Tomasz WÓJCICKI

Institute for Sustainable Technologies – National Research Institute, Radom tomasz.wojcicki@itee.radom.pl

THE CONCEPTION OF USING A BAYESIAN NETWORK FOR AIDING THE DESIGN OF MANUFACTURING PROCESSES OF SURFACE LAYERS

Key words

Surface layers, surface engineering, Bayesian network, probabilistic network, design.

Abstract

The paper presents a selected area of ongoing research on computer-aided design of manufacturing processes of surface layers with the use of modern information technologies. It describes the main problems related to the manufacturing of surface layers by mechanical, thermal, thermo-mechanical, thermo-chemical, electrochemical, and physical treatment, and information technologies used for these tasks. The paper presents an original methodology that uses a probabilistic Bayesian network, which is a directed graph, and it is based on the events and their associated probabilities representing the structure of cause and effect for the selected problem areas. The methods of determining the probability of events for specific network nodes and joint probability distribution for the whole structure of the graph are described. The model of the information system transforms the input values into output values, and this paper presents the range of information and the phases of the inference process, consisting of automatic technology identification of surface layer formations characterized by the expected properties and method of determining the process parameters for selected technology. The implementation of a model solution for selected application problems associated with the need to get a surface layer characterized by a certain hardness distribution and the results achieved are presented.

Introduction

The formation of surface layers, which enhance the exploitation properties of functional elements, is an important issue in the field of materials science. The surface layer is the part of the material that is limited on one side by the real solid surface or coating protection and from the other side by the material core, consisting of zones, characterized by varying thicknesses and different physical and chemical properties. Research related to the formation and exploitation of surface layers is carried out in a number of leading research centres located in Poland [1] and abroad [2]. By the formation of surface layers with the use of specific technologies, the durability of the elements that are parts of the machinery and other mechanical structures [3] can be substantially increased. There are many technologies for manufacturing surface layers which can be mechanical (burnishing, detonation deposition), thermal (hardening, tempering, annealing, remelting, hardfacing, melting), thermo-mechanical (saturation, alloying), thermo-chemical (spraying, spraying-remelting, plating, detonation hardening), electro-chemical (direct deposition, electrolytic deposition, conversion deposition), physical (vapour deposition, ion implantation, etc.). Technologies of surface layers are characterized by distinctive sets of process parameters and properties obtained from their use. For each type of surface layer, it is also necessary to prepare the substrate, which must take into account the specificity of the process. Exploitation properties of coatings depend on their chemical composition, metallographic structure, and the degree of adhesion to the substrate. The chemical composition, structure, and adhesion depend on the types and ratios of components. Moreover, some components may only be deposited on the substrate by specific methods. The same coatings made using different methods have different usable properties. PVD methods (Physical Vapour Deposition) [4] are used to produce coatings adhesively (and to a lesser extent by diffusion) connected to the substrate by using physical phenomena under reduced pressure involving ions. The PVD deposition mainly causes phase changes of the substance, and chemical changes occur in the technologically negligible extent [5]. The mechanism of deposition is controlled primarily by the choice of substrate temperature, atmospheric pressure, and the composition of the reaction atmosphere.

The tasks associated with the formation, modelling, and analysis of surface layers may be partially supported using advanced computational methods. Figure 1 presents the computational methods in the processes of modelling, formation, and analysis of the properties of surface layers.

Fig. 1. The scope of computational methods in the processes of modelling, formation, and analysis of surface layers Source: Author.

The effective selection of technology and parameter values of the formation of the surface layers is a key issue related to the area of surface engineering. Methods that reduce the time associated with the identification of technology and the values of specific properties of constituting layers significantly reduce operating costs of companies and research centres involved in the development of this area of research.

There are varieties of computational methods that may be used in the present task area. These methods include methods based on computational intelligence (CI), including artificial neural networks [6], genetic algorithms [7], fuzzy logic [8], etc. The modelling process aided by computational methods that use computer systems is presented in Figure 2.

Every single method has its advantages and limitations. Testing is also carried out using these systems [9], including the use of fuzzy logic [10] and artificial neural networks having a determined architecture [11].

In this paper, an original model using probabilistic Bayesian networks is presented. A characteristic feature of Bayesian networks is the use of *a priori* distribution for a specific set of analysed parameters. During the estimation stage, the initial knowledge is assumed to possess on the parameter values, and these values are changed in later processing. Bayes' theorem is used for events that depend previous events. The probability that is calculated using Bayes' theorem determines the extent to which the selected factor is the cause of the event. The "Naive Bayesian" classifier requires a probability calculation based on the training set, which consists of the examples described using attributes characterizing the input data and the conclusions that represent the output values.

Fig. 2. The modelling process aided by information systems in the field of surface engineering Source: Author.

1. Specificity of Bayesian network

A Bayesian network is a directed acyclic graph, which is composed of nodes, and connections called "edges" (Fig. 3). The nodes are variables that represent specific events and the edges are the relationships between events with

certain degrees of probability assigned to them. Bayesian networks reflect the causal effect structure of the chosen problem area.

Fig. 3. Bayesian network structure composed of four nodes and five edges Source: Author.

An important feature of Bayesian networks is the ability to calculate the probability distributions of defined variables (events) based on the status of the other variables. Assuming that *A* and *B* represent the events and the probability of event *B* is $P(B) > 0$, then the conditional probability of event *A* is determined from the following equation:

$$
P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}\tag{1}
$$

Assuming that *A* may have *n* states $\{a_1, a_2, ..., a_n\}$, then for the *i*-th state of the *a priori* probability of event *B* is determined according to the following equation:

$$
P(B) = \sum_{i=1}^{n} P(B | A = a_i) P(A = a_i)
$$
 (2)

The joint probability distribution of a Bayesian network that consists of *k* nodes is determined based on conditional probabilities of individual events for specific values of their predecessors:

$$
P(A_1, ..., A_m) = \prod_{k=1}^{m} P(A_k \mid parent(A_k))
$$
 (3)

where:

 $parent(A_k)$ – a set of nodes directly preceding node A_k .

For the network shown in Figure 3, a joint probability distribution is

$$
P(A_1, A_2, A_3, A_4) = P(A_1)^* P(A_2)^* P(A_3 | A_1, A_2, A_4)^* P(A_4 | A_1, A_2)
$$
 (4)

Nodes (events) A_1 and A_2 do not have to be directly preceding the other nodes; therefore, they may represent independent events. Nodes A_3 and A_4 have three and two preceding nodes and represent dependent events. The distribution of the dependent probabilities for each node is defined in the conditional probability tables (CPT). The tables contain the probabilities for each combination of events directly preceding the event being analysed. An example of a CPT array is shown in Figure 4.

| | А, | $P(A_4 A_1, A_2)$ |
|--------------|--------------|---------------------|
| TRUE | TRUE | 0.15 |
| TRUE | FALSE | 0.68 |
| FALSE | TRUE | 0.10 |
| FALSE | FALSE | 0.07 |

Fig. 4. An example of a CPT array for node *A*⁴ Bayesian network shown in Figure 3 Source: Author.

Based on the knowledge of the joint probability distribution, it is possible to conduct an inference process on the probabilities of events included in the network structure. Inference can be causal (for the mapping of events cause) and consecutive (related to events representing effects). The choice of inference depends on the type of problem, which maps the structure of the network.

In the case of complex problems related to hundreds of thousands of events, the network structure can be so complex that, for reasons of efficiency, algorithms are applied that can reduce the time of analysis. Two popular algorithms are the logical sampling method [12] and the weighted sampling method [13].

2. Model for the aided design of processes for manufacturing surface layers by means of a Bayesian network

In the proposed model solution, the identification method of the manufacturing technology of surface layers and the values of process parameters is based on systematic empirical knowledge and acyclic directed graph matrix that characterizes the specificity of each technology. A general model represents a system whose task is to transform the input values X_M in the output values Y_M using the operator F_M .

The formal model of the system is as follows:

$$
F_M: X_M \to Y_M \tag{5}
$$

where:

 F_M – operator of the model;

 X_M – space of input values;

YM – space of output values.

The space of input values X_M is a set of properties characterizing the surface layer and the material, and the empirical knowledge concerning the manufacturing processes of surface layers.

$$
X_M = \{X^p, X^e, X^w\}
$$
 (6)

where:

 X_M – space of input values; ${x_1^p, x_2^p, ..., x_i^p}$ $X^p = \{x_1^p, x_2^p, ..., x_i^p\}$ – set of properties of the surface layer; $\{x_1^e, x_2^e, ..., x_l^e\}$ $X^e = \{x_1^e, x_2^e, ..., x_l^e\}$ – set of properties of the processed material; X^w – empirical knowledge concerning the manufacturing processes of surface layers.

The space of output values Y_M is a collection of information on technologies and manufacturing process parameters of surface layers as follows:

$$
Y_M = \{Y^k, Y^c\} \tag{7}
$$

where:

YM – space of input values; $\{y_1^k, y_2^k, ..., y_n^k\}$ *n* $Y^k = \{y_1^k, y_2^k, \dots, y_n^k\}$ – set of information about technologies for the manufacturing of surface layers; $\{y_1^c, y_2^c, ..., y_m^c\}$ *m* $Y^c = \{y_1^c, y_2^c, ..., y_m^c\}$ – set of parameters of manufacturing processes of surface layers.

Inference process is carried out in two phases. The first phase is based on the expected properties of the surface layer and the material being processed, and the experiential knowledge accumulated in the directed graph of the

Bayesian network is the determined set of surface layer technology with an assigned probability of the use of each possible technology to realize the problem task. Then, the technology that is the most likely is selected. In the second phase, the process parameters are estimated which can produce the surface layer characterized by the expected properties. A functional model of this process is shown in Figure 5.

Fig. 5. Functional model of a process to aid in the manufacturing of surface layers with the use of a Bayesian network Source: Author.

Conditional probability, which describes nodes representing the surface layer manufacturing technologies in the first phase of the inference process, is represented by the following equation:

$$
P(y_f^k | x_1^p ... x_i^p, x_1^e ... x_i^e) = \prod_{g=1}^i P(x_g^p) \prod_{d=1}^r P(x_d^e), f = 1...n
$$
 (8)

The conditional probability for the appointed technology of the manufacturing of surface layer having specific properties is as follows:

$$
P(y_c^k | x_1^p ... x_i^p, x_1^e ... x_i^e) = \max((y_1^k | x_1^p ... x_i^p),
$$

(y_2^k | x_1^p ... x_i^p), ..., (y_n^k | x_1^p ... x_i^p)) (9)

The conditional probability describing the nodes representing the values of the parameters for the appointed technology of the manufacturing of surface layers in the second phase of the inference process is represented by the following equation:

$$
P(y_h^c \mid x_1^p \dots x_i^p, x_1^e \dots x_i^e) = \prod_{g=1}^i P(x_g^p) \prod_{d=1}^r P(x_d^e), h = 1 \dots m \tag{10}
$$

As a result of this inference process, information is obtained about the technology most likely to be used to manufacture the surface layer characterized by specific properties and about the values of the process parameters used during the processing of materials.

3. Verification of the model

For the purpose of the verification of the model, as well as the practical use of proposed solutions to support the manufacturing process of surface layers, the implementation of logical structures in the structures of the information model was made. The implementation was realized using Embarcadero Technologies tools and is designed for a MS Windows system platform.

The verification of the developed solution uses expert knowledge regarding the manufacture of surface layers obtained by the research process. The subject of the study was how to obtain a surface layer having a predetermined characteristic of the hardness distribution of the material, which was steel 18HGT (Fig. 6). Following the inference of the first phase, consisting in selecting the type of technology, it was found that the nitriding process gives the highest likelihood of obtaining the surface layer characterized by expected properties. In the next phase, inference values of process parameters were defined, which were the duration of the process *t*, temperature *T*, and the potential of nitric *Np*.

Figure 6a presents the expected distribution of hardness in the nitrided layer on the steel 18HGT for the following process parameters: $T = 530^{\circ}\text{C}$, $t = 8$ h, $N_p = 0.6$, whereas figure 6b shows hardness distribution in the nitrided layer obtained with the same values of parameters in the test process [11].

The proper operation of the model calculation for the selected problem area was confirmed by the appointment of the linear correlation between expected and actual values which were elements of the characteristics of hardness distribution in the surface layer of the selected material, and the correlation coefficient was 0.9899. The results are shown in Figure 7.

The results confirmed the usefulness of the developed model solution.

The difference between the expected and actual values expressed as a percentage is shown in Figure 8.

Fig. 6. The distribution of hardness in the nitrided layer on the steel 18HGT: a) the expected values, b) the actual values by [11] Source: Author.

Fig. 7. The correlation diagram between the expected values and the actual hardness distribution for the analysed surface layer Source: Author.

Fig. 8. The difference between the expected values and the actual distribution of hardness expressed as a percentage for the analysed surface layer Source: Author.

Conclusions

The aided design model for the manufacturing of the surface layers presented in this article is a significant improvement in the design processes of surface layer engineering. The proposed solution is characterized by the ability to conduct complex analyses, which reduces the expenditures of time and personnel that are necessary to identify the technology and process parameters for surface layers characterized by certain properties. The quality and quantity of accumulated empirical knowledge concerning the manufacturing processes of layers has an influence on the results. A limitation of the solution is the need to collect *a priori* knowledge for the use in the inference processes. The quality of the results depends on the quality of the source of knowledge that should be verified by adequate domain experts. Thanks to the automatic data processing, there is a reduction in risk associated with mistakes from the technology selection as well as the values of the process parameters. Because the method can be used at different stages in the manufacture of surface layers, it can greatly improve the efficiency of production or research. The developed IT solution in the form of computer software functioning on a popular system platform does not require additional capital expenditure on specialized high- -performance systems. The implemented computer application is very flexible in terms of design and functionality, so it can be widely used in a wide operating range.

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Koncepcja wykorzystania sieci Bayesa do wspomagania projektowania procesów wytwarzania warstw wierzchnich

Słowa kluczowe

Warstwa wierzchnia, inżynieria powierzchni, sieć Bayesa, sieć probabilistyczna, projektowanie.

Streszczenie

W artykule przedstawiono wybrany fragment realizowanych prac badawczych dotyczących wspomagania projektowania procesów wytwarzania warstw wierzchnich z wykorzystaniem nowoczesnych technologii informatycznych. Omówiono podstawowe problemy związane z wytwarzaniem warstw wierzchnich poprzez obróbkę mechaniczną, cieplną, cieplno-mechaniczną, cieplno- -chemiczną, elektrochemiczną i fizyczną oraz technologie informatyczne wykorzystywane do tego typu zadań. Zaprezentowano autorską metodykę wykorzystującą probabilistyczną sieć Bayesa, będącą skierowanym grafem opartym na zdarzeniach i przypisanych do nich prawdopodobieństwach odzwierciedlających strukturę przyczynowo-skutkową dla wybranych obszarów problemowych. Przedstawiono metody wyznaczania prawdopodobieństwa zdarzeń dla określonych węzłów sieci oraz łącznego rozkładu prawdopodobieństwa dla całej struktury grafu. Zaprezentowano model systemu informatycznego realizującego zadanie polegające na transformacji wielkości wejściowych na wielkości wyjściowe i wymagany do tego celu zakres informacyjny, a także fazy prowadzenia procesu wnioskowania, polegające na automatycznej identyfikacji technologii wytwarzania warstw wierzchnich, charakteryzujących się oczekiwanymi właściwościami, oraz sposób ustalania wartości parametrów procesowych dla wybranej technologii. Przedstawiono implementację rozwiązania modelowego dla wybranego problemu aplikacyjnego związanego z potrzebą uzyskania warstwy wierzchniej charakteryzującej się określonym rozkładem twardości, a także osiągnięte rezultaty.