Chapter

Fuzzy Logic and Fuzzy Expert System-Based Material Synthesis Methods

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Abstract

Analyzing a wide diversity of approaches to material selection and synthesis, one can observe a tendency to shift research efforts from physical experiments to systematic analysis based on mathematical models and computational schemes. The latter, in turn, evolves from traditional analytical methods and computational schemes to modern approaches that are based on collaboration of fuzzy logic and soft computing, machine learning, big data and other new methods. In this study, emphasis is put on modeling of fuzzy relationship between performance of new materials and affecting factors. This chapter includes applications of fuzzy model-based synthesis of different alloys. Fuzzy If-then rules based TiNiPt alloy synthesis problem, fuzzy expert system based synthesis of material for pressure vessel and other problems are considered.

Keywords: fuzzy logic, material synthesis, big data, fuzzy clustering, expert system

1. Introduction

Development of new materials is one of important tasks of theoretical and practical interest. Traditionally, this task is implemented mainly on the basis of intensive (and sometimes "ad hoc") experiments which are time- and resource consuming or even not practically implementable. Nowadays, it is well understood that more systematic and effective approaches are needed which are based on computer-guided synthesis of materials. Such approaches rely on data-driven mathematical models and knowledge base obtained from big data previously collected during intensive experiments. Existing computational approaches include methods based on phase diagrams, simulation modeling, theory of associated solutions, methods of microstructure modeling, random fields, etc. In [1], authors analyze the way data-driven techniques are used in deciphering processing-structure-property-performance relationships in materials, with examples of forward (property prediction) and inverse (materials discovery) models. Such analysis can noticeably improve cost-effective materials discovery as the aim of Materials Genome Initiative (MGI). It is shown that adding data sciences to the paradigms of materials science is important to deal with big data.

Agrawal et al. [2] used the Japan National Institute for Materials Science (NIMS) MatNavi database [3] to develop models for prediction of fatigue strength of steel. Prediction accuracy is important for a number of applications due to the significant complexity of fatigue testing and serious consequences of its failures. Actually, fatigue usually leads to more than 90% of all mechanical failures of structural components [4].

In [5], the authors processed the materials properties database for selecting and designing high-temperature alloys for solid oxide fuel cell (or SOFC) applications. Also, this work considers the selection of alloy compositions and properties, which are relevant to the SOFC application. The alloys of interest included such high-temperature alloys as Co, Ni, and Fe base superalloys, as well as stainless steels and Cr base alloys.

The fusion of clustering and regression methods with optimization approaches provides a new opportunity for materials discovery and design. In [6], they discuss the challenges and opportunities associated with materials research. The work [7] for the first time represents machine learning-based determination of viable new compound from true chemical white space, whereas no characterization was provided by promising chemistries. The authors consider an effective prediction model for materials properties that may be easily accessible and useful for researchers.

Existing works based on classical computational schemes used for material synthesis and selection provided good results. However, one important issue related to big data-based computerized material synthesis is that experimental data include measurement errors, partially reliable information, imprecise evaluations, etc. This mandates the use of fuzzy logic approaches for material synthesis. Let us consider some existing works in this regard.

Papers [8–10] show the necessity to account for nonlinearity and uncertainty factors that characterize modeling of material design problems. This requires searching for new ways in formalization of systematic approaches to material design. These papers are devoted to these factors.

Authors in [11] used a new combining tool with which it is possible to model and optimize new alloys that simultaneously satisfy up to 11 physical criteria. To develop a new polycrystalline nickel-base superalloy with the optimal combination of cost, density, gamma-primary phase and sol content, phase stability, durability, yield point, tensile strength, stress rupture, oxidation resistance, and elongation.

In [12], they have developed a rule-based fuzzy logic model for predicting shear strength of Ni-Ti alloy specimens which were produced using powder metallurgy method.

In [13], they applied the fuzzy set theory to knowledge mining from big data on material characteristics. The authors propose fuzzy clustering-generated If-Then rules as a basis for computer synthesis of new materials. These fuzzy If-Then rules describe relationship between material composition and material properties. Validity of the proposed approach is verified on an example of prediction properties of Ti-Ni alloy, and computer experiments of the proposed fuzzy model show its better performance than the physical experiment-based analysis.

In [14], ANFIS model is used to describe the high-temperature deformation behavior of Ni-based superalloy. The inputs of the ANFIS model are deformation temperature, strain rate, and true strain, and the output is true stress. The optimal numbers and types of membership function for the input variables are found. The results show that the constructed ANFIS model is effective in predicting the considered behavior of the Ni-based superalloy.

In this chapter, we propose fuzzy If-Then rule-based model to predict properties of new materials. The model is constructed on the basis of fuzzy clustering of big data on dependence between material composition and related properties. The motivation to use fuzzy model is inspired by the necessity to construct an intuitively well-interpretable development strategy from imperfect and complex data. The proposed approach is applied to synthesis of Ti-Ni-X alloys with required properties and synthesis of material for pressure vessel. Computer experiments of the proposed fuzzy models show better performance than the physical experiment-based analysis.

2. Statement of material synthesis problem and solution methods

The motivation to use fuzzy model is inspired by the necessity to construct an intuitively well-interpretable development strategy from imperfect and complex data. Analyzing a wide diversity of approaches to material selection and synthesis, one can observe a tendency to shift research efforts from physical experiments to systematic analysis based on mathematical models and computational schemes. The latter, in turn, evolutes from traditional analytical methods and computational schemes to modern approaches that are based on collaboration of fuzzy logic and soft computing, machine learning, big data, and other new methods. Uncertainty of materials properties requires to use fuzzy logic methods to more adequately model and predict possible material behavior. This will help to deal with imprecision of experimental data; partial reliability of experimental data, prediction results, and expert opinions; uncertainty of materials properties stemming from complex relationship between material components; and a necessity to analyze, summarize, and reason with a large amount of information of various types (numeric data, linguistic information, graphical information, geometric information, etc.).

Fuzzy logic methods have a good capability to effectively capture and process imprecise experimental data, that is, interpret, classify, learn, and compute with them. Fuzzy logic may help to improve abilities of big data principles to deal with a huge amount and variety of information. In this realm, fuzzy clustering and fuzzy logic-based knowledge bases and information search algorithms provide a bridge between complexity, imperfectness, qualitative nature of information, and research techniques. Particularly, this may help to get intuitive general interpretation of materials science results obtained by various techniques, and ways to get practical results would be then more evident.

Assume that big data on smart materials sourced from experiments is available. These big data describe relationship between alloy composition and its characteristics (**Table 1**) [13, 15, 16].

The problem is to extract knowledge-based model from the considered data and to find an alloy composition which provides a predefined alloy characteristics. We will consider fuzzy knowledge-based synthesis model [17–20]. The problem is solved as follows [21].

First, fuzzy clustering of the big data is applied to determine fuzzy clusters $C_1, C_2, \ldots, C_K$.

Second, fuzzy IF-THEN rule-based model is constructed from $C_1, C_2, \ldots, C_K$:

$$IF\, y_1\, is\; A_{k1}\, and, \ldots, and\, y_n\, is\; A_{kn}\; THEN\, z_1\, is\; B_{k1}\, and, \ldots,$$

Experiment	Alloy composition (in %)			Conditions			Alloy characteristics		
#	Metal 1, y_1	…	Metal n, y_n	Cond.1	…	Cond. l	Char. 1, z_1	…	Char. m, z_m
1	y_{11}	…	y_{1n}	T_{11}	…	T_{1l}	z_{11}	…	z_{1m}
⋮					⋮				
s	y_{s1}	…	y_{sn}	T_{s1}	…	T_{sl}	z_{s1}	…	z_{sm}

Table 1.
Big data of relationship between alloy composition and its characteristics.

$$and\, z_m\, is\, B_{km}, k = 1, \ldots, K \tag{1}$$

Third, fuzzy inference is implemented on the basis of the fuzzy IF-THEN rules to compute optimal values $B'_1, \ldots, B'_m$ of alloy characteristics $z_1, \ldots, z_m$. The fuzzy inference is mainly based on composition of a fuzzy input information on material constituents (and other conditions) and fuzzy relation which describes fuzzy IF-THEN rules. A different approach to fuzzy reasoning also exists and is applied in case of scarce rule base. This is based on fuzzy inference by using similarity of fuzzy input information and antecedents of existing fuzzy rules; a resulting output is then computed as linear interpolation of fuzzy rule consequents.

By using fuzzy inference, optimal values $B'_1, \ldots, B'_m$ are found as those closed to the ideal vector of characteristics $B^* = (B^*_1, \ldots, B^*_m)$. For material synthesis, also fuzzy expert system approach is used. In this case, fuzzy expert system ESPLAN implements IF-THEN rule base obtained from fuzzy clustering of data.

The use of fuzzy rules and fuzzy inference provides us important tools for transition from intensive experiments which deal with a physical model to a fuzzy logic-based mathematical model. Further experiments are conducted not by using physical model but by using fuzzy logic-based mathematical model.

3. Material synthesis of Ti-Ni-X alloys by using ideal vector of characteristics

3.1 Synthesis of Ti-Ni-Pd alloys with given characteristics

A problem of computational synthesis of Ti-Ni-Pd alloy with predefined characteristics is considered. A big data fragment describing dependence alloy composition and the corresponding characteristics is shown in **Table 2**.

A problem of computational synthesis is related to determination of alloy composition with corresponding values of the characteristics close to the target values:

$$z_1 = (302.3), z_2 = (323.3), z_3 = (347.1), z_4 = (331.3) \tag{2}$$

Thus, $B^* = (B^*_1, B^*_2, B^*_3) = ((302.3), (323.3), (347.1), (331.3))$ can be considered as an ideal solution.

In order to describe relationship between alloy composition and the characteristics values, the fuzzy IF-THEN rules were obtained by using FCM clustering of the considered big data:

IF Ni is L and Pd is A2

THEN M_f is A and M_s is A and A_s is aand A_f is A

IF Ni is Aand Pd is A1

THEN M_f is L and M_s is L2 and A_f is L2 and A_s is L

IF N_i is H2 and P_d is L1

THEN M_f is VL and M_s is VL and A_s is Land A_f isVL,

IF Ni is H1 and Pd is L2

THEN M_f is L and M_s is L and A_f is L and A_s is L

IF Ni is VH and Pd is VH

THEN M_f is H and M_s is H and A_f is VH and A_s is VH

The codebooks for inputs are shown in **Tables 3** and **4**.

The linguistic approximation of the inputs is shown in **Tables 5** and **6**.

The codebooks for the outputs are shown in **Tables 7–10**.

Composition			Transformation temperatures			
x_1 (Ni, %)	x_2 (Ti, %)	x_3 (Pd, %)	y_1 (martensitic finish temperature, K)	y_2 (martensitic start temperature, K)	y_3 (austenitic finish temperature, K)	y_4 (austenitic start temperature, K)
41	50	9	322.3	329.4	341.3	331.2
39	50	11	318.2	335.7	347.6	334.7
29	50	21	406.4	424.5	440.3	426.6
20	50	30	515.3	533.8	546.8	534.9

Table 2.
A big data fragment on Ti-Ni-Pd alloy composition [22].

No.	Linguistic value	TFN
1.	Very low (VL)	(3, 3, 13.5) (1)
2.	Low (L)	(3, 13.5, 24) (2)
3.	Average (A)	(13.5, 24, 34.5) (3)
4.	High (H)	(24, 34.5, 45) (4)
5.	Very high (VH)	(34.5, 45, 45) (5)

Table 3.
Codebook for input 1 (Ni).

No.	Linguistic value	TFN
1.	Very low (VL)	(3, 3, 13.75) (1)
2.	Low (L)	(3, 13.75, 24.5) (2)
3.	Average (A)	(13.75, 24.5, 35.25) (3)
4.	High (H)	(24.5, 35.25, 46) (4)
5.	Very high (VH)	(35.25, 46, 46) (5)

Table 4.
Codebook for input 2 (Pd).

No.	Linguistic value	TFN
1.	Very low (VL)	(0, 3.977, 19.2)
2.	Low (L)	(6.709, 18.6, 30.48)
3.	Average (A)	(14.53, 24.7, 34.86)
4.	High 1 (H1)	(21.16, 39.33, 57.51)
5.	High 2 (H2)	(20.88, 30.73, 40.59)

Table 5.
Linguistic terms for input 1 (Ni).

No.	Linguistic value	TFN
1.	Average 1 (A1)	(21.28, 30.03, 38.78)
2.	Average 2 (A2)	(15.9, 24.9, 33.9)
3.	Low 1 (L1)	(0, 10.58, 28.06)
4.	Low 2 (L2)	(9.962, 19.04, 28.13)
5.	Very high (VH)	(28.8, 43.21, 57.62)

Table 6.
Linguistic terms for input 2 (Pd).

No.	Linguistic value	TFN
1.	Average (A)	(394.8, 502.1, 609.5)
2.	Low 1 (L1)	(359.2, 451.3, 543.5)
3.	Very low (VL)	(199.3, 322.3, 445.2)
4.	Low 2 (L2)	(294.4, 386.8, 479.2)
5.	Very high (VH)	(475.4, 674.5, 873.5)

Table 7.
Linguistic terms for output 1 (Mf).

No.	Linguistic value	TFN
1.	Average (A)	(417.4, 523.8, 630.2)
2.	Low 1 (L1)	(369.6, 463.1, 556.6)
3.	Very low (VL)	(221.4, 338.8, 456.2)
4.	Low 2 (L2)	(306.8, 400.4, 494)
5.	Very high (VH)	(532.2, 717.8, 903.5)

Table 8.
Linguistic terms for output 2 (Ms).

No.	Linguistic value	TFN
1.	Average (A)	(414.3, 527.4, 640.5)
2.	Low 1 (L1)	(374.6, 466.5, 558.4)
3.	Very low (VL)	(246.3, 354.8, 463.3)
4.	Low 2 (L2)	(319.1, 409, 498.9)
5.	Very high (VH)	(536.5, 730.6, 924.7)

Table 9.
Linguistic terms for output 3 (As).

The constructed fuzzy model will be used to determine an input vector $A' = \left(A'_1, \ldots, A'_n\right)$ that induces the corresponding output vector $B' = \left(B'_1, \ldots, B'_m\right)$ maximally close to the ideal solution $B^* = \left(B^*_1, B^*_2, B^*_3\right)$.

We have found that the fuzzy optimal output vector B' induced by the fuzzy input vector $A' = \left(A'_1, A'_2, A'_3\right) = (19.5, 50.5, 30)$ is $B' = \left(B'_1, B'_2, B'_3, B'_4\right) = ((347.78), (364.86), (382.17), (375.22))$. It is the closest vector to the considered ideal fuzzy vector $B^* = ((302), (323), (347), (313))$. The distance is $D\ (B,B^*) = 94$. Thus,

#	Linguistic value	TFN
1.	Average (A)	(420.5, 537.7, 654.9)
2.	Low 1 (L1)	(360.5, 471.1, 581.6)
3.	Very low (VL)	(214.5, 344, 473.6)
4.	Low 2 (L2)	(301.9, 406.6, 511.3)
5.	Very high (VH)	(599.2, 771, 982.8)

Table 10.
Linguistic terms for output 4 (Af).

the computational synthesis based on the fuzzy model uncovers the following alloy composition: Ni is about 19%, Ti is about 51%, and Pd is about 30% with the characteristics $M_f = 347.78$, about $M_s = 364.86$, about $A_f = 382.17$, and $A_s = 375.22$.

3.2 Synthesis of Ti-Ni-Pt alloys with given characteristics

A problem of computational synthesis of Ti-Ni-Pt alloy with predefined characteristics is considered. A big data fragment describing dependence alloy composition and the corresponding characteristics is shown in **Table 11**.

The following fuzzy IF-THEN rules were obtained by using FCM clustering of the considered big data:

If x_1 is VL and x_3 is VH THEN y_1 is VH and y_2 is VH.
If x_1 is H2 and x_3 is L1 THEN y_1 is VL and y_2 is VL.
If x_1 is A and x_3 is L3 THEN y_1 is L2 and y_2 is L2.
If x_1 is L and x_3 is H THEN y_1 is H and y_2 is H.
If x_1 is H1 and x_3 is L2 THEN y_1 is L1 and y_2 is L.

Composition			Transformation temperatures	
x_1 (Ni, %)	x_2 (Ti, %)	x_3 (Pt, %)	y_1 (martensitic start temperature, K)	y_2 (austenitic start temperature, K)
30	50	20	539	544
20	50	30	833	867
15	50	35	953	1023
		…		
10	50	40	1173	1123

Table 11.
Transformation temperatures of Ti-Ni-Pt alloy [23].

No.	Linguistic value	TFN
1.	Very low (VL)	(5, 5, 13.75)
2.	Low (L)	(5, 13.75, 22.5) (2)
3.	Average (A)	(13.75, 22.5, 31.25) (3)
4.	High (H)	(22.5, 31.25, 40) (4)
5.	Very high (VH)	(31.25, 40, 40) (5)

Table 12.
Codebook for input 1 (x_1).

No.	Linguistic value	TFN
1.	Very low (VL)	(10, 10, 18.75) (1)
2.	Low (L)	(10, 18.75, 27.5) (2)
3.	Average (A)	(18.75, 27.5, 36.25) (3)
4.	High (H)	(27.5, 36.25, 45) (4)
5.	Very high (VH)	(36.25, 45, 45) (5)

Table 13.
Codebook for input 2 (x_3).

No.	Linguistic value	TFN
1.	Very low (VL)	(0, 7.535, 22.65)
2.	High 1 (H1)	(25.98, 35.17, 44.35)
3.	Average (A)	(19.27, 26.33, 33.39)
4.	Low (L)	(8.109, 17.64, 27.17)
5.	High 2 (H2)	(21.67, 30.06, 38.48)

Table 14.
Linguistic terms for input 1 (Ni).

No.	Linguistic value	TFN
1.	Very high (VH)	(27.18, 42.47, 57.75)
2.	Low 1 (L1)	(5.859, 14.84, 23.82)
3.	Low 2 (L2)	(14.14, 21.78, 29.42)
4.	High (H)	(22.63, 32.36, 42.08)
5.	Low 3 (L3)	(13.71, 19.75, 26.18)

Table 15.
Linguistic terms for input 2 (Pt).

No.	Linguistic value	TFN
1.	Very low (VL)	(363, 363, 565.5)
2.	Low (L)	(363, 565.5, 768)
3.	Average (A)	(565.5, 768, 970.5)
4.	High (H)	(768, 970.5, 1173)
5.	Very high (VH)	(970.5, 1173, 1173)

Table 16.
Codebook for output 1 (y_1).

The codebooks for inputs are shown in **Tables 12** and **13**.

The linguistic approximation of the inputs is shown in **Tables 14** and **15**.

The codebooks for the used outputs are shown in **Tables 16** and **17**.

We have found that the fuzzy optimal output vector B' induced by the fuzzy input vector $A' = \left(A'_1, A'_2, A'_3\right) = (40, 50, 10)$ is $B' = ((479.68), (488))$. It is the closest vector to the considered ideal fuzzy vector $B^* = ((363), (373))$. The distance between them is $D(B', , B^*) = 164$. The fuzzy model-based results show that the

No.	Linguistic value	TFN
1.	Very low (VL)	(373, 373, 585.5)
2.	Low (L)	(373, 585.5, 798)
3.	Average (A)	(585.5, 798, 1010.5)
4.	High (H)	(798, 1010.5, 1223)
5.	Very high (VH)	(1010.5, 1223, 1223)

Table 17.
Codebook for output 2 (y_2).

desired alloy composition is as follows: Ti is about 50%, Ni is about 37%, Pt is about 13%, and the obtained characteristics are about M_s = 479,6828 and about As = 488,1005.

4. Material synthesis by fuzzy expert system

A series of works exist on material synthesis by using fuzzy models [12, 24, 25]. In this study, to solve material synthesis problem for pressure vessel, two methods are used: possibility measure-based inference method (by ESPLAN shell, Aliev inference) and Mamdani inference method (by MATLAB environment, Fuzzy Toolbox) [26].

4.1 Statement of the problem

Defining the performance index for pressure vessel in material synthesis is a very important problem. The basic problem is to evaluate the performance index by using weighted performance indices.

For determining the performance index, we use data of alloys. There are many types of alloys.

The weighted performance index denoted *Out* is a compound index built from four characteristics each of which is extracted from the data set. The four characteristics are *in1*-scaled PREN, *in2*-scaled yield strength, *in3*-scaled weldability, and *in4*-scaled impact strength.

Using the abovementioned parameters, the performance index model can be expressed as.

IF x_1 is A_{11} and ..... x_n is A_{1n} THEN y is B_1.

IF x_1 is A_{21} and ..... x_n is A_{2n} THEN y is B_2.

... ...

IF x_1 is A_{m1} and ..... x_n is A_{mn} THEN y is B_m.

where $x_j = {}^j 1...n$ are the linguistic input variables, y is the output variable, and A_{ij} and B_i are the fuzzy sets, n = 4, m = 7.

Fragment of data set is given in **Table 18**.

4.2 Modeling of material data by fuzzy C-means clustering

To create this model, we use clustering approach, mainly fuzzy C-means. Data set contains 35 records extracted from big data. For modeling we use two-thirds of the given data and testing one-third. Inputs: x1, scaled PREN; x2, scaled yield; x3, scaled weldability; x4, scaled impact strength. Output: y, performance index. For simulation FCM-based clustering initial data are:

Scaled PREN	Scaled yield strength	Scaled weldability	Scaled impact strength	Performance index
26.60	3.60	18.40	5.00	53.50
29.70	4.40	23.00	8.60	65.60
19.80	3.60	23.00	5.00	51.30
22.30	3.20	23.00	8.60	57.10
26.00	3.60	18.40	6.80	54.70
22.30	5.40	13.80	11.30	52.70
...	...	...	...	...
47.00	4.60	18.40	13.50	83.50
29.70	4.40	18.40	15.80	68.30
20.40	12.00	18.40	5.00	55.80
21.00	9.80	23.00	4.50	58.30
23.50	4.60	23.00	13.50	64.60
11.80	2.50	18.40	9.00	41.60
15.50	2.50	18.40	8.80	45.10
22.90	5.80	13.80	7.10	49.50
26.60	6.20	4.60	3.20	40.50
...	...	...	...	...
18.60	2.90	18.40	8.80	48.60
32.20	6.20	18.40	6.00	62.70
42.70	4.30	23.00	15.20	85.10
21.00	2.50	18.40	8.80	50.70
21.60	9.50	18.40	4.50	54.00

Table 18.
Fragment of data set (extracted from big data).

Cluster numbers = 7.
Max iteration =1000.
Exponent = 2.
Min. improvement = 0.000001.

Obtained centers of the clusters are given in **Table 19**. Each row describes a cluster center as five-dimensional vector with coordinates x1 (scaled PREN), x2 (scaled yield), x3 (scaled weldability), x4 (scaled impact strength), and y (performance index). Columns describe the values of the coordinates of the cluster centers.

Representation of the extracted fuzzy rules from big data by using fuzzy c-means method fragment is given below and in **Figure 1**.

1. *IF Scaled PREN = about 18 and Scaled yield = about 3 and Scaled weldability = about 14.5 and scaled impact strength = about 10.8, THEN Performance index = about 46.5.*

2. *IF Scaled PREN = about 27 and Scaled yield = about 4.4 and Scaled weldability = about 21 and scaled impact strength = about 12 THEN Performance index = about 65.*

3. *IF Scaled PREN = about 26 and Scaled yield = about 5 and Scaled weldability = about 4.8 and scaled impact strength = about 3 THEN Performance index = about 38.5.*

4. *IF Scaled PREN = about 21 and Scaled yield = about 9 and Scaled weldability = about 21.2 and scaled impact strength = about 5 THEN Performance index = about 55.*

5. *IF Scaled PREN = about 25 and Scaled yield = about 3.6 and Scaled weldability = about 19 and scaled impact strength = about 6 THEN Performance index = about 53.5.*

6. *IF Scaled PREN = about 47 and Scaled yield = about 4.5 and Scaled weldability = about 18 and scaled impact strength = about 13 THEN Performance index = about 83.*

	x1	x2	x3	x4	y
Center 1	18.5215	3.0384	14.7548	10.7647	46.9898
Center 2	27.6395	4.4574	21.3502	12.6412	66.0559
Center 3	26.0329	4.9933	4.8428	3.2598	39.0312
Center 4	20.8528	9.7068	21.3952	5.0337	56.9826
Center 5	25.0287	3.5955	19.0063	6.3912	53.9372
Center 6	46.9418	4.5996	18.4040	13.4963	83.4416
Center 7	24.1544	6.2895	14.0802	9.7481	54.2839

Table 19.
Centers of the clusters.

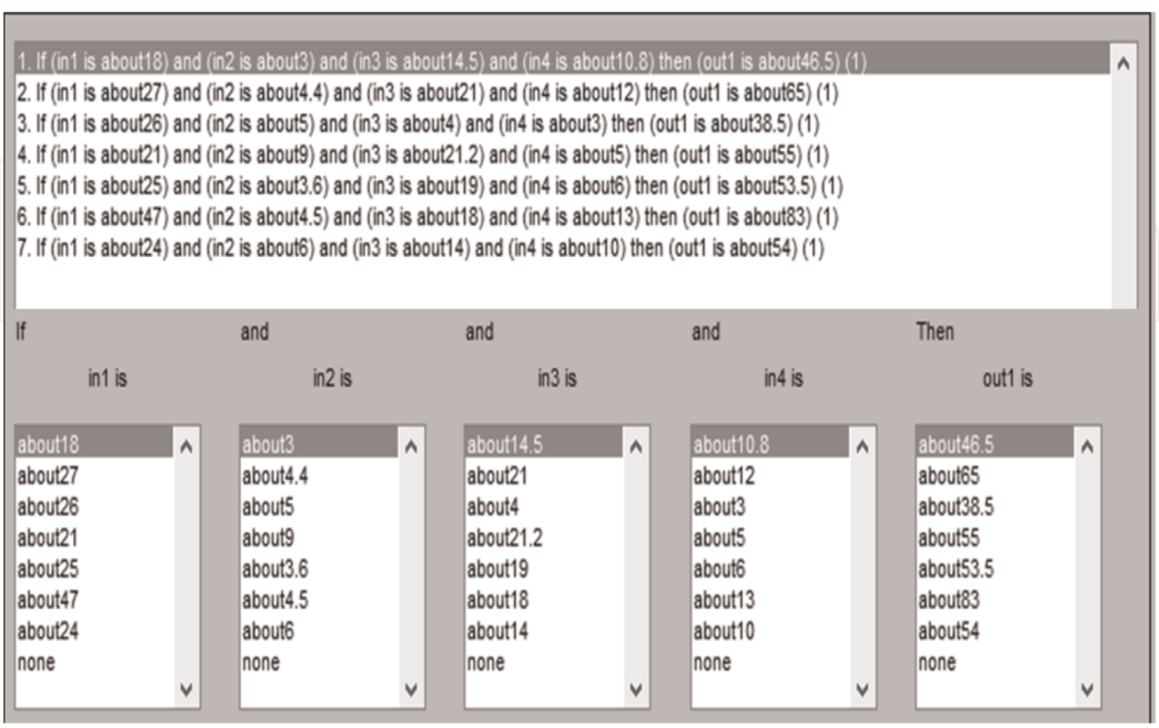

Figure 1.
Extracted fuzzy rules (by using fuzzy C-means method).

7. *IF Scaled PREN = about 24 and Scaled yield = about 6 and Scaled weldability = about 14 and scaled impact strength = about 10 THEN Performance index = about 54.*

Graphical representation of the linguistic terms of inputs and outputs of the rules as trapezoidal fuzzy numbers is given in **Figures 2–6**.

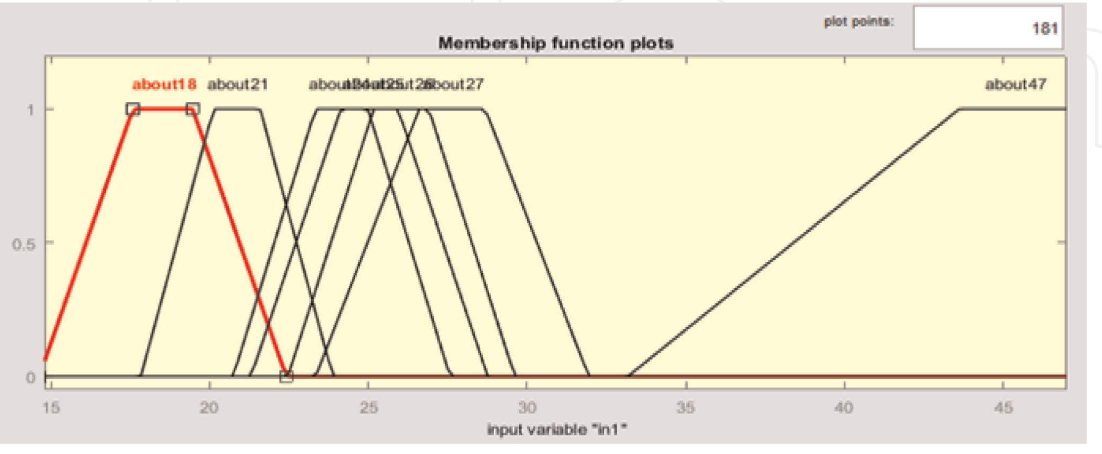

Figure 2.
Linguistic terms of input 1 (scaled PREN).

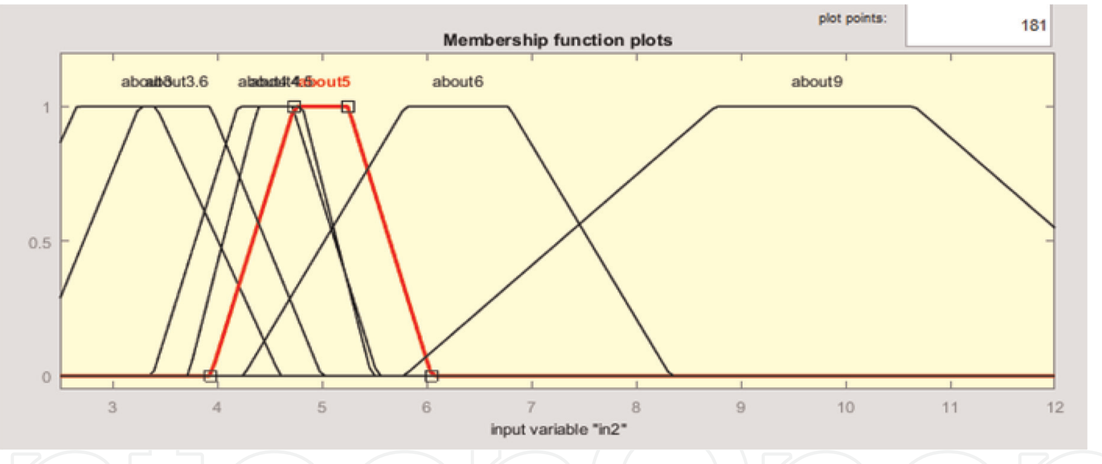

Figure 3.
Linguistic terms of input 2 or scaled yield strength.

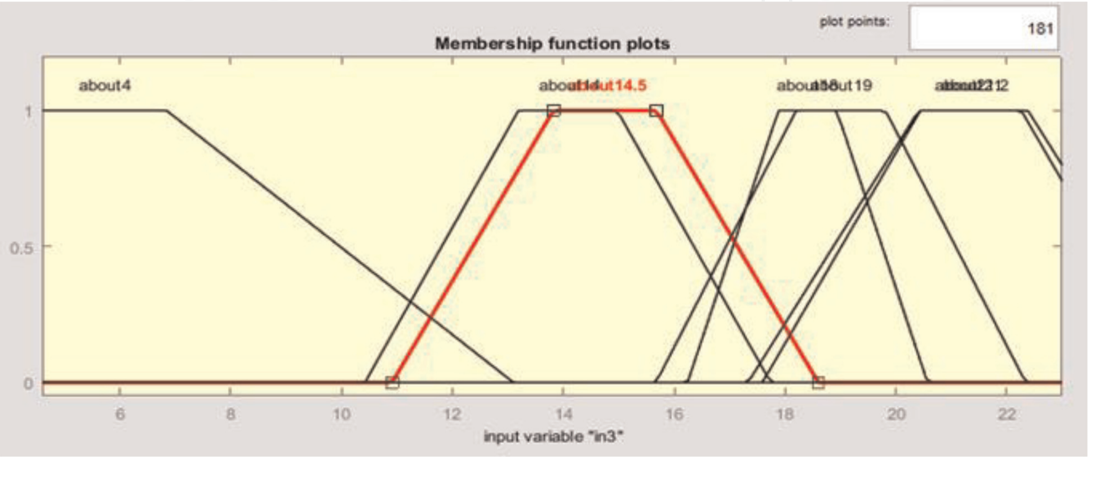

Figure 4.
Linguistic terms of input 3 or scaled weldability.

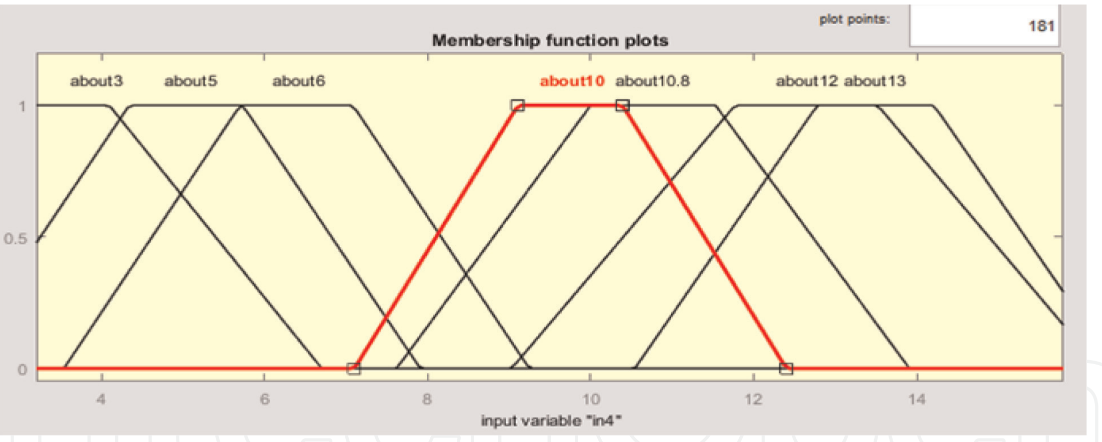

Figure 5.
Linguistic terms of input 4 or scaled impact strength.

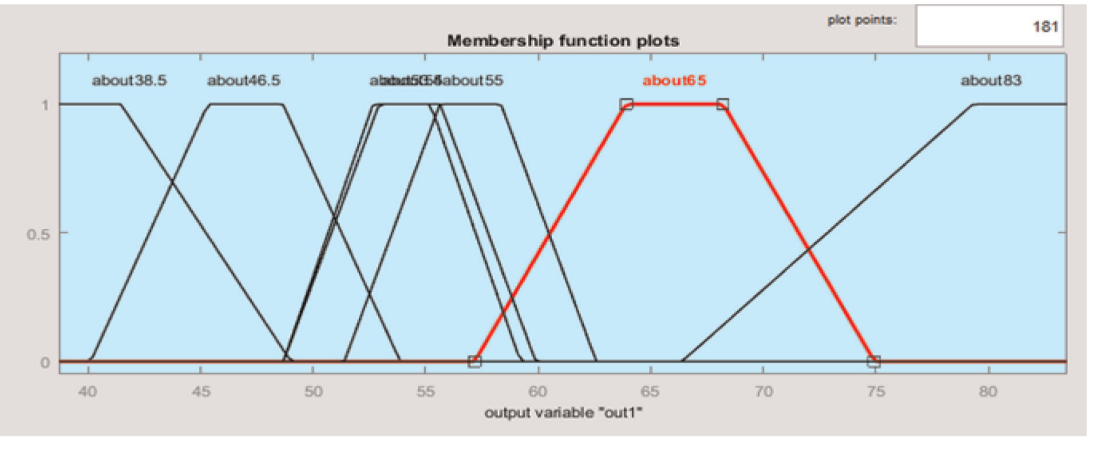

Figure 6.
Linguistic terms of outputs or performance index.

4.3 Solution of the problem

For solving the problem described in Section 4.1, we will use ESPLAN shell.

The problem is to determine material with the given level of performance index using the fuzzy model obtained in Section 4.2.

In this context we define basic objects and linguistic terms according to ESPLAN shell. The linguistic terms are described by trapezoidal fuzzy numbers. The rule base given above is put as knowledge base in ESPLAN shell. Then, different tests are performed.

TEST 1.

IF Scaled PREN = about 18 and Scaled yield = about 3 and.

Scaled weldability = about 21 and scaled impact strength = about 12.

THEN Performance index =?

ANSWER:

EXPERT system shell ESPLAN's result is "Performance index is about 46.5" **(alloy Monel-400)**.

The fuzzy rules were derived from alloy big data by using FCM method, and fuzzy inference within these rules is implemented in expert system shell ESPLAN. The obtained results confirm efficiency of the proposed approach.

Solution by using Mamdani inference method. General form of the abovementioned rules are as form (4.13). Mamdani fuzzy inference is most commonly used approximate reasoning methodology for fuzzy modeling. The method works with crisp input which is transformed into a linguistic value using the antecedent membership functions. After the aggregation process of consequents induced by antecedents, obtained final fuzzy set is defuzzified. We can describe fuzzy inference process in algorithmic view as follows:

1. Firing level for each rule is defined as follows:

$$\alpha_i = \min_{j=1}^{n}\left[\max_{x_j}\left(A_j'(x_j)\wedge A_{ij}(x_j)\right)\right] \quad (3)$$

where $A_j'(x_j)$ are current input values.

2. Outputs for each rule are calculated:

$$B_i'(y) = \min(\alpha_i, B_i(y)) \quad (4)$$

3. Calculate aggregative output:

$$B'(y) = \max\left(B_1'(y), B_2'(y), \ldots., B_m'(y)\right) \quad (5)$$

In our example the number of input variables is equal to 4, and for each variable, linguistic value number is equal to 7.

For example, scaled PREN variable is evaluated as (about 18, about 27, about 26, about 21, about 25, about 47, about 24).

Observing the relationship between input and output clusters, we may formulate the following linguistic descriptions—productions rules, for example:

1. *IF In1 about 18 and In2 = about 3 and In3 = about 14.5 and In4 = about 10.8 THEN Out = about 46.5.*

2. *IF In1 = about 27 and In2 = about 4.4 and In3 = about 21 and In4 = about 12 THEN Out = about 65.*

3. *IF In1 = about 26 and In2 = about 5 and In3 = about 4.8 and In4 = about 3 THEN Out = about 38.5.*

4. *IF In1 = about 21 and In2 = about 9 and In3 = about 21.2 and In4 = about 5 THEN Out = about 55.*

5. *IF In1 = about 25 and In2 = about 3.6 and In3 = about 19 and In4 = about 6 THEN Out = about 53.5.*

6. *IF In1 = about 47 and In2 = about 4.5 and In3 = about 18 and In4 = about 13 THEN Out = about 83.*

7. *IF In1 = about 24 and In2 = about 6 and In3 = about 14 and In4 = about 10 THEN Out = about 54.*

The obtained rules are put into Fuzzy Toolbox to perform tests by using the following data (**Table 20**):

Below, we provide some test results.

Test results. The following input data are given:

Scaled PREN	Scaled yield strength	Scaled weldability	Scaled impact strength	Performance index
18.60	2.90	18.40	8.80	48.60
21	2.5	18.4	8.8	50.7

Table 20.
Testing data (fragment).

In1 = 18.60, *In2* = 2.90, *In3* = 18.40 and *In4* = 8.

For these data, the following defuzzified output describing the alloy performance index is computed by using Mamdani fuzzy inference:

Out = 48.60.

This value fits the performance index of alloy 317 L (from the given big data).

Consider other values of the inputs:

In1 = 18.60, *In2* = 2.90, *In3* = 18.40 and *In4* = 8.80.

For these values, the defuzzified output is *Out = 50.3*. This result fits the performance index of alloy 317LM.

Consider also the following input values:

In1 = 26, *In2 = 3*.6, *In3* = 18.4, and *In4* = 6.8.

The computed output (performance index) is 54.7. The performance index computed for the third case and the performance index from big data set are shown in **Table 21**.

Deviation between testing and expert data is 0.18% or 0.0018.

Summarizing the findings in this chapter, we have to conclude that the discovery and design of new materials are driving forces for much of the research that takes place in multiple disciplines, including materials science and engineering, matter physics, materials chemistry, and emerging technologies such as fuzzy logic, soft computing, etc. However, this task is implemented mainly on the basis of time- and resource-consuming experiments. Thus, we consider to shift the approaches to material design investigations from physical experiments to experiments on the basis of fuzzy If-Then rule-based material model. The motivation to use fuzzy model is inspired by the necessity to construct an intuitively well-interpretable material design model based on imperfect and complex data. In this chapter we have considered three material synthesis problems which had shown that instead of carrying out complicated experiments, researchers can use fuzzy model-based computational synthesis approach utilizing digital twins of physical models. Applications of this approach have shown that fuzzy model-based experiments can give better results than physical experiments in terms of desirable characteristics of synthesized materials. The approaches suggested in this chapter are universal and may be applied not only in materials science but also in chemical engineering, drug design, and other fields. Complexity of material design problems mandates to combine fuzzy logic and efficient learning methods as artificial neural networks, evolutionary algorithms, and others to more adequately model and predict possible material behavior.

Scaled PREN	Scaled yield strength	Scaled weldability	Scaled impact strength	Computed performance index	Given performance index
26.00	3.60	18.40	6.80	54.70	54.8 (alloy 1925hMo)

Table 21.
Comparison of computed and given data.

5. Conclusion

In this chapter, we have used data-driven approach to construction of fuzzy model which is more effective than expert-driven approach. Consequently, we have used fuzzy C-means clustering to derive fuzzy If-Then rules from material data that describe material composition and related characteristics. In order to determine the required characteristics, computational experiments on the basis of fuzzy inference and fuzzy expert system were conducted. The expert opinions and some few physical experiments have proven validity of the obtained results. The main advantage of the fuzzy logic-based approach is a high interpretability of fuzzy If-Then rules. However, learning the ability of the fuzzy models is scarce. Thus, combination of fuzzy logic with deep learning methods, mainly, reinforcement learning methods, would help to achieve better results on material synthesis.

In future works, fuzzy materials paradigm may improve processing-structure--property-performance relationship in hierarchy of structural materials levels, from the atomic and electronic to the macrostructural levels. Another important application of fuzzy logic is fuzzy phase diagram construction for different alloy models using uncertain enthalpies and other thermodynamic parameters will be investigated, which opens a door to design new materials.

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References

[1] Agrawal A, Choudhary A. Perspective: Materials informatics and big data: Realization of the 'fourth paradigm' of science in materials science. APL Materials. 2016;**4**:1-10

[2] Agrawal A, Deshpande PD, Cecen A, Basavarsu GP, Choudhary AN, Kalidindi SR. Exploration of data science techniques to predict fatigue strength of steel from composition and processing parameters. Integrating Materials and Manufacturing Innovation. 2014;**3**:1-19

[3] National Institute of Materials Science. Available from: http://smds.nims.go.jp/fatigue/index_en.html [Accessed: January 12, 2016]

[4] Dieter GE. Mechanical Metallurgy. New York: McGraw-Hill Book Company; 1986

[5] Yang ZG, Stevenson JW, Paxton DM, Singh P, Weil KS. Materials Properties Database for Selection of High-Temperature Alloys and Concepts of Alloy Design for SOFC Applications. Richland, Washington: Pacific Northwest National Laboratory; 2002. 78 p

[6] Hill J, Mulholland G, Persson K, Seshadri R, Wolverton C, Meredig B. Materials science with large-scale data and informatics. Unlocking new opportunities. MRS Bulletin. 2016;**41**:399-409

[7] Gaultois MW et al. Perspective: Web-based machine learning models for real-time screening of thermoelectric materials properties. APL Materials. 2016;**4**(5):053213-1-053213-11. DOI: 10.1063/1.4952607

[8] Elishakoff I, Ferracuti B. Fuzzy sets based interpretation of the safety factor. Fuzzy Sets and Systems. 2006;**157**: 2495-2512

[9] Lee Y-H, Kopp R. Application of fuzzy control for a hydraulic forging machine. Fuzzy Sets and Systems. 2001; **99**:99-108

[10] Rao HS, Mukherjee A. Artificial neural networks for predicting the macromechanical behaviour of ceramic-matrix composites. Computational Materials Science. 1996;**5**:307-322

[11] Conduit BD, Jones NG, Stone HJ, Conduit GJ. Design of a nickel-base superalloy using a neural network. Materials & Design. 2017;**131**:358-365

[12] Tajdari M, Mehraban AG, Khoogar AR. Shear strength prediction of Ni–Ti alloys manufactured by powder metallurgy using fuzzy rule-based model. Materials and Design. 2010;**31**:1180-1185

[13] Babanli MB. Synthesis of new materials by using fuzzy and big data concepts. Procedia Computer Science. 2017;**120**:104-111

[14] Chen DD. Dislocation substructures evolution and an adaptive-network based fuzzy inference system model for constitutive behavior of a Ni-based super alloy during hot deformation. Journal of Alloys and Compounds. 2017; **708**:938-946

[15] Babanli MB, Huseynov VM. Z-number-based alloy selection problem. Procedia Computer Science. 2016;**102**: 183-189

[16] Babanli MB, Kolomytsev V, Musienko R, Sezonenko A, Ochin P, Dezellus A, et al. Thermodynamic properties and thermal stability of the multicomponent TiNi based alloy ribbons. Metal Physics and Advanced Technologies. 2001;**23**:111-124

[17] Zadeh LA. Fuzzy sets. Information and Control. 1965;**8**:338-353

[18] Babanli MB. Theory and practice of material development under imperfect information. In: Advances in Intelligent Systems and Computing. Vol. **896**. Springer; 2018. pp. 4-14

[19] Babanli MB, Prima F, Vermaut P, Demchenko LD, Titenko AN, Huseynov SS, et al. Material selection methods: A review. Advances in Intelligent Systems and Computing. 2018;**896**: 929-936

[20] Babanli MB. Fuzzy modeling of phase diagram under imprecise thermodynamic data. In: Proceedings of the Tenth World Conference "Intelligent Systems for Industrial Automation". b-Quadrat Verlag; 2018. pp. 265-266

[21] Babanli MB, Prima F, Vermaut P, Demchenko LD, Titenko AN, Huseynov SS, et al. Review on the new material design methods. Advances in Intelligent Systems and Computing. Cham, Switzerland: 2018;**896**:937-944

[22] Frenzel J, Wieczorek A, Opahle I, Maa B, Drautz R, Eggeler G. On the effect of alloy composition on martensite start temperatures and latent heats in Ni–Ti-based shape memory alloys. Acta Materialia. 2015;**90**:213-231

[23] Vafaeenezhad H, Seyedein SH, Aboutalebi MR, Eivani AR. Application of constitutive description and integrated ANFIS – ICA analysis to predict hot deformation behavior of Sn-5Sb lead-free solder alloy. Journal of Alloys Compounds. 2017;**697**:287-299

[24] Odejobi OA, Umoru LE. Applications of soft computing techniques in materials engineering: A review. African Journal of Mathematics and Computer Science Research. 2009;**2** (7):104-131

[25] Datta S, Chattopadhyay PP. Soft computing techniques in advancement of structural metals. International Materials Reviews. 2013;**58**:475-504

[26] Aliev RA, Aliyev RR. Soft Computing and Its Applications. New Jersey, London, Singapore, Hong Kong: World Scientific; 2001