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FUZZY REASONING SYSTEM DESIGN AND ASSESSMENT OF LOAD-BEARING ENDOPROSTHESES AND THEIR FABRICATION PROCESSES

SYSTEM WNIOSKOWANIA ROZMYTEGO DLA PROJEKTOWANIA I OCENY ENDOPROTEZ PRZENOSZĄCYCH OBCIĄŻENIE ORAZ PROCESU ICH PRODUKCJI

Five attempts of an application of a fuzzy reasoning approach to problems encountered in biomechanics and engineering of biomaterials are presented. They include: (A) assessment of maximum contact stress acting on endoprosthesis, (B) design of sintering plan to obtain a porous/scaffold implant, (C) design of oxidation plan to obtain nanotubular oxide structure on the Ti alloy, (D) and (E) design of deposition of hydroxyapatite coating on the Ti alloy. The fuzzy reasoning system is shown to well predict: the maximum contact stress estimation on acetabular surface of the load-bearing hip joint endoprosthesis for chosen and given Wiberg's angle values and patient's body weight; the optimal geometry of scaffold's architecture; the geometry of TiO_2 nanotubular layer on titanium surface and directions of the adjustment of fabrication conditions; the ratio of Ca/P and the coating crystallinity; effects of control factors (sintering temperature and content of ZnO) on mechanical properties of BHA-ZnO composite. A small deviation of the predicted values from those obtained in the course of experiments can be decreased by improvement of the proposed fuzzy model i.e. adjusting fuzzy membership functions of input and output variables.

Keywords: biomaterials, fuzzy reasoning, prediction

Zaproponowano pięć zastosowań podejścia rozumowania rozmytego do rozwiązania problemów w dziedzinie biomechaniki oraz inżynierii biomateriałów. Obejmują one: (A) oszacowanie maksymalnych naprężeń kontaktowych działających na endoprotezę, (B) zaprojektowanie procesu spiekania dla otrzymania porowatego implantu, (C) opracowanie planu utleniania w celu otrzymania struktury nanorurkowej na stopach Ti, (D) oraz (E) zaprojektowanie osadzania powłoki hydroksyapatytowej na stopach Ti. System wnioskowania rozmytego umożliwił poprawne oszacowanie: maksymalnych naprężeń kontaktowych na powierzchnię panewki w endoprotezie stawu biodrowego przenoszącej obciążenia dla wybranych wartości kąta Wiberg'a oraz masy ciała pacjenta; optymalną geometrię architektury rusztowania implantu; optymalną geometrię nanorurkowej warstwy tlenku TiO_2 na powierzchni tytanu oraz optymalizację warunków procesu jej wytwarzania; stosunek molowy Ca/P oraz krystaliczność powłoki; wpływ określonych czynników (temperatura spiekania oraz zawartość ZnO) na własności mechaniczne kompozytu BHA-ZnO. Zauważono niewielkie odchyłki przewidywanych wartości od parametrów uzyskanych w trakcie przeprowadzania eksperymentów, które mogą zostać zmniejszone poprzez odpowiednie dostrojenie modelu rozmytego, np. poprzez regulację rozmytych funkcji przynależności dla zmiennych wejściowych i wyjściowych.

1. Introduction

The biomechanics and biomaterials engineering encounter many problems in design of the experiments, assessment of results and design of proper technical solutions. The principal reasons include two: (i) difficult modelisation of a patient body and its parts because of a great number of unrepeatable features followed by only rough assessment of desired features, and (ii) huge amount of necessary tests resulted from wide range of inputs and their limits, and high costs of experiments which results could be then treated by non-parametric statistics or approximate reasoning methods, like the fuzzy reasoning method.

The fuzzy reasoning system enables to operate with quality knowledge, on the contrary to numerical calculations on data and using complicated mathematical models by traditional computer programs [1,2]. The fuzzy reasoning approach provides an efficient method to establish the relationships between an input and an output without the need of complex mathematical models. The fuzzy reasoning approach allows to handle problems in-

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volving ambiguity and vagueness by mapping an input to an output in a nonlinear way [1].

In this paper the five attempts of an application of the fuzzy reasoning method to the above problems are presented. They include: (A) assessment of maximum contact stress acting on endoprosthesis, (B) design of sintering plan to obtain a porous/scaffold implant, (C) design of oxidation plan to obtain nanotubular oxide structure on the surface of the Ti alloy, (D) and (E) design of deposition of hydroxyapatite coating on the surface of the Ti alloy.

The study (A) is focused on the hip joint endoprosthesis loosening resulting in the lost of implant stem or cup stability, which first of all, is the result of too high contact stress on upper part of endoprosthesis. As boundary (acceptable) value 3.0 MPa is assumed [3]. The maximum contact stress on the acetabular surface estimation method is presented, which means the area of load transfer on upper part of endoprosthesis taking into account Wiberg's angle (which describes the size of load transferring area) and patient's body weight. Two above parameters are taken into account; as it has been proven, the Wiberg's angle, especially it's small values adequate to reduction of a load transferring area, as well as the patient's overweight, can lead to an unfavorable phenomenon of aseptic endoprosthesis loosening and in consequence to revision of the hip alloplasty operation [3-7].

Titanium and titanium alloys are frequently used as implanting materials in orthopaedic applications in order to replace a damaged bone and to provide support for healing bone tissue and as such have been investigated in the three here described studies. The load-bearing scaffolds should mimic the properties of the native bone and possess adequate mechanical strength. Titanium biomaterials demonstrate some desirable properties, such as relatively low elastic modulus, good fatigue strength, formability and corrosion resistance [8]. Porous titanium implants provide three-dimensionally interconnected pores which permit the transportation of body fluids, vascularization and in-growth of bone tissue [9]. There are several processing techniques to fabricate titanium scaffolds, such as sintering of metal powders [10], space-holder method [9], replication of polymeric sponge [11], rapid prototyping technology, like three-dimensional fiber deposition (3DFD) [12], and many others. Among them, the powder metallurgy process with the creation of TiH_2 as pore forming agent has been used [12]. Using this method it is possible to obtain a porous Ti6Al4V structure with controlled porosity and uniform pore size with properties similar to that of the human cancellous bone. The pore size and porosity are affected by processing parameters, such as sintering temperature and pressure applied during powder compaction, what it has been an aim of the test (B).

Titanium and titanium alloys are frequently subjected to surface engineering. It may include as the first stage the creation of nanotubular oxide layers which demonstrate both excellent corrosion resistance and biocompatibility [13-15]. Incidentally, TiO_2 layers are mostly developed because of their other extraordinary surface properties usable gas sensing, photoelectronics, and photocatalysis applications. The efficiency of TiO_2 nanotubular layer depends on the geometry and surface area of nanotubes. The nanotubular oxide layer can be grown directly by cost-effective method such as electrochemical anodization of titanium in fluoride electrolytes [16]. Various electrolytes have been used to form TiO_2 nanotube arrays, such as HF/H_2SO_4, chromic acid/HF, $NH_4F/(NH_4)_2SO_4$ and H_3PO_4/HF mixtures [13,14,16]. The structure of nanotubular oxide layer on titanium substrate depends on fabrication conditions, like applied potential, pH value of electrolyte, and anodization time. The geometry of TiO_2 nanotube layer can be controlled by choosing optimal parameters of anodization process as shown in the test (C).

In order to enhance bioactivity and joining of an implant and a bone, hydroxyapatite coatings have been proposed and applied, mainly by thermal spraying method [17]. The hydroxyapatite (HA) coating crystallinity, dependent on the processing method and heat treatment, determines the dissolution rate of the coating. It is important to control the degree of crystallinity that should match the rate of bone growth around the implant, preventing the latter implant loosening. The molar ratio Ca/P close to 1.67 is beneficial for the bone in-growth [18]. The Ion Beam Assisted Deposition method (IBAD) has been taken into the account as the method which enables to control the microstructure and the crystallinity of the coating by controlled substrate heating during the deposition [19,20] in test (D).

The chemical form of phosphate is very important. The biologically derived hydroxyapatite (BHA), obtained from bovine bones or human teeth, is very interesting biomaterial clinically used for skeletal and dental restoration and treatments. The production cost is lower that of synthetic HA. Moreover, BHA accommodates several trace elements, which play an important role in biological performance of biomaterial after implantation [21-25]. It has been suggested that incorporation of ZnO in BHA matrix can improve mechanical (e.g. compressive strength, microhardness) and biological properties, since ZnO has positive effect on proliferation of osteoblastic cells and inhibiting effect on osteoclastic bone resorption [29]. This case is considered in the test (E).

2. Experimental

The common fuzzy reasoning system has been used [1,29]. The domains of input sets have been established based on literature data or own experimental data as shown later. Fuzzy output sets represent searched variables. Each of the sets corresponds to certain searched value, with given specific linguistic names expressing subjective differences in values for previously defined variability range. Input and output variable domains have been divided into fuzzy values, and membership functions for fuzzy sets were generated using the triangular and trapezoidal membership function form [1,2]. The rule base corresponds with the division of input and output space. It consists of several rules linking input values with output for certain parameters, which were introduced into the Matlab environment, the Fuzzy Logic Toolbox [2]. Rules in the form of "if – then" have been presented as the decision table. For resultant output value of the center of gravity, the defuzzyfication method has been used [1]. After the defuzzyfication process, only one value has been chosen, in response to given input values.

3. Results

3.1. Test (A)

Domains of input sets were established based on literature data [7,28,29] where variability ranges for geometrical parameters of femoral head – pelvis system were observed. Variability range for Wiberg's angle (v_{CE}) were in $0^0 \div 55^0$ range and for body weight (W_B) as 40÷85 kg based on study results demonstrated in [29] as shown in Table 1. Fuzzy output sets represent maximum contact stress on acetabular surface of the endoprosthesis (p_{max}) . Each of the sets corresponds to the certain stress range, with given linguistic names: "small, medium, large" for previously defined stress variability range 1.6÷12 MPa [29].

TABLE 1
Decision table of fuzzy rule base for maximum contact stress on acetabular surface of endoprosthesis [29]

Input values	Body weight [kg]			
	Variability range	X [40÷60]	Y [50÷70]	Z [60÷85]
Wiberg's angle [^{0}]	A [0÷10]	L	S	S
	B [5÷20]	M	M	M
	C [10÷30]	M	M	M
	D [20÷55]	M	M	M

As a result of approximate reasoning for chosen input variables values, the resultant output set were received (Fig. 1). After the defuzzyfication process, only one value was chosen, in response to given input values. As an example, maximum contact stress for hip joint with Wiberg's angle of v_{CE} $=25^0$ and patient's body weight of W_B =75 kg, was determined. The received maximum contact stress on acetabular surface of the hip is p_{max} =3.62 MPa. The obtained stress value was similar to the value 3.2 MPa achieved with an use of software HIPSTRESS [3], thus here proposed simple approach brings out the value relatively close to that obtained with more complicate tool.

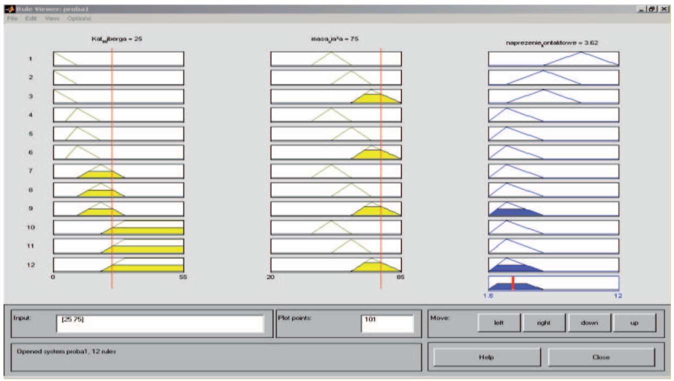

Fig. 1. Resultant maximum contact stress p_{max} =3.62 MPa based on the input Wiberg's angle magnitude v_{CE} $=25^0$ and body weight W_B =75 kg [2]

3.2. Test (B)

Fuzzy input and fuzzy output sets were established based on the research conducted by Gu *et al.* [8]. As input variables sintering temperature 840÷1100°C and compaction pressure 9÷88 MPa were chosen. Fuzzy output sets were: pore size 10÷200 μm and porosity 10÷70%. Input and output spaces were divided into fuzzy triangular and trapezoidal sets, with linguistic names: "very small (VS), small (S), medium (M), large (L), very large (VL)". The rule base was consisted of just 9 rules linking input values with output for certain parameters, introduced into Matlab environment, Fuzzy Logic Toolbox [2]. Rules in the form "if – then" are presented as decision Table 2.

Accordingly to approximate reasoning for chosen input variables values, the resultant output sets were received (Fig. 2). As a result of the defuzzyfication process, only one value was again chosen, in response to given input values. As an example, for the chosen input variables, applied sintering temperature of 970°C and compaction pressure of 45 MPa, the simulation results determined the outputs variables: pore size of 97.9 μm and porosity of 29.4%. Similarly, for the inputs variables, applied sintering temperature of 950°C and compaction pressure of 26 MPa, the outputs variables are the pore size of 50 μm and porosity of 30%. The obtained pore size dimensions and porosity are well in line with the experimental data achieved by Gu Y.W. *et al.* [8].

TABLE 2

Decision table of fuzzy rule base for fabrication of porous Ti6Al4V by powder metallurgy process [5], where: T – sintering temperature [°C], C – compression pressure [Pa], PS – pore size [μm], P – porosity [%]

Fuzzy input					Fuzzy output		
	T is VS		C is VS		PS is L		P is M
	T is S		C is M		PS is L		P is VL
	T is S		C is VL	Then	PS is VS		P is S
If	T is M	and	C is VS		PS is S	and	P is L
	T is M		C is S		PS is S		P is M
	T is M		C is M		PS is S		P is M
	T is M		C is L		PS is M		P is M
	T is M		C is VL		PS is VS		P is S
	T is L		C is M		PS is VS		P is S

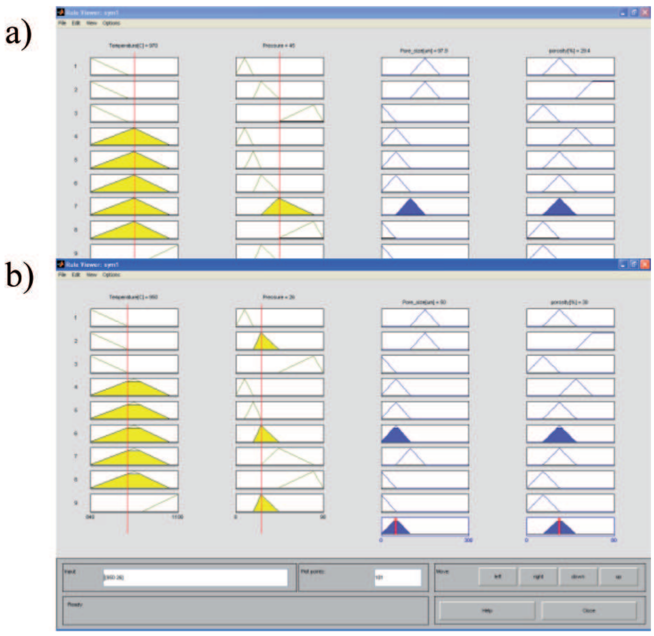

Fig. 2. Results of fuzzy reasoning system for fabrication of porous Ti6Al4V: a) the inputs – applied sintering temperature 970°C and compaction pressure 45 MPa, the outputs – pore size 97.9 μm and porosity 29.4%, b) the inputs – applied sintering temperature 950°C and compaction pressure 26 MPa, the outputs – pore size 50 μm and porosity 30%

3.3. Test (C)

As input variables, the applied potential 0÷25 V and anodization time 0÷12 h were chosen. Fuzzy output sets were set up as the nanotube diameter 0÷120 nm, and tube length 0÷1200 nm, based on experimental results presented by Bauer *et al.* [15]. Input and output space were divided into fuzzy triangular and trapezoidal sets, with linguistic names given: "very small (VS), small (S), medium (M), large (L), very large (VL)". The rule base corresponded to division of input and output space and consisted of 15 rules linking input values with output for certain parameters introduced into Matlab environment, Fuzzy Logic Toolbox [2]. Rules in the form "if – then" are presented as decision Table 3. For resultant output values of tube diameter and tube length, the center of gravity defuzzyfication method was used.

3.4. Test D

Domains of input sets were established based on results provided by Blalock *et al.* [19]. as shown in Table 4. In their investigations, the input values were the temperature of specially heated substrate and a distance between the ion beam and the substrate. The variability range of the substrate temperature was 450÷750°C, and of the distance from the substrate 0÷1000 nm. Fuzzy output sets represent the Ca/P ratio distribution over the thickness of the coating in range 0÷28 μm. For each fuzzy input and output variable corresponding fuzzy sets were established with given linguistic names: "very small (VS), small (S), medium (M), large (L), very large (VL)". Membership functions for fuzzy sets were generated using triangular and trapezoidal membership function form [2]. Rule base for fuzzy reasoning system consisted of 20 rules in form of 'if-then' statements. For resultant output value Ca/P ratio, the center of gravity defuzzyfication method was used [1]. Fuzzy variables and rule base have been introduced into Fuzzy Logic Toolbox in Matlab environment [2].

As a result of approximate reasoning for chosen input variables values, the resultant output sets were received (Fig. 3). As an example, for the chosen input variables, applied voltage of 10 V and the oxidation time 2 h, the diameter of TiO_2 nanotube of 53.5 nm and length of 600 nm were found. The potential increasing to 20 V resulted in change of nanotube diameter to 93 nm and its length to 970 nm. The simulation results are in accordance with the experimental data achieved by Bauer *et al.* [15].

TABLE 3

Decision table of fuzzy rule base for electrochemical oxidation in 1 M H_3PO_4 solution with an addition of 0,3 wt.% HF [15], where: V – applied potential, t – anodization time, φ – tube diameter, and th – tube length

	Fuzzy input				Fuzzy output		
	V is VS		t is S		φ is VS		th is VS
	V is VS		t is M		φ is VS		th is VS
	V is VS		t is L		φ is S		th is S
	V is S		t is S		φ is S		th is VS
	V is S		t is M		φ is S		th is S
	V is S		t is L	then	φ is S		th is S
If	V is M	and	t is S		φ is M	and	th is M
	V is M		t is M		φ is M		th is M
	V is M		t is L		φ is M		th is L
	V is L		t is S		φ is M		th is L
	V is L		t is M		φ is L		th is L
	V is L		t is L		φ is L		th is L
	V is VL		t is S		φ is M		th is L
	V is VL		t is M		φ is L		th is L
	V is VL		t is L		φ is L		th is L

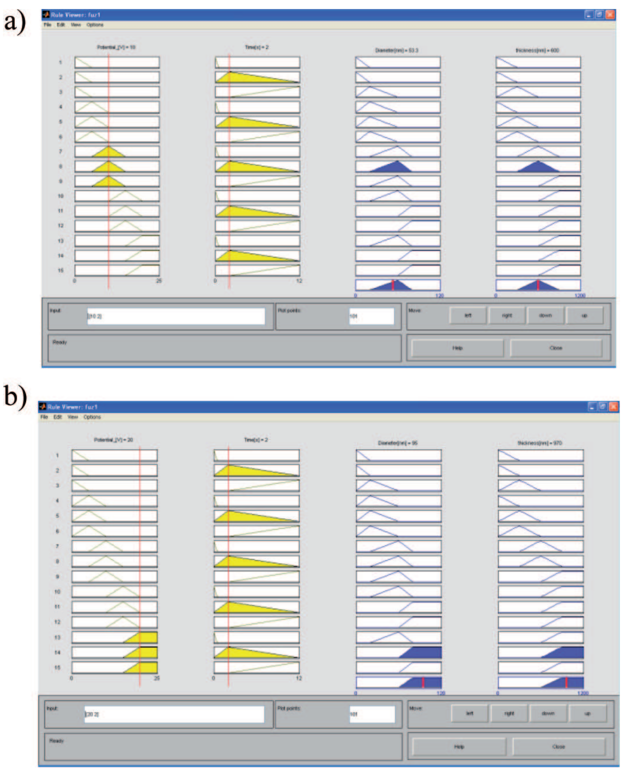

Fig. 3. Results of fuzzy reasoning system for TiO_2 layer formation: a) the inputs – applied potential 10 V and anodization time 2 h, the outputs – diameter 53.3 nm and tube length 600 nm, b) the inputs – applied potential 20 V and anodization time 2 h, the outputs – tube diameter 95 nm and the t length 970 nm

TABLE 4

Experimental results evaluated by STEM-EDS – the average atomic Ca/P ratio for sets substrate temperatures along the HA coatings thickness [19]

Distance from Ti substrate [nm]	Atomic Ca/P ratio			
	Substrate temperature [°C]			
	450	550	650	750
0	0	0	0	0
200	1.9	2.4	2.4	0
400	1.95	2.7	2.3	16
600	2	2.9	2	16
800	2.2	2.5	4.6	14
1000	–	–	4.1	26.3

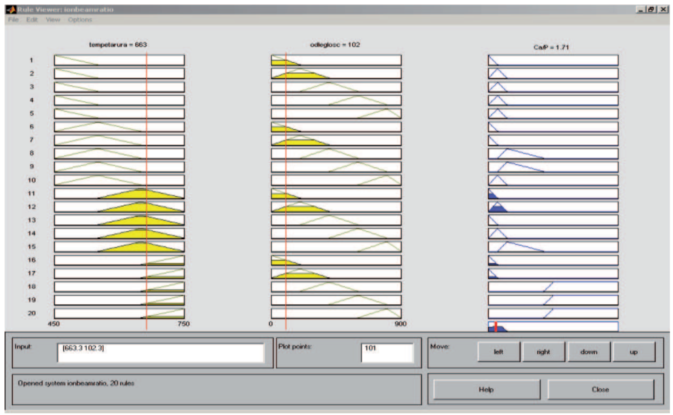

Fig. 4. Resultant Ca/P ratio 1.71 for inputs: substrates temperature 663°C and distance from the Ti substrate 102 nm

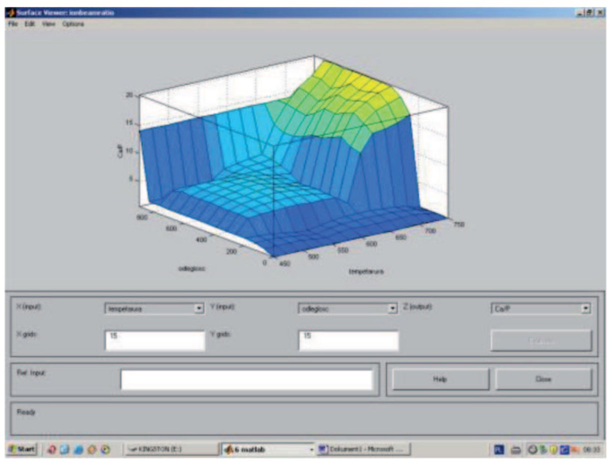

Fig. 5. Control surface for ratio Ca/P based on the rule base

Fig. 4 shows the resulting value of the Ca/P ratio 1.71 for a chosen input variables: substrate temperature 663°C and distance from the substrate 102 nm. Using fuzzy reasoning method it is possible to predict Ca/P ratio from the control surface (Fig. 5) for each combination of input parameters with deviation of 3% comparing to the results achieved by microstructure characterization techniques, like TEM and SEM examination techniques [19,30].

3.5. Test E

Domains of input sets have been established basing on the literature data shown in Table 5. As input variables, the sintering temperature (T) 1000÷1300°C and the amount of ZnO in range of 2.5÷10 wt.% were chosen. Fuzzy output sets were: the density of BHA-ZnO composite (d) 1.9÷3 g/cm^3, compressive strength (σ) 19÷75 MPa, and Vickers microhardness 49÷600 HV, based on experimental results presented by Gunduz *et al.* [21]. Input and output space were divided into fuzzy sets, with linguistic names given: "very small (VS), small (S), medium (M), large (L), very large (VL), and very very large (VVL)". For each fuzzy set a membership function was generated in triangular and trapezoidal form, and Mamdani fuzzy reasoning system was used [29]. The system has been based on 12 fuzzy rules in form "if – then" statements.

TABLE 5
Experimental results of influence of sintering temperature and the amount (wt.%) of ZnO on density, compressive strength, and Vickers microhardness of BHA-ZnO composites [21]

Temperature T [°C]	2.5 ZnO [wt.%]	5 ZnO [wt.%]	10 ZnO [wt.%]
		d [g/cm^3]	
1000	2.77±0.060	2.86 + 0.004	2.94±0.002
1100	2.82±0.002	2.17±0.030	2.94±0.002
1200	2.66±0.036	2.76±0.060	2.99±0.058
1300	2.74±0.004	2.82±0.060	2.93±0.069
		σ [MPa]	
1000	21.00±2.24	37.67±10.41	28.36±1.97
1100	39.45±2.38	37.31±2.380	27.99±5.03
1200	52.24±7.12	71.96±10.90	53.22±3.36
1300	35.41±7.88	37.45±12.60	32.99±8.68
		HV	
1000	49.02±6.990	58.84±5.570	67.87±10.87
1100	94.39±13.89	71.12±28.43	95.13±10.79
1200	208.20±40.870	226.88±11.300	203.10±22.000
1300	302.82±29.800	545.67±45.700	338.10±32.490

The results of fuzzy reasoning method used for predicting the mechanical properties: densification, compression strength and microhardness are shown in Fig. 6. For chosen input variables, namely the sintering temperature 1300°C and 2.5 wt.% ZnO in BHA matrix, simulation led to the following values of output variables: compression strength 30 MPa, density 2.7 g/cm^3, and Vickers microhardness 283 HV. Simulation results showed deviation of 4% comparing to the results achieved by experimental tests [21].

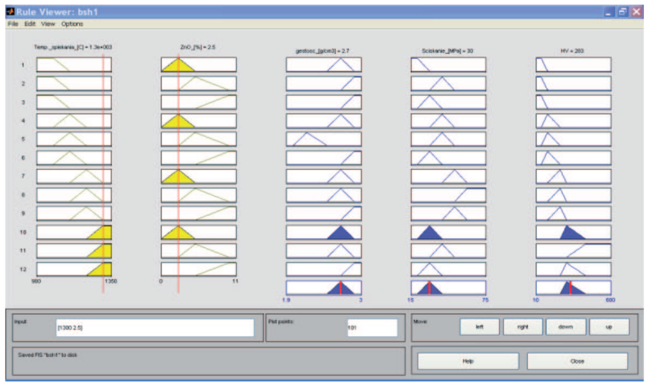

Fig. 6. Results of fuzzy reasoning system for BHA-ZnO composite, where inputs are: sintering temperature 1300°C and 2.5 wt.% ZnO, and outputs: compression strength 30 MPa, density 2.7 g/cm^3, and Vickers microhardness 283 HV

4. Discussion

The fuzzy reasoning system presented in this work is able to predict the maximum contact stress estimation on acetabular surface of the load-bearing hip joint endoprosthesis for chosen and given Wiberg's angle values and patient's body weight. The advantage of the presented method is a lack of necessity for the complicated mathematical models' creation.

The optimal geometry of the scaffold's architecture can be also well determined using the simple fuzzy reasoning method. It is possible to make the model more accurate by addition of fuzzy rules in order to make a better estimation of the scaffold's architecture, although just 9 fuzzy rules are enough to properly predict the scaffold's geometry. The proposed method provides a useful tool within the range of the area responses established, based on the selective and limited representative experimental data.

An another application of the fuzzy reasoning approach is the prediction and optimization of the geometry of TiO_2 nanotubular layer on titanium surface by adjustment of fabrication conditions, i.e. applied voltage and oxidation time during electrochemical anodization process.

The next example described in the work is the usage of the fuzzy reasoning system to predict properly the ratio of Ca/P as it constitutes an efficient way to attain robustness analysis of the coating crystallinity depending on the substrate temperature and the distance from the

Ti substrate along the coating's thickness obtained by IBAD technique.

Using fuzzy reasoning approach, the relationship between control factors (sintering temperature and content of ZnO) and response variables of mechanical properties of BHA-ZnO composite can be obtained. The small deviation of the predicted values from those obtained in the course of the experiments can be decreased by improvement of the proposed fuzzy model i.e. adjusting fuzzy membership functions of input and output variables.

5. Conclusions

In this study, the five attempts of an application of the fuzzy reasoning approach to the engineering of biomaterials are presented. In all cases the proposed system proved to be an efficient method to establish correct relationships between an input and output without the need of complicated mathematical models. Although there were some minor deviations of the predicted output values from those obtained from experiments, the results accuracy can be increased by modification of particular modules of the proposed system i.e. adjusting fuzzy membership functions of input and output variables or automatic learning the knowledge base from numerical information.

The proposed method offers reasonable prediction and assessment of the output of engineering processes as have been shown in the presented examples, limiting the amount of the measured data available from expensive and time-consuming experiments. Above that, the fuzzy reasoning system can be easily developed and modified according to different applications, especially during the early stage of any engineering process development.

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