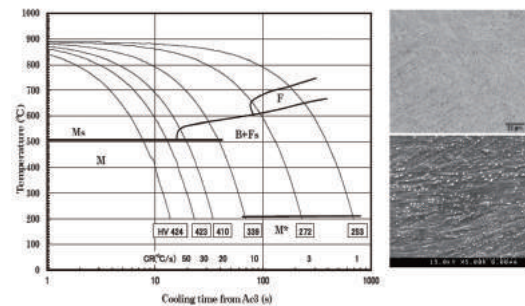


**TADASHI KASUYA**  
School of Engineering,  
The University of Tokyo



**SUSUMU TSUKAMOTO**  
National Institute for Materials Science

Microstructure is one of the most influential factors for the mechanical qualities of steels; however, its prediction is not simple. Several processes such as solidification and phase transformation have an influence on the microstructure and these processes strongly depend on the chemical compositions and thermal histories, which make the microstructure prediction very complicated. We are hence constructing the database of the CCT diagrams using the experiments and the data from the literature. The database is useful for the phase field calculations. In addition, the other microstructural data such as stress – strain curves of the HAZ and prior austenite grain observations are being obtained for the systems for materials microstructure and performance.



## Multi-scale and multi-physics based study on strength and toughness of steels

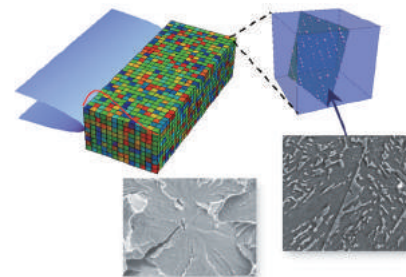
Keywords : steel, fracture mechanics, welding metallurgy, micromechanics, structural reliability

### SHUJI AIHARA

Department of Systems Innovation, Graduate School of Engineering, The University of Tokyo



Steels are required to exhibit higher strength and toughness to meet the demand for more stringent environments. Although control of microstructures, like grain-refinement, is well known to increase the steel toughness, the relationship between the microstructures and toughness has not been completely elucidated. Rather, it depends on empiricism. Specifically, the intrinsically stochastic nature of cleavage fracture has been making it difficult to establish a complete physical model of fracture, on the microscopic as well as macroscopic levels. Newly developed micro-fracture mechanics models, incorporating the weakest link mechanisms, are being applied to analyze the microstructure-toughness relationship and evaluate the reliability of welded steel structures.



## New approach for breakthrough of micro-mechanism of fracture in steel and proposal of new steel material by using optimum arrangement of microstructure

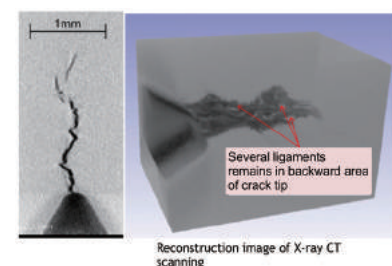
Keywords : steel, rapid fracture, micro-mechanism, optimum arrangement

### TOMOYA KAWABATA

Department of Systems Innovation, Graduate School of Engineering, The University of Tokyo



Steel continues to be the most important material for humans in terms of cost effectiveness and recycling efficiency. However, its fracture behavior is so complicated due to the multi-scale hierarchal microstructures that we have not fully understood the mechanisms of its complexity and high-speed behavior. Trial-and-error methods are dominantly used in development for improvement. A new approach for developing micro-mechanisms, including many in-situ observation techniques with the latest methods and appropriate numerical simulation tools, is being developed. The figure shows the in-situ observation of bridging, which is effective for crack arrest in steel structure, by using X-ray CT technology.



# Members of Research Domain D: Development of Materials Integration System

## 4DVar-based Data Assimilation for Massive Phase-field Models

Keywords : Data assimilation, 4DVar, Phase-field method

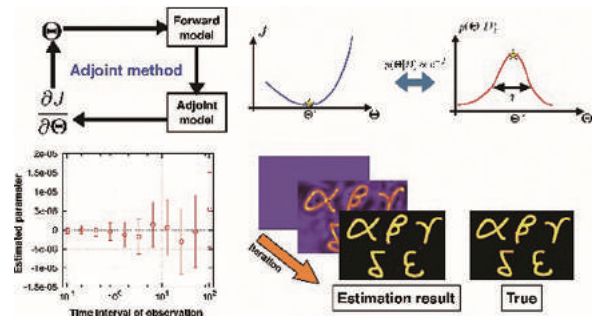
**HIROMICHI NAGAO**  
Earthquake Research Institute,  
The University of Tokyo



**SHIN-ICHI ITO**  
Earthquake Research Institute,  
The University of Tokyo



Data assimilation (DA) is a computational technique used to estimate parameters and predict future states, integrating simulation models and experimental data via Bayesian statistics. We have developed a new 4DVar-based DA methodology applicable to massive phase-field models towards predicting material composition and proposing new materials. Our method can rapidly evaluate uncertainties of objective quantities by the second-order 4Dvar, extracting the second-order information of a given posterior distribution. Such uncertainties provide significant information for proposing and optimizing experimental design.



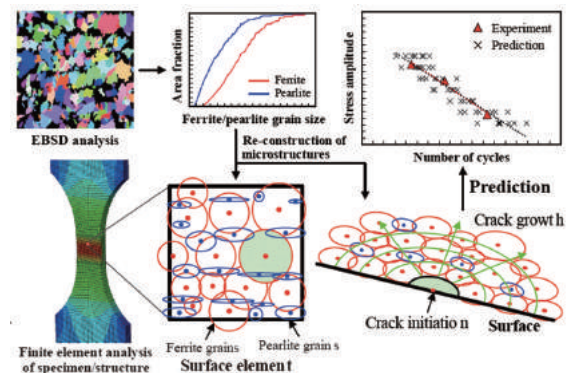
## Innovative modeling to predict fatigue strength of steels

Keywords : Fatigue, Prediction of life, Small crack, Multiscale modeling, Model synthesis

**KAZUKI SHIBANUMA**  
School of Engineering, The University of Tokyo



Fatigue is one of the most common failure modes of materials or structures. Quantitative prediction of fatigue life is therefore crucial for both material development and maintenance of existing structures. Although fatigue strength of steel is related to its microstructures, any models and methods to quantitatively predict the relationship has never been established. In particular, quantitative prediction of the behavior of a small crack, approximately the size of grain, has been an ongoing issue for more than 30 years. We are attempting to develop an innovative model to predict fatigue strength of steels using “the model synthesis approach” composed of (1) a crack growth model based on the interaction theory between a crack and grain boundaries, (2) a spatial distribution model of microstructures, and, (3) a macroscopic finite element analysis.



**HIDEHIRO ONODERA**  
Collaboration Coordinator

The ultimate target of computational materials science is to predict a material's microstructures and properties. However, many mechanisms are involved in the formation process of microstructures and the appearance of a material's properties, and the precise prediction of these factors has not yet been realized by computational simulation based on a single mechanism. Materials Integration is a new approach by combining knowledge, experimental data, and computational simulations. This challenge has been

enabled by the recent remarkable advances in the fields of theory, computational simulations, and information technology such as AI. I believe that very innovative research tools for materials science will be developed by this project.

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## Estimation of physical properties on the basis of atomistic simulations

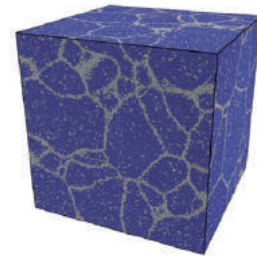
Keywords : Molecular dynamics; Large-scale simulation; Estimation of Physical Properties

### YASUSHI SHIBUTA

Department of Materials Engineering, School of Engineering, The University of Tokyo



Thanks to the recent progress in high-performance computational environments, the spatiotemporal scale in numerical simulations is rapidly expanding. The figure shows a grain distribution obtained by a large-scale molecular dynamics (MD) simulation (ca. 12 million atoms) of nucleation from undercooled melt iron. In the MD simulation, only atomic configurations are directly obtained from the simulation, from which the microstructure and related physical properties are extracted via multiple post-analyses. These processes are regarded as the data compression from the atomistic information to representative values of physical properties on a macroscale. Our goal is to establish the methodology for the estimation of physical properties based on the atomistic simulation from the point of view of the data compression.



## Development of workflows on secure virtual computer network

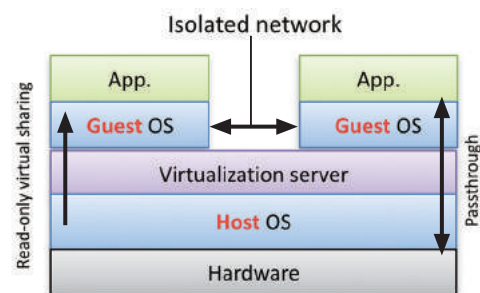
Keywords : Workflow, Cloud computing, Secure system

### KAITA ITO

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Flexible connectivity of a variety of software modules is required for MI systems in order to estimate the structure and properties of materials. In the initial stage of system development, many modules have been developed by several research groups with different operating systems and middle ware. Therefore, a workflow is necessary to provide creation and running of logical flows among these modules. Moreover, this workflow must be complete in a secure environment to ensure no data leakage. In this research, a private cloud which is completely isolated from external networks but is remotely -accessed will be constructed. An R&D environment consisting of virtual computers for this private cloud and the workflow is currently in development.



## Application study of the MI system

Keywords : Creep, Data science, Crystal plasticity

The MI system predicts the performance of materials by connecting several modules being developed in this project. The development of the modules is on track and some of them have been partly implemented.

In our group, we focus on the application study in which we actually connect the developed modules and tackle them with some practical examples. In particular, we will treat fracture problems in which the crystal plasticity modeling plays a critical role.

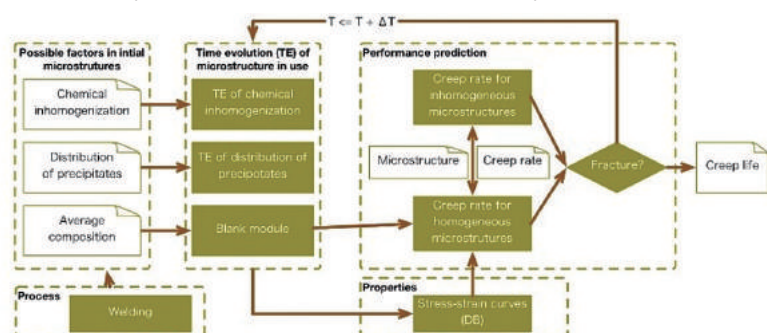
We will report feedback on what we will discover from those application studies to the other developing groups, such as the units for the integrated system, performance prediction, microstructure prediction, and data assimilation.



MASAHIKO DEMURA  
RCAST, U. Tokyo



HITOSHI IZUNO  
RCAST, U. Tokyo





## Members of Research Domain D: Development of Materials Integration System

### Evaluation and prediction of microstructures of high-temperature structural materials during creep deformation

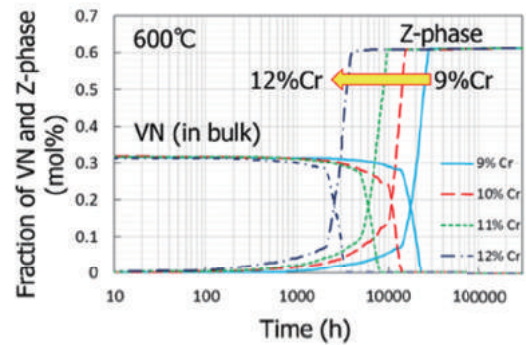
Keywords : Heat resistant steels, Creep, Precipitation, Simulation for precipitate, Quantitative stereology



#### SHOICHI NAMBU

Department of Materials Engineering, The University of Tokyo

The prediction of creep strength has been required in order to use high-temperature structural materials under higher temperatures and longer period. Since precipitations and sub-grain microstructures in materials are considered to be the factor affecting creep strength, not only the evaluation but also the prediction of change in these microstructures during creep deformation should be conducted. In this study, the microstructures are evaluated based on quantitative stereology and the relation to creep strength is examined. Also, the numerical simulation which can predict the nucleation and growth of precipitates including nucleation site is conducted and the prediction of creep strength is attempted.



### Development of calculation module for solidification microstructures based on phase-field model

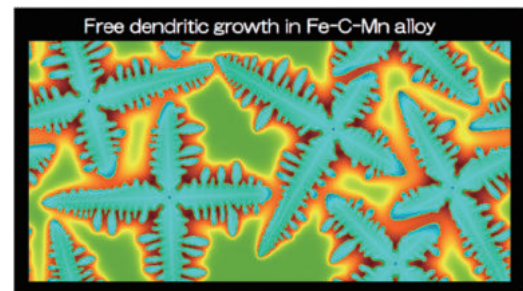
Keywords : phase-field models, dendritic growth, grain growth



#### MUNEKAZU OHNO

Faculty of Engineering, Hokkaido University

Calculation modules based on phase-field models is being developed to predict solidification microstructures in the weld pool and polycrystalline microstructures in heat-affected zones. The solidification module can be utilized for precise analyses of size and morphology of solidified grain structures and segregation behavior. This module is constructed by coupling a quantitative phase-field model, which correctly recovers the free-boundary problem of solidification in multi-component alloys, and the CALPHAD approach. The grain growth module is being developed based on a multi-phase-field model that is able to describe effects of non-uniform temperature distribution and pinning particles. Furthermore, an efficient numerical algorithm has been implemented for the acceleration of this module.



### Phase-field modeling of microstructure evolution during diffusional solid phase transformations in multicomponent steels

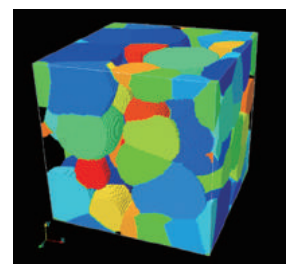
Keywords : Multi-phase-field method, solid phase transformation, steel



#### AKINORI YAMATAKA

Tokyo University of Agriculture and Technology

We have developed program codes for simulating three-dimensional microstructure evolution during diffusional solid phase transformations in multicomponent steels. In order to simulate the austenite-to-ferrite transformation during a continuous cooling process of the steels, the chemical-free energy functions obtained by the CALPHAD method are incorporated to the multi-phase-field model. Furthermore, to utilize experimental data for the estimation of the initial conditions and the parameters of the multi-phase-field simulation, the data assimilation technique for the phase-field simulation, using the ensemble Kalman filter, is being developed.



## Development of computational materials design system based on phase-field method and the parameter optimization by data assimilation

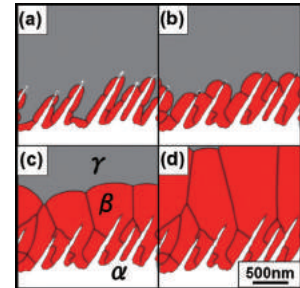
Keywords : phase-field method, simulation, phase transformation, welding, data assimilation

**TOSHIYUKI KOYAMA**

Graduate School of Engineering, Nagoya University



The phase-field method has been utilized in many fields of the material sciences as a powerful tool for predicting and modeling inhomogeneous microstructure changes in real materials. In this study, we are developing a computational environment for materials design for the the concept of materials integration based on the phase-field method, where we focus on the welding process of high-strength steel as a typical example of this approach. The figure shows the simulation result that indicates the formation and growth behavior of low-temperature hard phase  $\beta$ , such as pearlite and bainite, in  $(\alpha+\gamma)$  two-phase microstructure. Furthermore, the optimization method of materials parameters used in PF simulation is being developed by using the inverse-design method such as data assimilation techniques, because the precision of microstructure simulation depends on the accuracy of materials parameters used in the calculation.



## The Establishment of Simulator of Hydrogen Transportation Behaviors in Engineering Structure with the Site of Stress Concentration

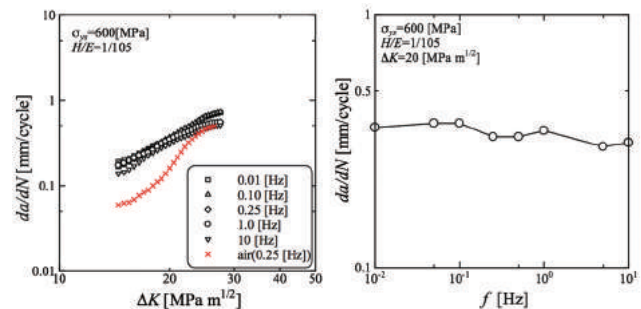
Keywords : hydrogen embrittlement, hydrogen diffusion, numerical analysis  $\alpha$  multiplication method, FEM-FDM method

**A.TOSHIMITSU YOKOBORI, Jr.**

Strategic Innovation Research Hub Laboratory of Strength of Material and Science, Teikyo University



Concerning hydrogen embrittlement, from the viewpoint of an engineering application, the accurate analysis of the hydrogen transportation in an engineering structure with stress concentration becomes important. Therefore, in order to realize the effect of local stress on the hydrogen diffusion and concentration behaviors,  $\alpha$  multiplication method has been proposed that incorporates a reasonable weight in to the stress driven term of the hydrogen diffusion equation. Furthermore, our group has developed a FEM-FDM hybrid method, where stress analysis is conducted by finite element method (FEM) and hydrogen diffusion analysis is conducted by finite difference method (FDM). On the basis of this method, reasonable hydrogen diffusion and concentration behaviors were calculated with reasonable accuracy and CPU time. This research project has entailed the coding of software programs on the analyses of hydrogen diffusion and concentration around a stress concentrated site in a structure. Furthermore, on the basis of this method, we are analyzing hydrogen embrittlement cracking during welding by collaborating with the material performance group.

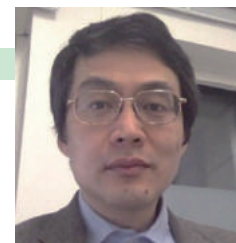


## Data and Knowledge Representation for Materials Science and Engineering based on the Semantic Web Technology

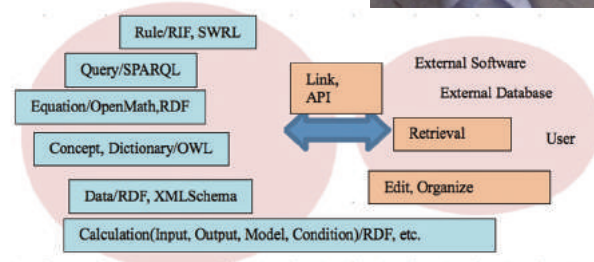
Keywords : Data and Knowledge Representation, Ontology, Semantic Web

**TOSHIHIRO ASHINO**

Faculty of Regional Development Studies, Toyo University



There is a great amount of knowledge, rules, and equations that describes structural materials performance, and there have been many trials to develop advanced systems. However, because there are so many semantic gaps among material process, micro structure, property, and performance, it is impossible to build a monolithic system. We are developing data representation and its platform based on the semantic web framework to store and retrieve heterogeneous information resources, such as data, equations, rules for materials science and engineering, and the connections between these sources.



## Members of Research Domain D: Development of Materials Integration System

### Web user interface for MI system

Keywords : Design information system, Simulation system, educational technology

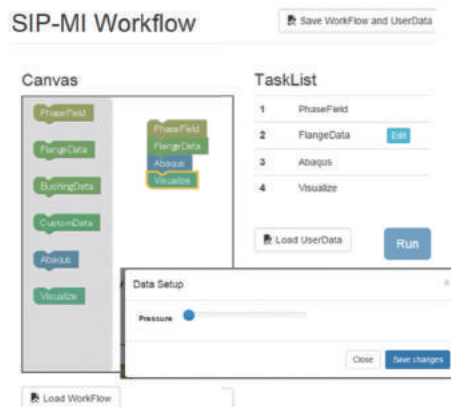


**HIROSHI SAKUTA**  
Aoyama Gakuin  
University



**DAI HASEGAWA**  
Aoyama Gakuin  
University

This team aims to build a prototype system that is organized by various loosely coupled server modules based on knowledge of distributed server systems. The purposes of the research are to improve visualized workflow, which includes individual functions, user interfaces, and API to archive and share them. It is expected that this prototype will be applied to a Workbench for consideration of functional specifications for the main server system and professional education models. The right figure is an example of workflow design of an outcome of 2015, in which a sequence of workflow was designed, executed, and archived.



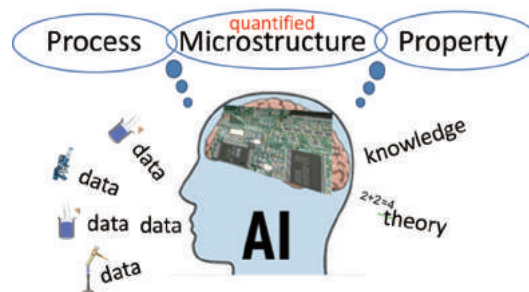
### Artificial intelligence materials science (AI-MS)

Keywords : Artificial intelligence, image recognition, 3D4D, materials genome, deep learning, steel

**YOSHITAKA ADACHI**  
Kagoshima University



This study highlights the fusion of advanced artificial intelligence (AI) with materials science. As an approach, attention is placed on "data science" in combination with modelling. In order to understand the relationship between "cause (microstructure)" and "result (property)", conventional machine learning (such as Bayesian inference, neural network, support vector machine, etc.) is applied to material science. Furthermore, deep learning based on a convolutional neural network is incorporated into microstructural image recognition. I also aim to develop a fully automated serial section 3D microscope to extract material genomes from a 3D image.



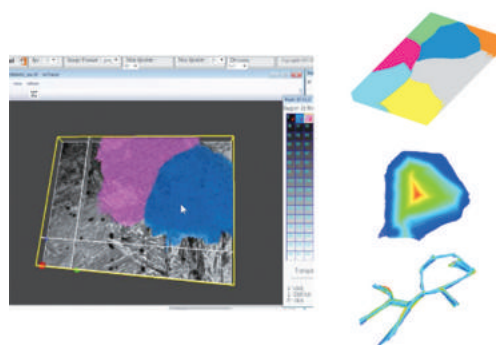
### Computational feature expression of 3D material structure using image processing

Keywords : Image processing, 3D feature expression, material structure

**HIDEO YOKOTA**  
RIKEN, Image processing research team



Our group has studied developing numerical expression methods of 3D features of material structures based on 3D images using image processing. Recent advancement of 3D measurement methods has enabled us to obtain 3D image data of steel structures. Since the 3D structures relate to their macroscopic performances, it is essential to quantify their features without relying on the subjective judgment of researchers. We have developed computational methods of 3D geometric expression of the structures. For the next step, we will develop advanced methods by introducing metallurgical knowledge. Furthermore, we will supply image processing environments for other groups. Using accumulated knowledge, we will try to establish useful feature extraction methods.



## Reproduction of weld microstructures and Validation of creep performance prediction for commercial steels

Keywords : Heat-resistant steel, Creep, Data acquisitions

IHI Corporation Corp. R&D, Production Engineering Center



HIROTO YAMAOKA



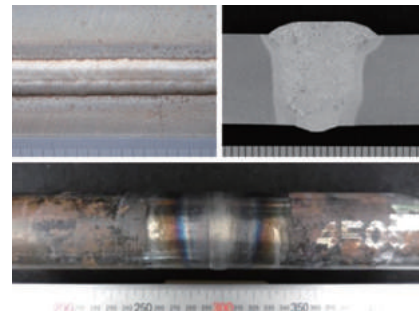
KOUTAROU INOSE



TAKAASI MATSUOKA

This research focuses on the development of a reproduction technique for weld microstructures and the validation of the system for microstructure, as well as the development of an optimization technique for joint performance evaluation and the validation of the system for performance.

Reproductions of weld microstructures for various welding methods and data acquisition and the validation of the system for microstructure are conducted using commercial steels. Welding of Cr-Mo steel and creep tests are conducted. Testing under the simulated stress distribution conditions of an actual structure will also validate the practical usability of systems for performance. Figures show appearances of joint and cross-section of round-robin specimens, as well as the appearance of a creep test sample of inner pressure type for a 1Cr-0.5Mo steel joint



## Prediction of Microstructure and Performance of Aluminum Welded Structural Materials.

Keywords : Aluminum, Welding, Heat Affected Zone, Microstructure, Mechanical Properties

UACJ Corporation, Research & Development Division



KOICHI TAKAHASHI



TOSHIYA OKADA



SHINGO IWAMURA

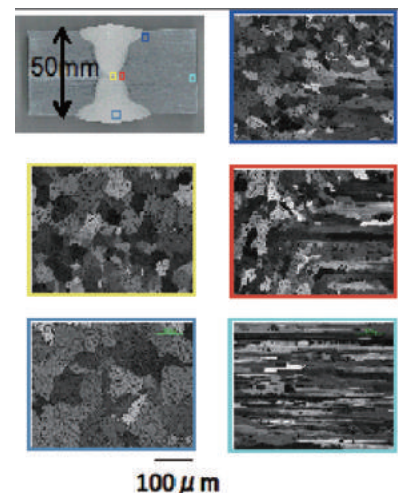


SYOHEI YOMOGIDA



TOSHIO ARAKI

Aluminum welded structural materials are widely used for ships and automobiles. Change in the mechanical properties of the welded material by different alloys, welding methods, or welding conditions cannot be completely predicted. The achievement of an accurate prediction of material performance from several production process conditions will make a powerful and positive impact on the manufacturing industry. The target of this study is to integrate the system for predicting the microstructure and performance of Al-Mg alloy welded by MIG welding. Final goals are: ① Prediction of microstructure of welded part and heat affected zone (HAZ) from the components of base material, welding material, and the welding conditions; ② Prediction of the mechanical strength properties of welded part and HAZ; and, ③ Prediction of the fatigue performance of the welded joint. Our company takes a role in collecting the data of microstructure and mechanical properties for integrating and verifying the availability of the system.



# Members of Research Domain D: Development of Materials Integration System

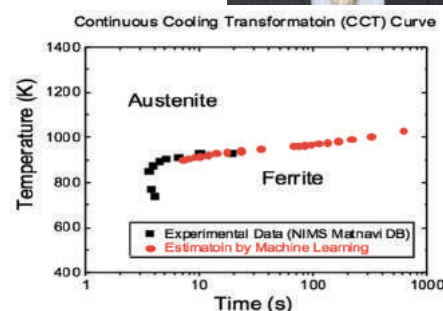
## Development of Machine Learning Modules for MI system based on Materials Database

Keywords : Machine Learning, Bayesian estimation, Multiple Regression Analysis, CCT, Creep



**MAKOTO WATANABE**  
National Institute for Materials Science

Predictions of microstructure and mechanical properties require various material parameters and criterions. However, such parameters are not always available in a database or published references. In order to develop an MI system, it is of crucial importance to develop the modules that can estimate and provide parameters to various analytical modules, such as phase field simulation and finite element analysis. In this work, the estimation modules for material parameters will be developed by applying machine learning techniques to a structural material database. Firstly, the modules for a continuous cooling transformation curve and creep strain rate will be investigated. In future research, generalized estimation modules for material engineering will be developed and combined into the MI system.



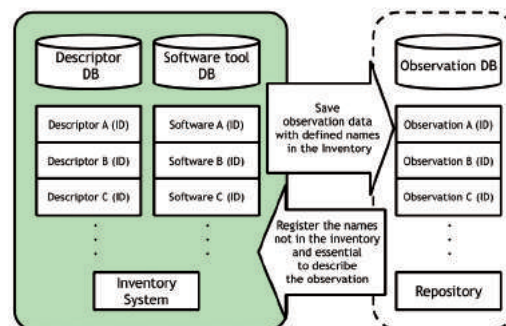
## Development of the data-inventory for MI system

Keywords : Data-inventory, Descriptors, Ontology



**TAKUYA KADOHIRA**  
National Institute for Materials Science

One of the most important goals of this project is the realization of a self-growth MI-system. To achieve this goal, it is necessary to establish a mechanism that will gain new insights by incorporating the knowledge of various users of the system as well as intelligently utilizing the information handled by the system. The cornerstone of such a mechanism is the centralized register of the various features of materials, software tools for simulation and/or prediction, etc., that are used in the system, which we call "data-inventory." Any application running on the system, by referring to the information in the data-inventory, can contribute to the goal. In the present study, we aim to build such a data-inventory by using the collective intelligence of all users.



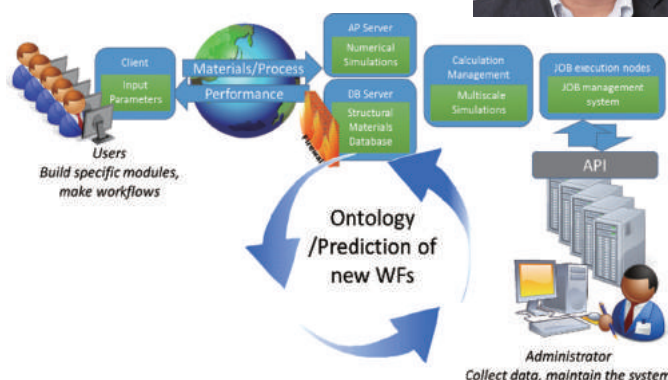
## Development of the integrated system

Keywords : Multiscale Simulations, Integration of modules and database, inventory system



**SATOSHI MINAMOTO**  
National Institute for Materials Science

In this project, we aim to develop the MI-system to predict performance, such as material fatigue life. To that end, as well as conventional experience equations, a high analysis module of the precision based on theory and reliable experimental data will be connected to techniques such as the machine learning. Furthermore, it is necessary to realize systems processing such as the connectivity of data, error evaluation, and scale conversion, because it is necessary to deal with the phenomenon as multi-scale. In this way, we aim to construct a system that can suggest an evaluation method of materials performance for various materials, based on the request of the users.

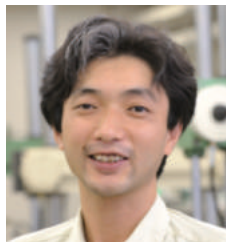


## Development of Local/Physical Fatigue Database for Heat Affected Zone (HAZ) of Weld Joint

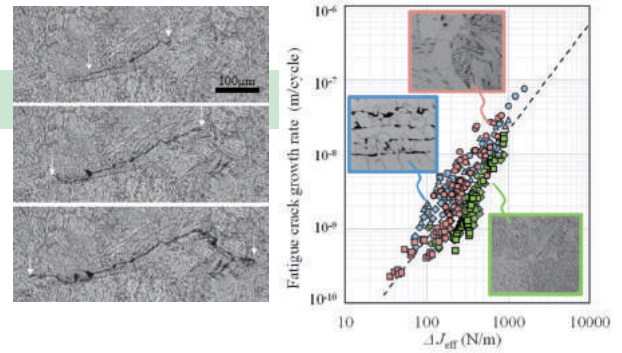
Keywords : Fatigue crack initiation and growth, Weld heat affected zone, Fracture mechanics



**HIDEAKI NISHIKAWA**  
National Institute for Materials Science



**YOSHIYUKI FURUYA**  
National Institute for Materials Science



Research theme/Development of Fatigue Database Module Initiation and early growth life of fatigue cracks, which are a large part of fatigue life, are sensitive to microstructure. The relationship between microstructure and fatigue property is important in order to improve the fatigue life estimation accuracy. This is especially true for weld, which has variable heat affected microstructures. We will construct a new fatigue database using simulated HAZ heat treated specimens to clarify the effect of HAZ microstructure for fatigue performance of weld. Furthermore, a fatigue database divided into fatigue crack initiation and growth life will be developed for physical and mechanical modeling of fatigue process. Figures show an example of fatigue initiation to early growth and a microstructurally small fatigue crack rate of a simulated HAZ specimen, which indicates microstructure-dependent crack growth resistance.

## Evaluation for creep damage and fracture of high temperature component

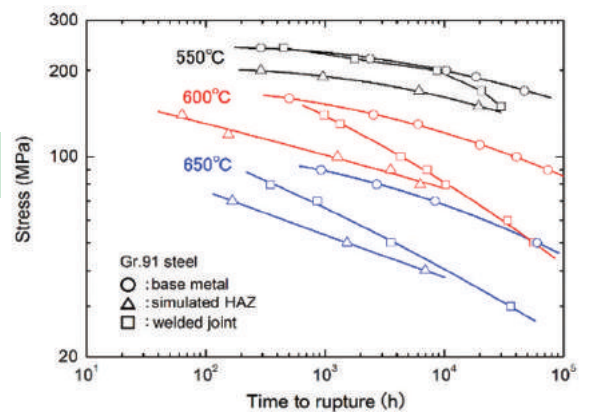
Keywords : Heat resisting steel, Welded joint, Creep, Damage mechanics, Fracture mechanics



**MASAAKI TABUCHI**  
National Institute for Materials Science



**TETSUYA MATSUNAGA**  
National Institute for Materials Science



Improvement in the efficiency of coal-fired power plants has been a critical issue in order to reduce CO<sub>2</sub> emissions. In the ultra-super critical (USC) power plant with highest efficiency, high Cr heat resisting steels with excellent creep strength have been used as the main structural components. The creep strength of their weld, however, decreases for long-term operation, as shown in the figure. In the present research, computational modules based on the damage mechanics and fracture mechanics and database module to predict creep life of high temperature weld components are developed and integrated into the MI system. It also aims to improve the accuracy of life prediction methods in cooperation with the "Microstructure prediction system" and "Data assimilation system."

## Members of Research Domain D: Development of Materials Integration System

### Development of thermodynamic databases of structural materials and prediction of microstructures by phase-field model coupled with databases.

Keywords : Phase diagram, CALPHAD, Microstructure, Computer simulation, Phase-field model

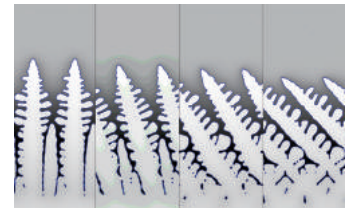
**IKUO OHNUMA**  
National Institute for Materials  
Science



**MACHIKO ODE**  
National Institute for  
Materials Science



Phase equilibria among the liquid,  $\gamma$ ,  $\alpha(\delta)$  and compound phases in steel materials are determined by experimental investigations using methods such as FE-EPMA, TEM, STEM, thermal analysis, etc. Thermodynamic parameters are evaluated by the CALPHAD (Calculation of Phase Diagrams) method by using obtained experimental data. Based on the phase-field model coupled with the CALPHAD databases, we are developing a computer simulation system for predicting the microstructure evolution, such as microstructures of the welded metal and heat affected zone (HAZ) at welded joints, in structural materials. The numerically obtained microstructural data are incorporated into the materials performance prediction system as one of the input parameters.

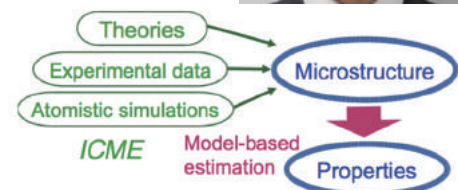


### Strengthening model based on heterogeneous microstructure in metals

Keywords :Continuum mechanics, micromechanics, ICME

**IKUMU WATANABE**  
National Institute for Materials Science

A theoretical framework will be established to couple between bulk properties and heterogeneous microstructure on the basis of homogenization theories and constitutive models of microscopic constituents in metals. The experimental materials database, metallurgical knowledge, dislocation theory, and computational results of atomistic simulations are integrated into the mathematical models at micro-scale to capture the material behaviors from underlying mechanisms and validated data.



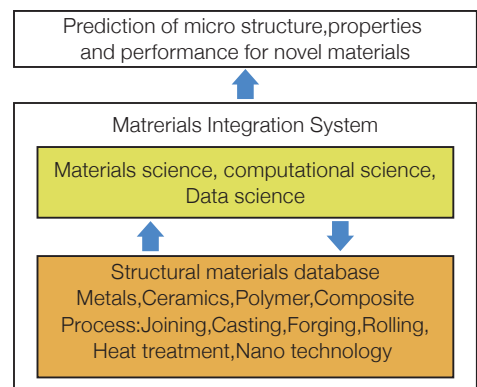
### Structural Material Database

Keywords :Chemical composition, Process, Mechanical property, Fatigu, Creep, Defusion

**MASAYOSHI YAMAZAKI**  
National Institute for Materials Science



**JUNKO HOSOYA**  
National Institute for Materials Science



This research aims to create a structural material database by developing the core data of fatigue and creep on structural material datasheets of the National Institute for Materials Science and to collect existing data from literature. In addition, the SIP-MI project obtained information about ceramics, polymers, composite material and their manufacturing process.

We also aim to build an integrated structural material database. Simulation software and machine learning use the data for the prediction of property and performance through the interface of a structural materials database in the Materials Integration system.

## Development of Visualization System based on Cloud Networking and Web Graphics Technologies in the field of Structural Materials

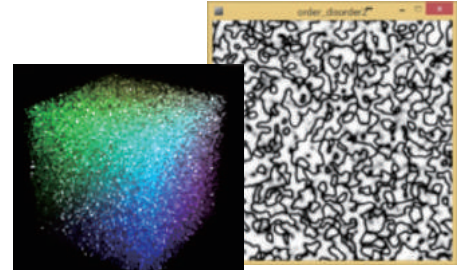
Keywords : Computer Graphics, Virtual Reality, Cloud Networking

**MAMORU ENDO**

Graduate School of Information Science, Nagoya University



This research is focused on the development of a visualization system based on Cloud networking and Web graphics technologies in the field of structural materials. In order to reduce the time required for structural materials development, simulation results output from the multi-systems are shared between networks to promote efficient use of data. By utilizing Web graphics technology, a possible high-speed drawing visualization module in a 2D/3D space on a web browser will be developed. Standardization work of the data structure assuming visualization for the data transmitters between the networks while ensuring interoperability is important. In addition, while an open network environment in the integrated system is necessary, it is also crucial to ensure confidentiality. Therefore, the system has been developed in consideration of information security.



## Development of microstructure data base and fatigue and cold cracking models for high strength steel welds

Keywords: weldment, microstructure, fatigue, cold cracking, non-destructive inspection

Steel Research Laboratory, JFE Steel Corporation



**NOBUYUKI  
ISHIKAWA**



**SATOSHI  
IGI**



**TOSHIFUMI  
KODAMA**

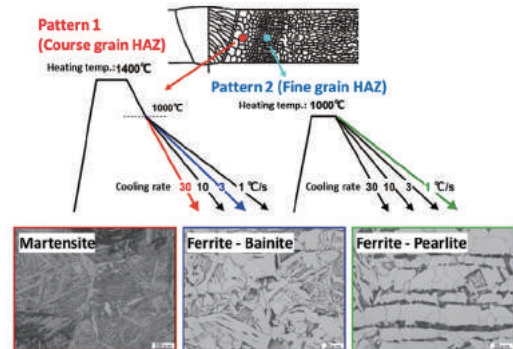


Figure. 1 Typical microstructures of high strength steel welds

A system to estimate the microstructure of materials is being developed by establishing the relevant microstructure data base for high strength steel welds and the validation of microstructure evolution in the weldment. Fatigue and cold cracking properties are being investigated with microscopic analysis of crack initiation and propagation behavior. With the materials property data base and non-destructive inspection technique, the validity of the materials performance estimation system will be confirmed and improved for higher accuracy.

## Characterization and analysis of high strength welded metal microstructures and verification of numerical model to predict brittle fracture properties

Keywords: Welding metallurgy, Brittle fracture, Defect detectability, Ultrasonic testing

KOBE STEEL, LTD.



Materials Research Laboratory  
**YOSHITOMI  
OKAZAKI**



Production Systems  
Research Laboratory  
**HIROYUKI  
TAKAMATSU**

Prediction systems for material performance are expected to reduce manufacturing costs and development times. The aims of this work are to construct databases for predicting the formation of microstructure in welded joints, and to reveal the relationship between the microstructures and fracture behavior. For this purpose, we

investigated the influences of Martensite-Austenite constituents and grain sizes on the brittle fracture initiation of high strength welded joints. We also focused on defects that affect fatigue properties, and revealed the defects detectability in ultrasonic testing by actual measurements and an ultrasonic scattering simulation for various weld structures.

