MI Technology in Developing and Utilizing Materials

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Abstract

Materials Informatics/Materials Integration (MI) technology is gaining attention as a method to advance the development of new materials efficiently. Kobe Steel is actively utilizing MI technology, exemplified by AI and simulations, in developing and utilizing a wide range of metal materials and their associated technologies. This article explains some representative cases: one involves using AI to predict material properties based on experimental data for welding materials and thin steel sheets, enabling the discovery of materials that achieve target properties by exploring chemical composition and heat treatment conditions. The other case explains how MI was used to obtain a material patent with few embodiments. Also explained is a case where simulations were constructed to evaluate the atomic-level material structure, properties, and processability into parts for thick steel plates and copper alloys. This allowed the development to be conducted on the desk. Finally, this article discusses the outlook for broadly utilizing MI to its fullest potential.

Introduction

Circumstances surrounding environmental issues are undergoing drastic change, for example, in the relatively new objective of carbon neutrality. Alongside this phenomenon, the requirements for materials and components are growing in terms of variety, complexity, and performance, with competition in the area of development intensifying. Working against these parameters are a declining birthrate and a population that is shrinking in number and advancing in age. Because these factors will likely make experts in the requisite areas of development scarcer, it is critical to be able to develop new materials more efficiently.

Conventional materials development has primarily relied on experiments, theory, and the experience and intuition of researchers, often requiring a massive amount of time and effort. Recently, however, materials informatics/materials integration (MI) has been attracting attention as a new materials development methodology that can overcome this challenge. Research into MI in the United States began in 2011 with the Materials Genome Initiative. In Japan, such research began in the mid-2010s with nationally run projects such as the Materials Research by Information Integration Initiative (MI^2I) for functional materials, and SIP-MI[1), 2)] (Cross-ministerial Strategic Innovation Promotion Program, materials integration) for structural materials. This propagated the use of MI in industry, with materials manufacturers using MI in the development process and suppliers of IT products beginning to offer a variety of related services.[3)] Kobe Steel, in particular, is working to reform materials development using MI as part of the company's DX strategy.

MI refers to two innovation methodologies: materials informatics and materials integration. Materials informatics involves applying information science (AI, machine learning) to materials science. Materials integration denotes the blending of information science with experimentation, theory, and computation/simulation (promoted by, e.g, SIP-MI). Further, there are two primary techniques for using MI in materials development. The deductive approach is theory-based and involves developing physical models to capture actual phenomena via simulation. In the inductive approach, data from experiments and simulations are analyzed by AI to find relationships between design data (e.g., chemical composition) and material properties.

Simulation techniques are selected based on the scale of the phenomenon being studied and include micro-scale (atomic-level) calculations using first-principle calculations and molecular dynamics, mesoscale calculations of material structures and properties using metallurgical theory and phase-field methods, and macro-scale calculations using the finite element method (FEM) to evaluate the workability and strength of components. One established subset of AI technologies uses regression methods such as linear regression, Gaussian process regression, and neural networks to learn from design data to create material property prediction models (forward problem analysis). Another subset uses optimization techniques (e.g., Bayesian optimization) to search for the design data most likely to achieve the desired material properties (inverse problem analysis)[4), 5)].

Kobe Steel has a deep understanding of chemical

composition and manufacturing process conditions related to a wide range of metal materials such as steel, aluminum alloys, copper alloys, and welding materials. This expertise is how the company develops materials that meet the desired material properties. We are also well versed in materials utilization, as proven in our components made of carefully designed materials, as well as our structural designs that rely on component performance. Further, we use MI technology in an exceptionally precise manner in developing the various metal materials we specialize in, as well as their applications (**Fig. 1**).

Examples of materials development covered in this paper describe the use of AI to predict material properties and explore chemical composition and heat treatment conditions using experimental data. Covered as well are examples of the use of AI in combination with micro- and macro-scale simulations. The areas of focus are welding materials (Section 1), thin steel plates (Section 2), thick steel plates (Section 3), and copper alloys (Sections 4 and 5).

1. Welding material development using experimental data and AI

This section introduces a case study in which AI was taught experimental data in a material property prediction model for flux-cored wire, a welding consumable used in arc welding. AI was used to research chemical composition to arrive at a material

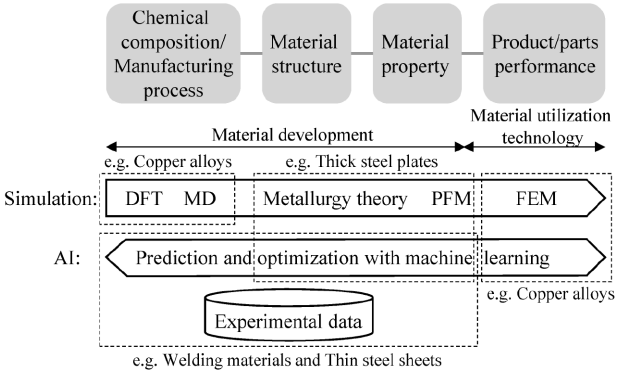

Fig. 1 Application of MI technology for material development and utilization

with an excellent balance of strength and toughness.

Fig. 2 shows a diagram of the AI-based prediction and search technology developed for this initiative. Conventional welding material development accounts for relationships between (1) raw material composition, (2) the chemical composition of welding materials made up of multiple raw materials (weld material composition), (3) the chemical composition of the weld metal after welding (weld metal chemical composition), and (4) the mechanical properties of the weld metal (weld metal properties). We developed MI technology that accounts for these hallmarks of welding material development in the form of AI prediction and search technology that connects every element, from (1) through (4), from both the forward and reverse perspectives.[6] The models within our prediction technology compute in the forward direction from (1)→(2), (2)→(3), and (3)→(4). Chaining the results of the individual models yields the overall prediction of (1)→(4). Our search technology also uses the prediction models for computations in the reverse direction, that is, (4)→(3)→(2)→(1). Described next are the details of the prediction and search technologies.

First, we modeled the prediction of (2) weld material composition from (1) raw material composition by taking advantage of the associated linear relationships. Next, we searched for (1) raw material composition from (2) weld material composition based on a convex optimization method that is effective for linear models. Gaussian process regression, a machine learning method, was then applied to experimental data to construct the prediction models for (2) weld material composition to (3) weld metal chemical composition and for (3) weld metal chemical composition to (4) weld metal properties. We chose this method because it is still difficult to define clear relationships based on theoretical physics due to complex welding phenomena and material microstructure morphology. The prediction model contains dozens of types of explanatory variables for weld material composition and weld metal chemical composition. As such, it is difficult to achieve high prediction accuracy simply by applying machine learning

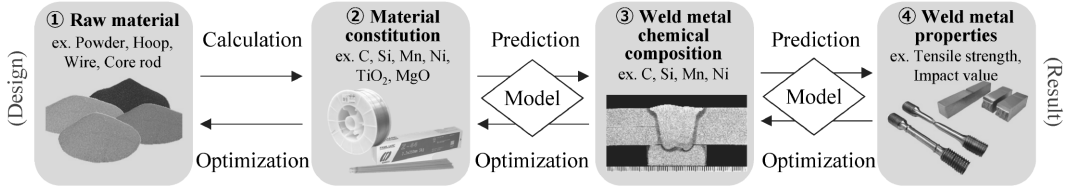

Fig. 2 Concept of MI application for welding material designing

methods to limited experimental data. We reduced the number of explanatory variables by excluding constituents known to have little effect based on our expertise in materials. We also incorporated the relationship between test temperature and brittle fracture rate into the model to predict toughness, a weld metal property. Through these measures, we improved the accuracy of our unique prediction model. Bayesian optimization, which is compatible with the Gaussian process regression used in the prediction model, was selected to search for (3) weld metal chemical composition and (2) weld material composition based on (4) weld metal properties. We applied this technology to flux-cored wire for arc welding of high-strength steel used in structural components.

First, we collected thousands of experimental data points in a range of strength classes for teaching to a prediction model. Next, we searched for raw material compositions predicted to achieve the weld metal's verification metrics of a tensile strength (TS) of ≥ 830 MPa and a 0℃ toughness (vE0℃ - energy absorbed upon Charpy impact test at 0℃) of ≥ 90 J. We made a prototype wire based on the results and evaluated its weld metal properties. Verification results were incorporated into the experimental data, and the process was iterated several times. **Fig. 3** shows the results based on conventional methods (white points) and based on MI (black points). Through MI, we uncovered a bold new design involving several composition changes compared with designs stipulated by conventional methods. One material satisfied the target properties by optimizing the balance between tensile strength and vE0℃. In short, we used MI to efficiently pinpoint a material that achieves the target properties, thereby revealing the value of using compositions different from those recommended by conventional design guidelines.

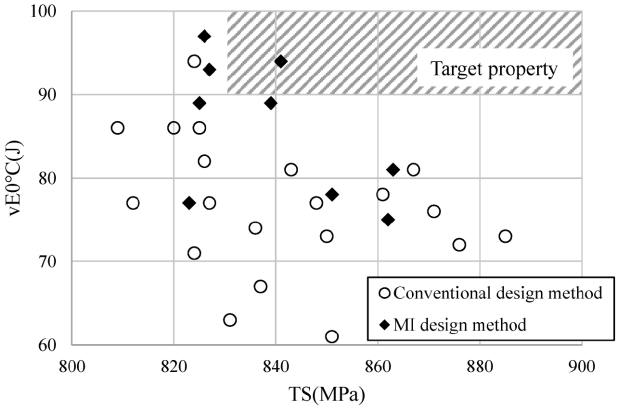

Fig. 3 Comparison of material properties between conventional design method and MI design method

2. Materials development using AI and experimental data on thin steel sheets

This section introduces a case study in which we used the experimental data Kobe Steel has amassed through developing ultra-high-tensile strength steel for vehicles to develop an AI-based property prediction model, which we then used to search for candidate materials, find a material that satisfies target properties, and obtain a patent with few embodiments.

Ultra-high-tensile strength steels for automotive applications must have high tensile strength for collision safety alongside mechanical properties in opposition to this, such as good total elongation (EL) and hole expandability (λ), which ensure formability. Although mechanical properties tend to improve with an increase in added elements, steel composition cannot be endlessly modified without sacrificing weldability and machinability. The cost and labor expenditure to develop and test ultra-high-tensile strength materials with excellent mechanical properties, given these constraints, is enormous. Our objective was therefore to find a suitable material using MI technology and few trials.

First, we constructed an AI-based property prediction model using 369 experimental data points accumulated by Kobe Steel on ultra-high-tensile strength steels. In addition to steel composition and heat treatment conditions, explanatory variables include the difference between the Ae_3 point and the uniform heat treatment temperature (T_1), and the difference between the Ms point and the cooling stop temperature (T_2). These parameters were introduced to capture changes in the material structure more directly and to improve the accuracy of mechanical property predictions. The Ae_3 point and Ms point can be calculated from composition information using the thermodynamics calculation software Thermo-Calc.[7] The objective variables were TS, EL, and λ, and Gaussian process regression was used as the prediction method. **Fig. 4** shows the relationship between the predicted and experimental values for TS and EL; both parameters were predicted with high accuracy.

Then, using the prediction model and Bayesian optimization, we searched for materials that satisfy the target properties of TS ≥ 950 MPa, EL ≥ 22%, and λ ≥ 20% within the composition ranges of C, Si, and Mn established for the verification material. We used Bayesian optimization to identify compositions and heat treatment conditions predicted to have the highest probability of achieving the desired properties. We then produced prototype materials and evaluated their properties. The first search

revealed 18 materials. We added the experimental data obtained based on this search to the training data and ran a second search, which revealed two additional materials. Materials satisfying the target properties were discovered via the second search.

Subsequently, we initiated the process to obtain a patent with a few embodiments for the composition and heat treatment conditions discovered via our AI-based property prediction model. The exact flow is described next. (1) We constructed an AI model that uses a large amount of experimental data to predict properties based on composition and heat treatment conditions. Further, we demonstrated the reliability of the model's predictions by comparing predicted and experimental values. (2) We used the AI model to create virtual data predicting properties based on composition and heat treatment conditions within and outside the scope of patent claims, and defended the validity of the claims. (3) We provided an embodiment and a comparative example using experimental data. **Table 1** shows the experimental and virtual data reported in the patent application. A circle in a property column of the virtual data section indicates that the target property was met; an 'x' indicates that it was not met. The embodiments of a patent claim must typically be based on a large amount of experimental data with great variation within each parameter. However, by substituting most of the required experimental data with virtual data predicted by AI, we were able to secure a patent, granted in October 2022[8], with only two sets of actual experimental data.

3. Materials development using metallurgical and fracture mechanics models and AI in thick steel plates

Large structures such as vessels and architectural steel frames are made up of welded thick steel plates. The heat-affected zone (HAZ) of a steel plate is generally less tough than the base metal, so ensuring the toughness of the HAZ is critical to the structure's safety. Evaluating the effects of compositions and welding conditions on HAZ toughness via experimentation is a complex process. The steel plate must be melted and rolled, and a simulation of heat treatment or thermal history during welding must be made available, entailing costly prototype production. Therefore, instead of using AI to predict HAZ toughness based on a vast repository of experimental data, we developed technology to predict HAZ toughness based on physical models and used inverse problem analysis to design the composition of the HAZ of thick steel plates. These projects are detailed next.

Inverse problem analysis requires a forward

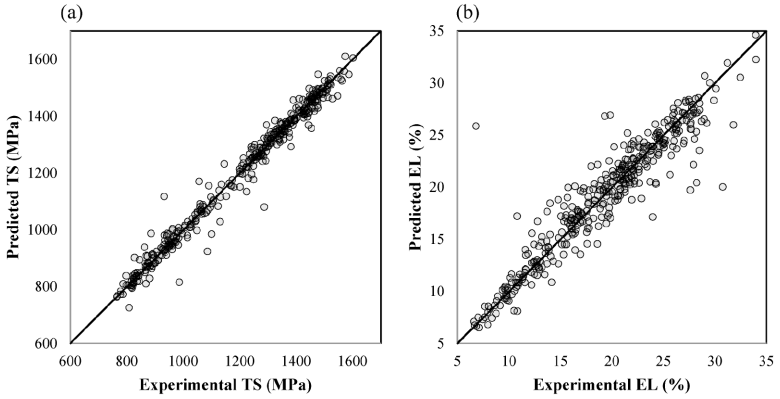

Fig. 4 Relationship between predicted and experimental values of each property - (a) Tensile strength, (b) Total elongation

Table 1 Experimental data and virtual data used for patent acquisition

Data No	Chemical compositions of materials								Annealing condition parameters						Mechanical properties		
	C	Si	Mn	Al	Ti	Ni	Mo	Cr	T_1-Ae_3	T_{preAT}	Ms-T_2	T_{postAT}	t_{preAT}	t_{postAT}	TS	EL	λ
	(mass %)								(℃)				(s)		(MPa)	(%)	(%)
Experimental-Data 1	0.20	0.8	2.0	0.04	0.00	0.0	0.0	0.5	-9	500	180	400	10	300	983	24.2	39.0
Experimental-Data 2	0.24	0.6	2.4	0.60	0.00	0.0	0.0	0.0	24	450	218	460	90	20	933	19.1	42.2
Virtual-Data1	0.20	0.8	2.0	0.04	0.00	0.0	0.0	1.0	130	500	50	400	10	300	○	×	○
Virtual-Data2	0.20	0.8	2.0	0.04	0.08	0.0	0.0	0.0	110	500	100	400	10	300	×	○	○
Virtual-Data3	0.40	2.0	2.0	0.04	0.00	0.0	0.0	0.0	48	380	5	380	100	450	○	×	×
Virtual-Data4	0.20	0.8	2.0	1.2	0.00	0.0	0.0	0.0	-12	450	200	400	23	300	×	○	○
Virtual-Data5	0.20	0.8	2.0	0.04	0.00	0.5	0.0	0.0	130	450	100	400	5	300	×	×	○
Virtual-Data6	0.20	0.8	2.0	0.04	0.00	0.0	0.2	0.0	110	500	50	400	5	300	×	×	○

※○: achieve target property. ×: not achieve target property

prediction model that predicts HAZ toughness from the composition and thermal history. Two models were linked together for forward prediction. One model calculates phase transformations based on composition and thermal history as well as structural characteristics, such as the hard second-phase microstructure that is the origin of fracture, based on transformation temperature information. The other model determines the occurrence of a brittle fracture based on the weakest link theory.[9] The model reproduces the phase transformation behavior of the HAZ at various cooling rates in thick low-carbon steel plates with different chemical compositions. It enables the use of the microstructure's characteristics in the HAZ to calculate the energy absorbed upon Charpy impact testing in the temperature range where brittle fracture is most likely to occur.[9] The predicted strength and toughness of the base metal corresponding to the quenching and tempering process are also modeled.[2]

To reduce the time required for optimization calculations during inverse problem analysis, more than 10,000 forward calculations with random chemical compositions were performed using our forward problem model, and an approximate function was learned by a neural network. Using this AI model to perform optimization calculations under specified constraints automates the design of steel composition and welding conditions (one pass). As a verification metric for inverse problem analysis, we researched the composition and process conditions (welding heat input) for steel plates with a strength of 980 MPa and low-temperature toughness in both the base metal and HAZ. Lower limits for base metal strength and base metal toughness and upper limits for alloy cost and equivalent carbon content were specified as optimization constraints. Given these constraints, we searched for the chemical composition that maximizes HAZ toughness in the heat input range of 4 - 8 kJ/mm. **Table 2** shows the steel plate composition for the verification test that was output by inverse problem analysis. Steel plates corresponding to the target composition in Table 2 were produced by melting, rolling, quenching, and tempering. These plates then underwent tensile and Charpy impact testing. HAZ toughness was evaluated using material subjected to a recreated HAZ thermal cycle. The toughness evaluation index is the transition temperature at which the absorbed energy upon the Charpy impact test reached 50 J. **Table 3** shows the results of the experimental verification and the properties obtained by inverse problem analysis.[2] Although the difference between the predicted and experimental HAZ toughness values was relatively large, the experimental verification results were satisfactory for each property. While it is impossible to completely eliminate the need for prototyping, the method used appears to be effective for defining material design guidelines. Our models will improve the efficiency of developing steel plates that meet various specifications and constraints.

Table 2 Chemical composition of steel plate for verification test

(mass%)

C	Si	Mn	Ni	Cr	Mo
0.06	0.4	1.6	2.0	1.0	0.5

Others Cu, Nb, V, Al

4. Materials development using molecular dynamics in copper alloys

Copper alloys exhibit excellent thermal and electrical conductivity, making them ideal for applications such as electronic devices, terminals in automotive electronics, and machinery cabling. However, the demand for lighter and smaller products is driving the need to develop copper alloys with higher strength and electrical conductivity. Solid solution strengthening is one way to increase the strength of a copper alloy. One of the many theories proposed as the mechanism of solid solution strengthening is the size effect theory[10]. The size effect theory starts with the explanation that when an element (solute) is dissolved in a solid material of another single element (solvent), the difference in atomic radii (solute vs. solvent) causes lattice distortion.

Table 3 Inverse problem analysis verification test results

	Base material		HAZ
	Tensile strength (MPa)	50 J transition temperature (℃)	50 J transition temperature (℃)
Predicted value	1,090	-44	-91※
Experimental result	1,011	-45	-58～-70
Target property	> 980	< -40	< -50

※Worst value in the heat input range for calculating HAZ toughness

Dislocations then adhere to the solute atoms (pinning), suppressing the movement of dislocations and thereby increasing strength. Experimental data show that the larger the difference between the atomic radii of the solute and solvent, the greater the effect of solid solution strengthening. However, the atomic-level mechanism of the size effect theory is not well understood. Therefore, we developed a simulation model for a binary copper alloy to calculate the force required to depin a dislocation from a solute atom using the molecular dynamics (MD) method, which can analyze the dynamics of a large number of atoms[11]. Furthermore, we extracted factors closely related to depinning force and developed a prediction formula to easily calculate depinning force. An example[12] is detailed next.

First, we created models to which we could apply MD methods. Specifically, we created Cu-Ni and Cu-Mo models with crystalline structures containing Cu as the solvent, one Ni or Mo atom as the solute, and one edge dislocation. Dislocations in a face-centered cubic lattice (FCC), such as those exhibited by Cu can expand into two partial dislocations and stacking faults, a phenomenon that can be reproduced. We used the MD method to determine the depinning force required for the partial dislocation to detach from the solute atom by increasing the force applied in the slip direction of the model. Results showed that the depinning force required for the Cu-Mo model was about 10 times higher than that of the Cu-Ni model (**Fig. 5**). The atomic radius of Mo is greater than Ni, which is similar in size to Cu. The results therefore line up with the tendency that the larger the difference in atomic radii between solute and solvent, the more intense the solid solution strengthening, making it possible to compare the depinning forces.

However, to calculate via the MD method, the interatomic potential must be known for each element. This entails enormous computational costs,

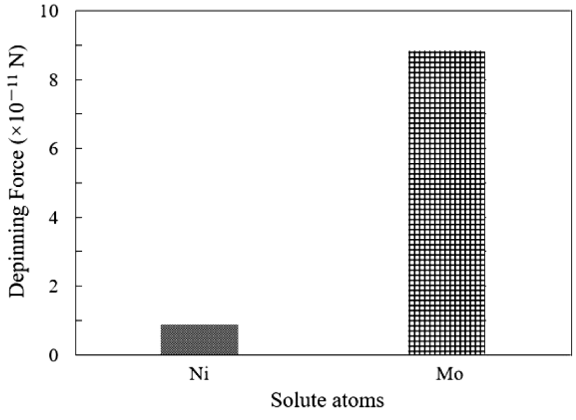

Fig. 5 Depinning force required for partial dislocation to move away from solute atom

making it difficult to simulate solid solutions of a large number of different elements. We therefore set out to develop a simple equation for prediction. The results of the MD method indicated that the maximum volumetric strain around the solute atom and the misalignment between the solute and solvent atoms calculated by first-principle calculations are related to the depinning force. As such, we developed Equation (1) to predict the depinning force F_V.

Equation (1): $F_V = \alpha|\Omega|Gb^2|\varepsilon_V^{max}|$

Here, α is a fitting parameter, Ω is the alignment between the solute and solvent atoms calculated by first-principle calculations, G is the shear modulus, b is the Burgers vector, and ε_V^{max} is the maximum volumetric strain. These parameters are element specific and can be determined via a simple simulation. In using this prediction equation to calculate the depinning force F_V when elements undergo solid dissolution, it is possible to screen for added elements that are highly effective for solid-solution strengthening via theoretical calculation. We anticipate that this will serve as a new guideline for designing high-strength copper alloys.

5. Developing materials application technology using finite element analysis and AI in copper alloys

This section introduces a case study in which AI and simulation via finite element analysis were jointly applied to optimize a multi-stage bending process for copper alloy sheets used in terminals for automotive electronics[13].

Conductivity is an essential property in terminals used for automotive electronics. When the pin-shaped male terminal is inserted into the female terminal, the leaf spring inside the female terminal deforms, generating counterforce from the contact pressure and thus ensuring conductivity. Terminals in automotive electronics have been made smaller in recent years to conserve space, entailing shorter leaf springs and therefore lower spring constants. To maintain the same contact pressure as before, spring deformation must be increased to compensate for the decrease in spring constant. However, if the leaf spring deforms to the point of plastic deformation, the desired contact pressure will not be achieved. Therefore, the material of the leaf spring must be strong enough to preclude plastic deformation. The stronger a material, though, the lower its bend formability, with breakage and creasing being more likely to occur during manufacturing. One way to improve bend formability is to

ensure manufacturing conditions are conducive to effective bending processes. However, there are many relevant process condition parameters, and determining the appropriate set of conditions through experimentation is costly. This drove us to develop a technique for efficiently exploring optimal bending conditions by combining optimization techniques with technology for evaluating bending formability through simulation.

Fig. 6 shows an FE model for contact bending as a simulation to evaluate bend formability. Contact bending is a four-stage bending process (1st through 4th stage) with six main process condition parameters: 1st bending radius R_1, 1st bending angle θ_1, 2nd bending clearance C, 2nd bending radius R_2, 2nd bending punch radius R_p, and 3rd bending angle θ_3. Experience shows a correlation between bending strain and the degree of breakage and creasing on the plate surface. Therefore, the maximum bending strain ε_{max} generated on the plate surface after the 4th bending stage was used for the simulation to evaluate bend formability. We used the explicit dynamics software LS-DYNA[14] for FEA. CATIA V5[15] (CAD software) and HyperMesh[16] (mesh creation software) were used to modify the FE model in response to changes in the process condition parameters.

This simulation was used to search for process condition parameters that would reduce the maximum bending strain ε_{max} via optimization techniques. Since a simulation takes about 30 minutes, we chose Bayesian optimization for its greater likelihood of obtaining an optimal solution within fewer runs of the simulation. The overall calculation flow was to acquire initial data by running a simulation with process condition parameters based on experimental design, search for process condition parameters using Bayesian optimization, modify the FE model, and rerun the simulation. The search process involves adding newly acquired data and repeating the calculations in an iterative process.

To verify the effectiveness of this technology, we ran experiments using dies for contact bending under three different conditions: (a) conventional condition, (b) manually adjusted condition, and (c) optimized condition. **Fig. 7** shows the contact bending surface under each condition. The copper alloy sheets in this experiment were tin plated. Under the conventional and manually adjusted conditions, the tin plating peeled off, exposing a large area of copper substrate. The optimized condition suppressed exposure of the copper substrate, confirming that this bending condition is favorable. This technology is a promising solution for quickly providing optimal bending conditions for copper alloy sheets with varying properties.

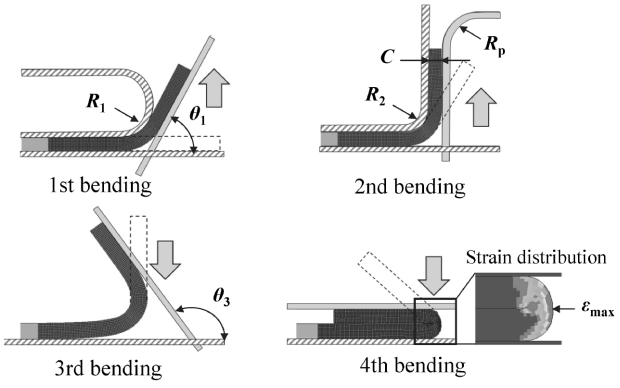

Fig. 6 FE model for contact bending evaluation

Conclusion

This paper describes examples of materials development and utilization as applied to various metal materials using MI technologies such as AI and simulation models. To use MI effectively in the discovery of new materials, we gathered extensive experimental data (from experiments conducted by Kobe Steel, patents, and publications), constructed physical models that capture physical phenomena on each scale, produced data through theoretical simulations of various conditions to overcome barriers to experimentation, and used AI to explore this large amount of high-dimensional data

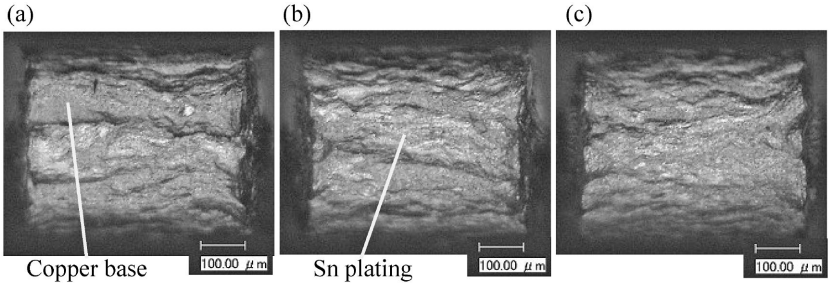

Fig. 7 Observation of contact bending outside surface experimented under each condition - (a) Conventional condition, (b) Manually adjusted condition, (c) Optimized condition

to an extent beyond human capabilities. We are continuing to develop our cloud-based platform DataLab® to foster the comprehensive utilization of MI, as this requires a platform with a database for storing experimental data and tools that enable materials engineers to use AI and simulation technologies without programming expertise. For details regarding DataLab®, see "Building and Utilizing Company-wide Data Analytics Platform, DataLab®" (pp.4-8 of this issue). While our application of DataLab® began with the development of welding materials[6], we will expand its scope by creating a development system that can respond quickly to the varying needs of our customers.

Our research was conducted in part under the Cross-ministerial Strategic Innovation Promotion Program (SIP) "Materials Integration for Revolutionary Design System of Structural Materials" of the Council for Science, Technology and Innovation, Cabinet Office, Government of Japan (managed by JST, Japan Science and Technology Agency).

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