

DESCRIPTION

Title of Invention: MATERIAL PROPERTY PREDICTION SYSTEM AND
MATERIAL PROPERTY PREDICTION METHOD

5

Technical Field

[0001]

The present invention relates to a technology that
supports experiments in materials science among others.

10 Background Art

[0002]

Along with development of a statistical processing
technology regarding data analysis, there is a rising
demand for carrying out data analysis in materials science
as well. Particularly, in a field of materials science, a
method called screening is known in which a selection of
candidates for a next experiment is made based on known
data to perform development of new materials efficiently.

15

[0003]

20 In Patent Literature (PTL) 1, a design support method
is described in which knowledges in a nanoscale domain are
linked and structured in a same concept scheme
independently of material types and applied usefully to new
material design independent of material types.

25

[0004]

In PTL 2, descriptions are provided as below: through the use of quantum statistic values that are obtained through statistic processing of quantum thermodynamics state quantities specific to elements constituting a reaction system, out of substances with the same number of elements, for which the number or percentage of elements that constitute a reaction system differs, a selection is made of only those substances that have the same physical property value; by inducing multiple simultaneous linear equations that are as many as or more than the number of elements constituting each of those substances and finding a solution of the equations, it is enabled to design the material of a metallic or non-metallic substance having targeted physical and chemical properties and functionality.

[0005]

As a screening method, various sorts of experimental data are input to an information system, a model is built for predicting an experiment result through machine learning, and screening is performed based on prediction through the model. For this prediction, a method that takes various parameters regarding material design as arguments and evaluates a function that returns a material property by a regression analysis is well known.

Citation List

Patent Literature

[0006]

PTL 1: Japanese Patent Application Laid-Open No. 2003-
178102

PTL 2: Japanese Patent Application Laid-Open No. 2004-
5 086892

Summary of Invention

Technical Problem

[0007]

10 In material development, increasing the accuracy of
predicting material properties makes it possible to
identify a promising potential of a candidate for a new
material more exactly and, by dispensing with unnecessary
experiments, it is expected that efficient material
development can be conducted.

15 [0008]

In the regression analysis, variables that correspond
to arguments of a function are called explanatory variables
and a value that corresponds to a return value of the
function is called an objective variable. In predicting a
20 property of a material, the material property is taken as
the objective variable and explanatory variables
representing the features of the material are selected so
that the material property can be predicted. Increase or
decrease in the accuracy of the prediction depends on how
25 to select the explanatory variables and, therefore, it is

important to prepare a variation of explanatory variables to be adaptable for prediction of a wide range of material properties.

[0009]

5 An attempt to predict material properties using past data is disclosed in PTL 1 and PTL 2. However, a general process for material development starts development with certain compositions and a manufacturing process and, for a material found to have an effective property, further takes
10 measures with its related composition and manufacturing process.

[0010]

 In fact, there is a problem in which, in an initial phase of development, only a very small amount of data can
15 be used for a task that has just begun. When attempting to use information of past data, in most cases, data representing well-prepared material properties is only such data available for the task to address, because material properties that are targeted differ task by task. In
20 addition, in some cases, even experiments that aim at finding like properties use different measurement methods and it is often hard to repurpose resulting data straightforwardly.

[0011]

25 A problem that is addressed by the present invention

is to provide a method that improves the accuracy of predicting material properties by making effective use of past data.

Solution to Problem

5 [0012]

One preferred aspect of the present invention resides in a system to carry out prediction of material properties by processing task data including a plurality of records, each including a material composition, an experimental
10 condition, and a material property. This system includes a material property prediction presenting unit, a cross-task compatible feature value generating unit, and a material property predicting unit. The material property prediction presenting unit accepts a specification of first task data
15 that includes a record in which a material property is unknown and is to be a target of material property prediction through a first predictive model. The cross-task compatible feature value generating unit predicts feature values from material compositions in the first task
20 data by using a second predictive model. The material property predicting unit generates the first predictive model by using the material compositions, experimental condition, feature values, and the known material property in the first task data. Also, the material property
25 predicting unit inputs the material composition, the

experimental condition, and the feature value in a record in which the material property is unknown in the first task data to the first predictive model and predicts the unknown material property.

5 [0013]

Material composition is at least information about the composition of a material and, more preferably, information about the structure of a material, e.g., its structural formula.

10 [0014]

Another preferred aspect of the present invention resides in a method for predicting material properties by an information processing device including an input device, a storage device, and a processor. When generating a first
15 predictive model for predicting a first material property from first data including first feature values, the method executes the following steps. The method executes, namely, a first step of preparing, from the first feature values, a second predictive model that is to predict a second
20 material property defined different from the first material property; a second step of predicting the second material property by applying the first data to the second predictive model; and a third step of generating the first predictive model, taking the first feature values as a
25 first explanatory variable, the second material property as

a second explanatory variable, and the first material property as an objective variable.

Advantageous Effects of Invention

[0015]

5 It is possible to improve the accuracy of predicting material properties by making effective use of past data.

Brief Description of Drawings

[0016]

 Figure 1 is a functional block diagram depicting an
10 example of an outlined configuration of an example.

 Figure 2 is a block diagram depicting an example of a physical implementation configuration of the example.

 Figure 3 is a conceptual diagram illustrating an example of procedures for using the example.

15 Figure 4 is a flowchart illustrating an example of a material DB update process in the example.

 Figure 5 is an image diagram illustrating an example of a screen that is displayed for accepting experimental data in the example.

20 Figure 6 is a tabular diagram illustrating an example of the structure of experimental data in the example.

 Figure 7 is a tabular diagram illustrating an example of an experimental data table in a material DB in the example.

25 Figure 8 is a conceptual diagram illustrating an

example of task data.

Figure 9 is an explanatory diagram illustrating a concept of cross-task compatible feature values.

Figure 10 is a flowchart illustrating an example a
5 material property prediction process in the example.

Figure 11 is an image diagram illustrating an example of a material property prediction display in the example.

Figure 12 is a tabular diagram illustrating an example of the structure of data for predicting material properties
10 in the example.

Description of Embodiments

[0017]

An embodiment is now described in detail with the aid of the drawings. However, the present invention should not
15 be construed to be limited to the following description of the embodiment. Those skilled in the art will easily appreciate that a concrete configuration of the present invention may be modified without departing from the idea or spirit of the present invention.

20 [0018]

In a configuration of the invention which will be described hereinafter, for identical parts or parts having like functions, identical reference numerals are used in common across different drawings and duplicated description
25 of those parts may be omitted.

[0019]

Multiple elements having the same or like functions, if any, may be assigned the same reference numeral with different subscripts and described. However, when it is not necessary to individualize those multiple elements, the subscripts may be omitted in describing them.

[0020]

Notation of "first", "second", "third", etc. herein is prefixed to identify components, but it is not necessarily intended to confine the components to a certain number, sequence, or contents. In addition, numbers to identify components are used on a per-context basis; a number used in one context does not always denote the same component in another context. Additionally, it is not precluded that a component identified by a number also functions as a component identified by another number.

[0021]

In some cases, the position, size, shape, range, etc. of each component depicted in a drawing or the like may not represent its actual position, size, shape, range, etc. with the intention to facilitate understanding of the invention. Hence, the present invention is not necessarily to be limited to a position, size, shape, range, etc. disclosed in a drawing or the like.

<Example 1>

[0022]

<1. System configuration>

Figure 1 depicts an example of a material property prediction device of Example 1. The material property

5 prediction device (101) of the present example is a device that accepts operation by a user (102) and includes an experimental data accepting unit (111) that receives experimental data from the user and a material database (DB: Data Base) (112) on a per-task basis in which the
10 features and properties of materials are stored. Here, a task means a set of data that a user can define freely; e.g., data obtained from an experiment and a development and assumed to be created by different persons and for different purposes.

15 [0023]

The material property prediction device (101) also includes a material property predicting unit (113) that generates a material property predictive model to predict material properties and predicts unmeasured material
20 properties using a material property predictive model and a material property predictive model DB (114) to store material property predictive models.

[0024]

The material property predicting unit (113) generates
25 a material property predictive model by using feature

values obtained from data of measured values of a material property from the material DB (112) and feature values obtained from a cross-task compatible feature value generating unit (115) and predicts an unknown property.

5 The cross-task compatible feature value generating unit (115) generates new feature values from data in the material DB (112) and the material property predictive model DB (114). A material property prediction presenting unit (116) presents a result of a prediction made by the material property predicting unit (113) to the user (102).
10 [0025]

In the present example, the material property prediction device (101) was assumed to be configured as an information processing device like a server including an
15 input device, an output device, a storage device, and a processing device. Computation and control functions among others are implemented by carrying out a defined process in cooperation with other elements of hardware in such a manner that a program stored in the storage device is
20 executed by the processing device. Figure 1 illustrates functional blocks instead of the hardware configuration of an information processing device. As the respective functional blocks, programs to be executed by a computer or the like, their functions or means for implementing the
25 functions may be referred to as "functions", "means",

"sections", "units", "modules", etc.

[0026]

Figure 2 depicts an example of a physical implementation configuration of Example 1. The material property prediction device (101) can be implemented by using a commonly used computer; that is, a device including a processor (201) having computational performance, a DRAM (Dynamic Random Access Memory) (202) which is a volatile and temporary memory with areas readable and writable at high speed, a storage device (203) that provides for permanent storage areas using a HDD (hard disk device), a flash memory, etc., an input device (204) which is a mouse and a keyboard, etc. for user operation, a monitor (205) for presenting an operation to the user, and an interface (206) such as a serial port for communication with an external entity.

[0027]

In Figure 1, the experimental data accepting unit (111), the material property predicting unit (113), the cross-task compatible feature value generating unit (115), and the material property prediction presenting unit (116) can be implemented in such a manner that the processor (201) executes programs recorded in the storage device (203). The material DB (112) and the material property predictive model DB (114) can be implemented in such a

manner that the processor (201) executes a program to store data into the storage device (203).

[0028]

The configuration of Figure 2 may be configured on a single computer or any part thereof may be configured on another computer connected via a network. In other words, the same system as discussed herein may be configured with a plurality of computers.

[0029]

Figure 3 schematically illustrates procedures for using the system of Example 1. Example 1 enables the execution of two procedures as follows: material data inputting (S310), i.e., a user inputs data concerned in predicting material properties; and prediction result viewing (S310) to check a result of predicted material properties.

[0030]

Material data inputting (S310) is a procedure of inputting experimental data (600) which is a data set in which data of a material for which an experiment was conducted and data of a material for which an experiment is going to be conducted have been stored to the material property prediction device (101). In response to this data, the material property prediction device executes a material DB update process (S311), thereby updating internally

stored information.

[0031]

In the prediction result viewing (S320), the material property prediction device executes a material property prediction presenting process (S321) in response to a request of the user (102) and presents a material property prediction display (322) which is a screen in which a result of predicted material properties is visualized.

[0032]

10 <2. Material data inputting process>

Figure 4 illustrates an example of a processing procedure of the material DB update process (S311). In the material DB update process (S311), the experimental data accepting unit (111) first receives experimental data (600) from the user (102) and recognizes or adds a task ID (S401). Then, the process updates or adds the corresponding data per task to the material DB (112) (S402).

[0033]

Figure 5 illustrates an example of a screen that is displayed on the monitor (205) for receiving experimental data (600) from the user (102) in the first step (S401) of the material DB update process (311). In Example 1, the user (102) pre-stores experimental data in a file and specifies the file location in a text box (501); in this way, the user passes experimental data (600). In the file

that is passed, tabular data is described in a CSV (Comma Separated Value) format which is publicly known and its interpreted result rendered in a tabular form is displayed in a table screen (502).

5 [0034]

In Figure 5, illustrated is a table with the following columns: "ID" which is the identifier of an experiment whose information is described; "Temp" that indicates temperature when the experiment was conducted; "SOL" that
10 indicates water solubility measured at that time; and "SMILES" which is a string representing the structural formula of a material. Water solubility is a material property that an experimenter wants to predict in this example and blank data in the SOL column indicates a
15 nonexperimental condition. Note that this way of passing data to the device is exemplary and another method may be applicable using any format in which, as information convertible to a tabular form, experimental data including structural formulas of materials and a material property
20 can be passed to the device. Information is displayed in the table screen (502) and saved in the material DB (112) using a button (503).

[0035]

Figure 6 illustrates an example of the structure of
25 one record of the experimental data (600). One record is

created for one material having a particular composition and obtained in a manufacturing process. In the present example, the experimental data (600) is information in which one record includes the following pieces of

5 information: material property (601), material structural formula (602) which is information that can express the material structural formula, such as, e.g., in the SMILES format, and experimental condition (603) indicating a condition when the experiment was conducted, such as
10 temperature and pressure. The experimental data (600) is a collection of one or more such records. These pieces of information correspond to the respective column items of the table screen (502) in Figure 5. In the present example, correspondence between each item and which element is
15 determined by correspondence to a predetermined item name. The user (102) may be prompted to input this correspondence relationship from the screen. Moreover, as for the material property (601), a value revealed by the experiment or the like is stored or a blank is stored if it is
20 nonexperimental. Other information such as a task name may be added to the experimental data (600).

[0036]

The first step (S401) of the material DB update process (S311) of Figure 4 interprets and formats the
25 experimental data (600) and stores it as an experimental

data table in the material DB (112).

[0037]

Figure 7 illustrates information in one record of an experimental data table. This data includes experiment ID (701) assigned to each experiment in a serial numbering scheme or the like so that the experiment can be identified uniquely, material property (702) derived from the material property (601) of the experimental data (600), material structural formula (703) derived from the material structural formula (602) of the experimental data (600), and experimental condition (704) derived from the experimental condition (603). Information from which these items of data are derived may be converted in units and formats and transformed into a coherent representation.

[0038]

A task ID (700) is an identification number that uniquely identifies a task. In Example 1, it is assumed to handle one file as one task and, therefore, a task ID corresponds to a filename of a real data file. A task ID (700) should be added in a serial numbering scheme when registering in the material DB (112). If correspondence between a file and a task is not fixed, its registration may be made in the following manner: when registering in the material DB (112), a question that "a file you are going to upload now corresponds to what task?" is presented

to the user to ask the user to input the correspondence.

The format of the experimental data table is required to be the same for registered data and added data. The user can define the material property (702) and the experimental
5 condition (704) optionally and also can set the number of material properties and experimental conditions freely.

[0039]

<3. Cross-task compatible feature values>

A feature of the present example is improving the
10 accuracy of predicting material properties by using data of existing tasks even in a situation where there are few data pieces. In an initial phase of a material development process, the amount of available data is very small. Before explaining a concrete example, a concept of the
15 present example is described.

[0040]

Figure 8 illustrates an example of task data that is stored in the material database (112) on a per-task basis. As illustrated in Figure 8, when attempting to use
20 information of any other task, in most cases, data representing well-prepared material properties is only such data available for the task to address, because material properties that are targeted usually differ task by task. In addition, in some cases, even experiments that aim at
25 finding like properties use different measurement methods

and it is often hard to repurpose resulting data straightforwardly.

[0041]

In the example of Figure 8, a past task A and a past
5 task B have data under different experimental conditions,
temperature, and humidity, and for different material
properties, A and B; therefore, their data cannot be used
interchangeably for property prediction as it is. In the
present example, it is enabled to increase the number of
10 explanatory variables by using past task data as
"information for creating feature values". Here, feature
values that are newly created are referred to as "cross-
task compatible feature values".

[0042]

15 A process that uses information about past tasks as
"information for creating feature values" is described with
Figure 9. Using data of the past task A (901), the process
first generates (learns) a predictive model (902) to
predict a material property A from structural formulas,
20 assuming the objective variable as the material property A
of a known material and the explanatory variables as the
structural formulas. This model can be generated through
supervised machine learning which is known, by using, e.g.,
regression trees, random forests, support vector regression,
25 Gaussian process regression, neural networks, etc.

[0043]

The process then predicts the material property A by applying the structural formulas in the data of the past task B (903) to the predictive model (902). The process
5 adds the material property A to the data of the past task B, thus generating a new data set (904). If the same structural formula as in the past task B is included in the past task A, its material property in the past task A may be added as is to the new data set. This material property
10 A corresponds to cross-task compatible feature values.

[0044]

Upon having obtained the new data set (904), the process generates a predictive model (905) to predict a material property B, taking known data of the material
15 property B (item Nos. 1, 2, and 3) in the data set as teacher data. At this time, the explanatory variables are the structural formulas, experimental condition (humidity), and the material property A and the objective variable is the material property B. The predictive model (905) can be
20 generated through supervised machine learning which is known.

[0045]

The process inputs data (item No. 4) for which the material property B should be predicted to the generated predictive model (905) and obtains the material property B.
25 By adding the material property A as new feature values

(cross-task compatible feature values), it can be expected to improve the prediction accuracy in comparison with when the past task B data is used as it is. This is considered as effective particularly when there is a correlation
5 between the material properties A and B.

With the understanding of the concept discussed above, a flow of a concrete process for prediction result viewing is described.

[0046]

10 <4. Process for prediction result viewing>

The material property prediction presenting process (S321) for prediction result viewing (S320) is described with Figure 10. In the following description, a description in relation to the concept illustrated in
15 Figure 9 is also provided with a reference numeral in a series of 901 to 905 in Figure 9.

[0047]

First, the material property prediction presenting unit (116) presents the material property prediction
20 display (322) to the user (102) and receives the specification of an experimental data table as a target of property prediction (S1001). At this time, a task ID is used to specify the designation of an experimental data table stored in the material DB (112). Here, it is assumed
25 that experimental data has already been stored in the

material DB (112).

[0048]

Figure 11 illustrates an example of a screen displayed on the monitor (205) for accepting a request from the user (102) and a screen for the material property prediction display (322) in which a result of predicted material properties is visualized.

[0049]

In a drop-down box (1101) in the figure, the designation of an experimental data table is displayed as a candidate. When the user specifies a task ID and presses the predicted value update button (1102), the material property prediction presenting unit (116) sends a command to execute interpolation by a predicted value for blank data of material property (702) in the records of the experimental data table (Figure 7) to the material property predicting unit (113), and a result is to be displayed in the screen (1103). Underlined values of the material property in Figure 11 are those obtained by the interpolation of blank data.

[0050]

Upon receiving the above command to execute interpolation from the material property prediction presenting unit (116), the material property predicting unit (113) retrieves the data of the experimental data

table specified by the task ID (700) from the material DB (112) (S1002). Also, in the screen (1104) in Figure 11, any other task is selected that is used to generate cross-task compatible feature values. The material property predicting unit (113) retrieves a predictive model (902) related to the selected other task from the material property predictive model DB (114) (S1003).

[0051]

Data retrieved in the processing step (S1002) as described with the flowchart of Figure 10 corresponds to the data of the past task B (903) in Figure 9. The predictive model related to the task retrieved in the processing step (S1003) corresponds to the predictive model (902) generated from the data of the past task A (901) in Figure 9.

[0052]

In the above description, it is assumed that the predictive model (902) has already been created and is called by the task ID (700) from the material property predictive model DB (114). If the corresponding predictive model (902) does not exist in the material property predictive model DB (114), learning and creating the predictive model (902) should be executed, assuming the material structural formulas in the data of the past task A as the explanatory variables and the material property of a

known material as the objective variable, as illustrated in Figure 9.

[0053]

Then, the material property predicting unit (113)
5 generates data for predicting material properties (S1004).
This processing corresponds to predicting the material
property A by applying the structural formulas in the data
of the past task B (903) to the predictive model (902) and
adding the material property A to the data of the past task
10 B, thus generating a new data set (904). At this time, the
cross-task compatible feature value generating unit (115)
executes prediction of the material property A (cross-task
compatible feature values) by using the predictive model
(902) retrieved in the pressing step (S1003).

15 [0054]

Figure 12 illustrates the structure of one record
(1500) of the data for predicting material properties. The
contents of one record take over the task ID (700),
experiment ID (701), material property (701), and
20 experimental condition (704) in the experimental data table
(Figure 7) of the data of the past task B (903). The
record also includes feature values derived from structural
formulas (1201). The feature values derived from
structural formulas are computed from the material
25 structural formulas (703). As a method for computing

feature values from structural formulas, there is a publicly known method such as fingerprinting.

[0055]

The data for predicting material properties includes
5 feature values (1202, 1203) created through the predictive
model (902) related to any other task, i.e., cross-task
compatible feature values. The description with regard to
Figure 9 assumes that any other task is another one, the
past task A, and cross-task compatible feature values are
10 of one material property A to be predicted. However,
feature values created through the predictive model (902)
related to any other task may be those of one material
property or any number of material properties. Also,
multiple other tasks may be used.

15 [0056]

From the data for predicting material properties
except for records in which material property (702) is
unmeasured, i.e., blank, the material property predicting
unit (113) assigns items excepting task ID (700),
20 experiment ID (701), and material property (702) to the
explanatory variables and the material property (702) to
the objective variable, executes a regression analysis
which is publicly known, obtains a prediction function, and
learns a predictive model (905) (S1005). The created
25 predictive model (905) is stored into the material property

predictive model DB (114) together with the task ID of the data from which the predictive model (905) was generated.

[0057]

Given that the prediction function is written as $y = f(x_1, x_2, \dots)$, where y is the objective variable and $x_1, x_2, \dots$ are the explanatory variables, this procedure means defining the function form of f , i.e., defining $x_1, x_2, \dots$ so that y can be predicted. In the case of the present example, supposing the use of the data for predicting material properties in Figure 12, the predictive model (905) is generated through learning of a regression analysis on the function: [material property (702)] = f ([feature values derived from structural formulas (1201)], [experimental condition (704)], [feature values about task [1] (1202)], [feature values about task [2] (1203)]).

[0058]

This learning corresponds to generating the predictive model (905) in the bottom row of Figure 9. Although experimental condition (704) is one type that is humidity in Figure 9, there may be any number and any type of experimental conditions, provided that relevant data exists. As experimental conditions, there are, e.g., material manufacturing conditions; however, they may be omissible if there is no relevant data. Also, as noted previously, although cross-task compatible feature values are of one

material property A to be predicted, as illustrated in Figure 9, there may be a plurality of items of such values, as in the formula provided above.

[0059]

5 Algorithms for the regression analysis may be those that are publicly known; regression trees, LASSO, random forests, support vector regression, Gaussian process regression, neural networks, etc. can be used. Note that an increase in the number of explanatory variables is made
10 in the present example and regression trees, and random forests are suitable for increasing the number of explanatory variables rather than support vector regression. Particularly, with nonlinear random forests, prediction at high accuracy can be expected.

15 [0060]

After thus generating the predictive model (905), the material property predicting unit (113) selects a record in which material property (702) is unmeasured, i.e., blank and computes a predicted value of the material property
20 (702) using the foregoing prediction function $y = f(x_1, x_2, \dots)$ (S1006).

[0061]

The computed predictive value is displayed by the material property prediction presenting unit (116) in the
25 screen on the monitor (205), as illustrated in Figure 11

(S1007). Note that, although feature values of spatial structures and experimental conditions are only used as explanatory variables in the present example, in fact, any other amount (e.g., molecular weight or charge) may be derived, added, and used.

[0062]

Although structural formulas are used when creating feature values about any other task in the example discussed hereinbefore, data of composition and others may be used as long as the data is common across tasks data. Additionally, a method in which prediction can be made using structural formulas as such is also publicly known and the scheme is the same in that case as well.

[0063]

According to the example described hereinbefore, using data stored when material properties were predicted in any other past task, a model is created that is compatible with a prediction that is executed currently and the accuracy is improved by increasing the number of explanatory variables through the model. Although, e.g., a task (the past task B in Figure 9) in the beginning of research and development has few data pieces, the present example enables it to make good use of data of a past task (the past task A in Figure 9) for which, e.g., research and development are complete and the amount of data is large. This can overcome a

problem in which, when prediction of material properties is performed, its accuracy is low due to a small amount of data. Accordingly, more accurate prediction can be performed in the phase of prediction and evaluation for screening in an experiment plan. In consequence, experiment plans will become easy to make and, furthermore, a good material can be developed with a reduced number of times experiments are performed. For example, it is possible to find out a parameter that is predicted to improve a property and do work, prioritizing the experimental condition of the parameter.

Reference Signs List

[0064]

101: material property prediction device

15 102: user

111: experimental data accepting unit

112: material DB

113: material property predicting unit

114: material property predictive model DB

20 115: cross-task compatible feature value generating unit

116: material property prediction presenting unit

{Claims}

1. A material property prediction system that is a system
to carry out prediction of material properties by
5 processing task data including a plurality of records, each
including a material composition, an experimental condition,
and a material property, the system comprising a material
property prediction presenting unit, a cross-task
compatible feature value generating unit, and a material
10 property predicting unit,

wherein the material property prediction presenting
unit accepts a specification of first task data that
includes a record in which a material property is unknown
and is to be a target of material property prediction
15 through a first predictive model;

the cross-task compatible feature value generating
unit predicts feature values from material compositions in
the first task data by using a second predictive model;

the material property predicting unit generates the
20 first predictive model by using the material compositions,
the experimental condition, the feature values, and the
known material property in the first task data; and

the material property predicting unit inputs the
material composition, the experimental condition, and the
25 feature value in a record in which the material property is

unknown in the first task data to the first predictive model and predicts the unknown material property.

2. The material property prediction system according to

5 claim 1,

wherein the task data can be retrieved from a material database;

the material database stores a plurality of tasks data pieces and data on the experimental condition and the
10 material property includes data in which different conditions and properties are defined across the tasks data pieces;

the material property prediction presenting unit accepts a specification of second task data different from
15 the first task data;

the cross-task compatible feature value generating unit retrieves the second task data from the material database and generates the second predictive model by using material compositions and a known material property in the
20 second task data; and

the cross-task compatible feature value generating unit predicts feature values based on a material property that is defined in the second data from material compositions in the first task data.

3. The material property prediction system according to claim 2, including the material database in which the following are stored:

the first task data including a plurality of records,
5 each including a material composition, a first experimental condition, and a first material property; and

the second task data including a plurality of records,
each storing a material composition and a second
experimental condition defined different from the first
10 experimental condition.

4. The material property prediction system according to claim 2, including the material database in which the following are stored:

15 the first task data including a plurality of records,
each including a material composition, a first experimental condition, and a first material property; and

the second task data including a plurality of records,
each storing a material composition and a second material
20 property defined different from the first material property.

5. The material property prediction system according to claim 2, provided with a material property predictive model database storing at least one of the first predictive model
25 and the second predictive model.

6. The material property prediction system according to claim 5, wherein the second predictive model is managed in relation to the second task data.

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7. The material property prediction system according to claim 1, wherein the first predictive model is configured using a random forest.

10 8. A material property prediction method that is a method for predicting material properties by an information processing device including an input device, a storage device, and a processor,

wherein, when generating a first predictive model for
15 predicting a first material property from first data including first feature values, the method executes:

a first step of preparing, from the first feature values, a second predictive model that is to predict a second material property defined different from the first
20 material property;

a second step of predicting the second material property by applying the first data to the second predictive model; and

a third step of generating the first predictive model,
25 taking the first feature values as a first explanatory

variable, the second material property as a second explanatory variable, and the first material property as an objective variable.

5 9. The material property prediction method according to claim 8, wherein the method executes a third step of predicting the first material property by using the first predictive model and the first data.

10 10. The material property prediction method according to claim 8, wherein the first feature values are the feature values based on material structural formulas.

11. The material property prediction method according to
15 claim 8, wherein the second predictive model is a model learned using second data including the first feature values and the second material property.

12. The material property prediction method according to
20 claim 11, using a material database on a per-task basis,
wherein first task data regarding a first task and second task data regarding a second task are stored in the material database;

the first task data includes a plurality of records,
25 each including material structure related information and

the first material property;

the second task data includes a plurality of records,
each including material structure related information and
the second material property;

5 the method generates the first feature values from the
material structure related information;

the method generates the first data from the first
task data; and

the method generates the second data from the second
10 task data.

13. The material property prediction method according to
claim 12, wherein the first task data further includes
first information about material manufacturing conditions.

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14. The material property prediction method according to
claim 13, wherein the second task data further includes
second information defined different from the first
information about material manufacturing conditions.

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15. The material property prediction method according to
claim 8, wherein a random forest is used as the first
predictive model.