

CLAIMS

1. A material property prediction device for predicting a material property using a case-by-case material database storing a plurality of case databases,

5 the case database including a plurality of records recording structural information about material structures in association with material properties about properties of materials, the device comprising:

10 a chemical space designation unit receiving a designation of at least one case database stored in the case-by-case material database;

15 an autoencoder learning unit generating an autoencoder for converting structural information corresponding to the case database received by the chemical space designation unit to multi-variables; and

20 a material property prediction unit predicting material properties using the multi-variables converted by the autoencoder generated by the autoencoder learning unit.

2. The material property prediction device according to claim 1,

25 wherein the autoencoder is a model having a property of enabling the structural information to be restored from the multi-variables after converting the structural information to the multi-variables.

3. The material property prediction device according to claim 1,

wherein the material property prediction unit

5 inputs training data including the plurality of records recording the structural information about the material structures in association with the material properties about the properties of the materials,

10 inputs structural information corresponding to the training data to the autoencoder and converts the structural information to multi-variables as explanatory variables, and

15 sets material properties corresponding to the training data as objective variables and trains a prediction model using the explanatory variables and the objective variables.

4. The material property prediction device according to claim 3, further comprising:

20 a material property prediction receiving unit receiving structural information about structures of materials having properties to be predicted,

wherein the material property prediction unit

25 inputs the structural information about the structures of the materials having the properties to be predicted to the autoencoder and converts the structural information

to multi-variables as explanatory variables, and

inputs the explanatory variables to the prediction model and predicts properties that are the objective variables.

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5. The material property prediction device according to claim 1,

wherein the chemical space designation unit has a function of searching the case database with a keyword.

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6. A material property prediction method, executing:

a first step of preparing a first database including a plurality of records recording structural information about material structures, wherein a case-by-case material database storing a plurality of case databases is used, and at least one case database is selected from the case-by-case material database as the first database;

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a second step of extracting structural information from the first database prepared in the first step;

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a third step of training an autoencoder for converting structural information to multi-variables using the structural information extracted in the second step;

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a fourth step of preparing a second database including a plurality of records recording structural information about material structures in association with material properties about properties of materials;

a fifth step of extracting structural information from the second database prepared in the fourth step;

a sixth step of converting the structural information extracted in the fifth step to multi-variables using the autoencoder;

a seventh step of obtaining explanatory variables on the basis of the multi-variables converted in the sixth step and obtaining objective variables on the basis of material properties extracted from the second database; and

an eighth step of generating a prediction model for assuming the objective variables from the explanatory variables using the explanatory variables and the objective variables.

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7. The material property prediction method according to claim 6,

wherein in the case-by-case material database, text information is stored in association with the case database, and

in the first step,

a user searches the text information and selects at least one case database.

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8. The material property prediction method according to

claim 6,

wherein in the first step,

the case database includes a plurality of records
recording structural information about material
structures in association with material properties about
properties of materials,

and

in the fourth step,

at least one case database is selected from the case-
by-case material database as the second database.

9. The material property prediction method according to
claim 8,

wherein the material properties included in the
records of the first database and the material properties
included in the records of the second database are
material properties having different definitions.

10. The material property prediction method according to
claim 6,

wherein in the autoencoder,

a model having a property of enabling the structural
information to be restored from the multi-variables after
converting the structural information to the multi-
variables is used.

11.The material property prediction method according to claim 6, further executing:

a ninth step of preparing structural information about material structures having properties to be predicted;

5 a tenth step of converting the structural information prepared in the ninth step to multi-variables using the autoencoder;

an eleventh step of obtaining explanatory variables on the basis of the multi-variables converted in the tenth step; and
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a twelfth step of assuming material properties that are the objective variables by applying the explanatory variables obtained in the eleventh step to the prediction model.
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12.The material property prediction method according to claim 6,

wherein at least one of the autoencoder and the prediction model is stored in a storage device and reused.
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13.The material property prediction method according to claim 6,

wherein both of the first database and the second database include the plurality of records recording the structural information about the material structures in
25 association with the material properties about the

properties of the materials, and record data having different definitions or types with respect to the material properties.