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A strategy for the selection of multiple materials and processes fulfilling inherently incompatible functions: The case of successive surface treatments

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ABSTRACT

Multiple surface treatment technologies are used as an example of: (i) simultaneous selection of materials and processes; (ii) selection of multiple materials each of which fulfills different functions; and (iii) selection of materials with incompatibility issues. A questionnaire-based screening algorithm uses a small surface treatment database mostly filled in with Booleans to address these issues. It relies on the fact that functions can be brought by the first treatment, the latest treatment, all treatments or at least one treatment, like for corrosion resistance. Functions are associated with attributes and combinations of treatments are suggested. The system is illustrated for four examples (automobile corrosion protection, electronic packaging, aluminum die casting and wear protection of gears) and successfully proposes candidates from literature as well as alternatives. It can be used as an exchange tool between the users and the providers of surface treatments, as a marketing tool for a specific family of processes or as a complement to industrial drawing software.

1. Introduction

Several computerised approaches exist, in order to automatically select bulk materials, surface treatments, forming processes or other material-related items. In case the requirements can be expressed by mathematical functions of attributes, the user needs a tool:

- Connected to a database of physical properties.
- Able to express these mathematical functions.
- Able to select the items that optimise them.

CES standard software combines such features with binary filters to select individual materials for a wide range of applications, using a "free searching" strategy and merit factors [1,2]. Design for multiple constraints or objectives [3] is made possible, as well as design of hybrid materials that fill gaps in the universe of materials [1,4–6]. However, this chart method assumes the existence of a model to describe the performance of the materials or the hybrid materials. The lack of homogeneous data or physical models makes more complex the design for properties like wear or corrosion resistance [2]. Other approaches for the material screening have been reviewed and compared in [2,7] and their study has been pursued, especially for multi-criteria selection [8–11]. When final ranking is not mandatory, and when requirements are of "go–no go" type, a "questionnaire" approach may be suitable [7]. Bréchet et al. suggested it for surface treatments and described the migration from a chart method to a questionnaire [3].

In order to address the high level of diversity of surface treatments, various strategies were proposed in the past. They range from the selection of anticorrosion layers to tribological treatments. In the first case, they comprise a real database, but no calculator [12–15]. In the second case, like in TRIBSEL [16], PRECEPT [17,18] and TRIBEX [19,20] or in more recent works [21,22], they do not fully predict the tribological performances, but comprise several tools based on physical considerations as well as a database.

More generalist algorithms that can be reattached to the "questionnaire" type were also proposed: ST2S [23–25] and Apticote-Isis [26], based on little or no quantification of the properties that are mostly expressed in a Boolean way. These expert systems succeed in accounting for the following specificities of surface treatments:

- The same "chemical substance" can be deposited through several processes, leading to different microstructures and different properties.
- A given "couple (layer, process)" is not compatible with any substrate, because the layer does not adhere or the process cannot be applied. An extreme example is the one of diffusion layers (like

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nitriding) that are by definition applied onto steel or, in specific cases, onto a few other metals [1,26].

However, these systems are not designed to propose multiple treatments, even though it is a frequent practice in the surface treatment field. Such "multilayers" can be reattached to at least one of the following approaches: (i) multilayers aimed at optimising one specific property; (ii) multi-purpose multilayers, i.e., each layer aims at fulfilling one or several of the functional purposes; (iii) multilayers in which one of the treatments aims at making possible other treatments (like bond coats), let's say "compatibility treatments".

Approach (i) is formalised yet for the design of optical multi-coatings, using a calculator and alternating several times two or three layers, with a tailored thickness [27–31].

Approaches (ii–iii) were illustrated in early work of Voevodin et al., in a systematic algorithm for selecting PVD multi-layers. However, the proposed stacking procedure implies to compare the relative intensities of corrosive, mechanical and thermal aggressions with each other, which, again, cannot be made quantitatively. Besides, even if additional layers are suggested in the case of cyclic solicitations, deep surface modifications used to improve fatigue resistance cannot be handled using the proposed heuristics [32].

In this paper, a pre-selection algorithm generating multi-treatments from approaches (ii–iii) is proposed, based on the logical analysis of the relevant surface properties and industrial examples. Then, it is discussed for practical examples using a re-engineering of home-made software "EXPESURF".

2. Method

Present system contains a small database and a search algorithm. Sections 2.1 and 2.2 are dedicated to the database itself (processes, additions and attributes). Section 2.3 shows the link between attributes and the desired functions of the product. Section 2.4 shows how multiple functions are dealt with (approach (ii) in Introduction section). Sections 2.5 and 2.6 detail how approaches (ii) and (iii) are implemented in the algorithm.

2.1. Covered additions and treatments

The database is designed to include the following types of processes:

- Structural transformations, i.e., superficial heat treatments, mechanical treatments like shot peening, …
- Diffusion treatments, like nitriding or carburizing.
- Conversion layers, like anodizing, phosphating, …
- Coatings, like thermal spray, PVD, CVD, electroless and electrochemical coatings, …

In the case of structural transformations, *additions* are mechanical or thermal. In the other cases, additions are chemical as well. The combination of additions and processes is named *treatment* in this paper.

2.2. Covered attributes

A distinction is made between the attributes of individual additions, the attributes of the process, the functions of the obtained treatment and the functions of a sequence of multiple treatments.

Attributes are expressed in a database, τ, while the questions to the user and the algorithm determine the functions of the treatments that depend on the end-use. In the case of multiple treatments, the function of the same treatment can change, depending on its position in the sequence. For instance, phosphate conversion layers can be used as a solution to reduce friction, when it is used as a top coat, while it is an adequate undercoat for painting.

Attributes of individual additions and *attributes of processes* are given on the left side of Fig. 1. An attempt was made in separating the two kinds of attributes in distinct tables, to save space. However, it leads to a complex database management, with various exceptions. For instance, for diffusion treatments, diffusing boron or nitrogen into steel is not made at the same temperature. In present database, these attributes are entered case per case (Table 1).

A particular case of attribute, named *compatibility* in present paper, depends both on the addition and the process. It refers to the practical feasibility of a treatment onto a substrate or onto another treatment, respectively *treatment/substrate compatibility* and *treatment/treatment compatibility*. The second type of compatibility is inherent to the presence of combinations of successive treatments in present algorithm. For instance, nitriding can usually be made only onto steel and stainless steel. It is feasible on other metals, but in different conditions and with different properties. Classical nitriding is therefore listed as incompatible with all the substrates, except steel and stainless steel. In some cases, a treatment is not feasible on a material, but a solution consists in inserting another layer between them, often named bond coat. For instance, plasma sprayed zirconia is listed as not feasible onto steel, but a NiCrAlY coating is listed as a solution to this incompatibility (Table 2).

Most attributes are given in a Boolean way. Quantifying the quality of a treatment in a given function is extremely complex if the treatment is a building block of a multiple treatment. For instance, ranking multiple treatments with respect to corrosion or wear resistance requires physical laws that do not exist yet.

2.3. Covered functions

The final *functions* for the multiple treatments are listed on the right side of Fig. 1 and connected to relevant attributes.

Functions that involve transport phenomena play a special role: since multiple treatments generate highly textured materials, the queries must express the direction of transport, perpendicular or parallel to the surface. When it comes to barrier properties, we assume that the barrier property applies perpendicular to the surface (diffusion barrier, thermal insulation, electrical insulation). Enhanced transfer of matter is not included in the algorithm, but electrical and heat conduction can be either desired perpendicularly or parallel to the surface.

Similarly, in the case of corrosion resistance, a distinction is made between additions that resist to a given medium (attribute), and treatments that protect the underlying materials (function). In some multiple treatment architectures, it is sometimes adequate to put a resistant but not protective coating on top, and to provide corrosion protection in underlying treatments. Therefore, resistant additions are listed as attributes of additions, while protective treatments can be selected only among the intersection of resistant additions and treatments that lead to dense layers, without open porosity.

2.4. Solving problems with multiple functions

When the desired functions cannot be met using a single treatment, a decision must be taken to stack these functions. Since present problem considers 12 functions, random assembly of layers followed by adequate filtering requires exploring factorial of 12 generic architectures, i.e. $>4.10^8$. To simplify the problem, functions can be divided into 5 types:

(i) Functions inherently brought by the latest treatment.
(ii) Functions inherently brought by the first treatment.
(iii) Functions brought by one treatment located anywhere in the sequence.
(iv) Functions that imply a constraint on all the treatments.
(v) Functions that imply a constraint on at least one treatment.

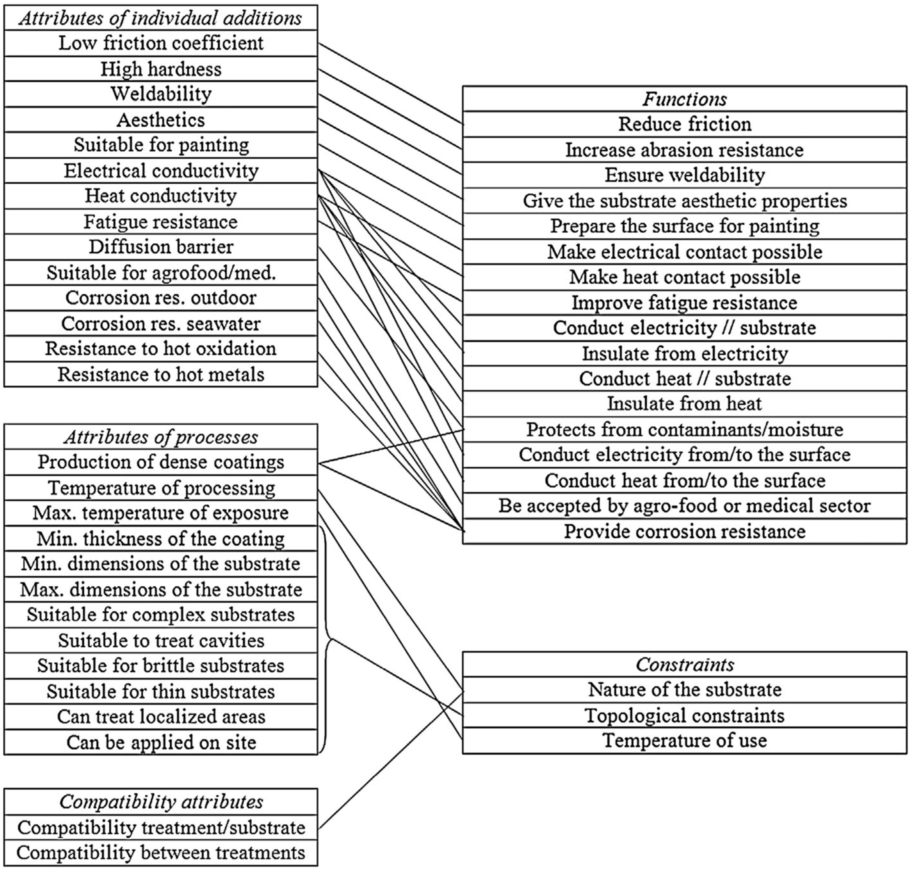

Fig. 1. Functions and attributes included in present algorithm.

Functions of type (i) are intrinsic to the contact of the component with its environment. That is, if the treatment must provide the component with a certain colour, wear resistance and the possibility to be welded, all these requirements will have to be met by the same treatment. They are denoted as "S" for "surface".

Only one function is known to be of type (ii): fatigue resistance, denoted as "F".

We limit present algorithm to four functions of type (iii):

- Thermal/electrical insulation perpendicularly to the surface or conduction parallel to the surface, denoted as "H" for "heat" and "E" for "electricity".
- Diffusion barrier, "B".
- Corrosion resistance, "C".

Functions of types (i–iii) are sketched in Fig. 2. Denoting function 1/ … /function i/function n all the functions from the outer world to the substrate, denoting π the permutations of an ensemble, one gets the following 24 possibilities, if all these functions are required:

$$\eta = S/\pi(B/C/E/H)/F. \tag{1}$$

Functions of type (iv) include thermal and electrical conduction perpendicularly to the surface. For instance, to be able to extract heat from the substrate, all the treatments of the stack that generate heat insulating layers must be rejected from the database in preliminary to any selection.

Corrosion resistance belongs not only to type (iii), but to type (v) as well. Assuming a protection by a dense layer that does not let the corrosive medium contaminate the underlying materials (see type (iii)), further resolution must reject from the database all the materials that do not resist the medium. For instance, for the stack: S/E/C/H/F, the treatments dedicated to functions S and E must be selected only within the treatments that also resist to the desired medium. Note that the system is not yet designed to select corrosion protection layers using sacrificial mechanism.

2.5. Algorithm

The algorithm consists of the following steps:

1. *Questionnaire*: the user expresses the functions to fulfil and the practical constraints (brittle component, dimensions, expected temperature of use, …).
2. *Architecture generation*: the number of possible η is reduced, so as to eliminate unneeded functions and duplicates.
3. *Importation of database* τ.
4. *Selection of individual processes*: this consists of saving in separate tables τ_i the treatments able to fulfil each function i from η, based on the attributes listed in τ.
5. *Combination*: all the permutations of treatments from τ_i are stored in the table of solutions, denoted as σ, each line $\sigma(i)$ of which consists of a multiple treatment:

$$\sigma(i,1)/\ldots/\sigma(i,j)/\ldots/\sigma(i,n), \tag{2}$$

where $n \leq 6$ with present assumptions. Note that further steps will make possible that $n > 6$, as well as sequences of different lengths. A high number of solutions are rapidly reached: in case (1) is not simplified and 10 treatments are given in each τ_i, σ contains 24,000,000 lines.

6. *Compatibility check*: using τ, for each of the $\sigma(i,j)$, it is verified that $\sigma(i,j)$ is compatible with $\sigma(i,j+1)$. If it is true, the algorithm goes to treatment $j + 1$. If it is false, line i in σ is rejected. If it is false,

Table 1
Excerpt of table τ: attributes of the additions (yellow) and of the processes (in green). For Booleans, “x” indicates that the treatment possesses the attributes. “−x” stands for the opposite property.

Nr.	Addition	Process	Low friction coefficient	High hardness/Wear resistance	Weldability	Suitable for aesthetic applications	Suitable for painting	Electrical conductivity	Heat conductivity	Fatigue resistance	Diffusion barrier (H2O, O2)	Suitable for agrofood/medical appl.	Corrosion res. in outdoor atmosphere	Corrosion res. in seawater	Resistance to hot oxidants	Resistance to molten metals	Production of dense coatings	Temperature of processing	Max. temperature of exposure	Min thickness (μm)	Min. size of the substrate (m)	Max. size of the substrate (m)	Suitable for complex substrates	Suitable to treat cavities	Suitable for brittle substrates	Suitable for thin substrates	Can treat localized areas	Can be applied on site
1	Compressive stress	Mech. treat.		x						x								20	200	0	3 10^{-2}	5^{10-1}						x
2	N	Diffusion (nitriding)		x						x								500	700	10	0	1000	x	x	x			
3	B	Diffusion (boriding)		x							x					x	x	900	900	10	0	1000	x	x	x			
4	C	Diffusion (carburizing)		x														900	900	10	0	1000	x	x	x			
5	Zn	Diffusion (galvanizing))						x	x				x	x			x	400	400	40	0	1000	x		x			
6	ZrO2 (porous)	Thermal spray						-x	-x				x	x	x	x		300	2500	20	3 10^{-2}	1000			x	x	x	x
7	NiCrAlY (porous)	Thermal spray						x	x		x		x	x	x	x		300	2700	20	3 10^{-2}	1000			x	x	x	x
8	CrN	PVD		x							x		x	x		x	x	200	700	2 10^{-1}	0	1000			x	x	x	
9	DLC	CVD	x	x				-x	x				x	x				600	400	5 10^{-1}	0	1000	x	x	x		x	
10	Zn	Electroplating											x	x			x	100	400	1	0	1000			x	x	x	x
11	Zinc phosphate	Chemical conversion	x				x						x	x			x	100	200	2	0	1000	x		x	x	x	x
12	Organic	Painting				x							x	x				20	100	30	3 10^{-2}	1000			x	x	x	x
13	Anodizing (Al, phosp. acid)	Electrochemical conversion	x			x	x	-x					x	x				20	1750	5	0	1000	x		x	x	x	x

Table 2
Excerpt of table τ: compatibility attributes. Blue columns correspond to generic substrates. Orange columns refer to the number of treatments given in first column. "x" indicates that the treatment given in left can be done onto the treatment or material given above. Numbers inside the cells refer to the treatment than can be used to ensure compatibility. For instance, painting can be made onto aluminum if treatment nr. 13 (anodizing) is performed first.

Nr.	Addition	Process	Comp. on steel	Comp. on stainless steel	Comp. on aluminium	Comp. on nickel	Comp. on ceramics	Comp. on polymers	Comp. on 1	Comp. on 2	Comp. on 3	Comp. on 4	Comp. on 5	Comp. on 6	Comp. on 7	Comp. on 8	Comp. on 9	Comp. on 10	Comp. on 11	Comp. on 12	Comp. on 13
1	Compressive stress	Mech. treat.	x	x	x	x			x												
2	N	Diffusion (nitriding)	x	x						x											
3	B	Diffusion (boriding)	x	x							x										
4	C	Diffusion (carburizing)	x	x								x									
5	Zn	Diffusion (galvanizing))	x	x									x								
6	ZrO2 (porous)	Thermal spray	7	7	7	x	7	7	7	7	7	7	x	x	x	7	7	x			7
7	NiCrAlY (porous)	Thermal spray	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
8	CrN	PVD	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
9	DLC	CVD	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
10	Zn	Electroplating	x	x		x			x				x		x			x			
11	Zinc phosphate	Chemical conversion	10	10		10			10				x		10			x	x		
12	Organic	Painting	x	x	13	x	x	x	x	x	x	x	11	x	x	x	x	11	x	x	x
13	Anodizing (Al, phosp. acid)	Electrochemical conversion			x																x

but if τ provides a treatment σ^* that fixes the problem, Eq. (2) is replaced by:

$$\sigma(i,1)/\ldots/\sigma(i,j)/\sigma^*/\ldots/\sigma(i,n). \tag{3}$$

Incompatibility of σ(i,n) with the substrate is solved similarly.

7. *Simplification*: in solutions where two successive treatments are identical, these treatments are regrouped. Duplicates are also rejected.
8. *Filtering candidates from* σ: solutions have to be rejected in the following situations:

(i) Type (iv) functions cannot be fulfilled: for instance, if electricity must be conducted from the substrate to the outer layer, any solution with at least one non electrical layer must be rejected.
(ii) Type (v) function cannot be fulfilled, which means that a non-corrosion resistant treatment was inserted above the corrosion protection treatment.
(iii) Temperature of any process exceeds the maximum allowed temperature of the underlying treatments or the substrate, both given in τ. For instance, this removes solutions where thermal spray coatings is performed onto organic coatings. At the same time, solutions that are thermally incompatible with the substrate are removed as well.
(iv) Temperature of use exceeds the maximum allowed temperature of any treatment.

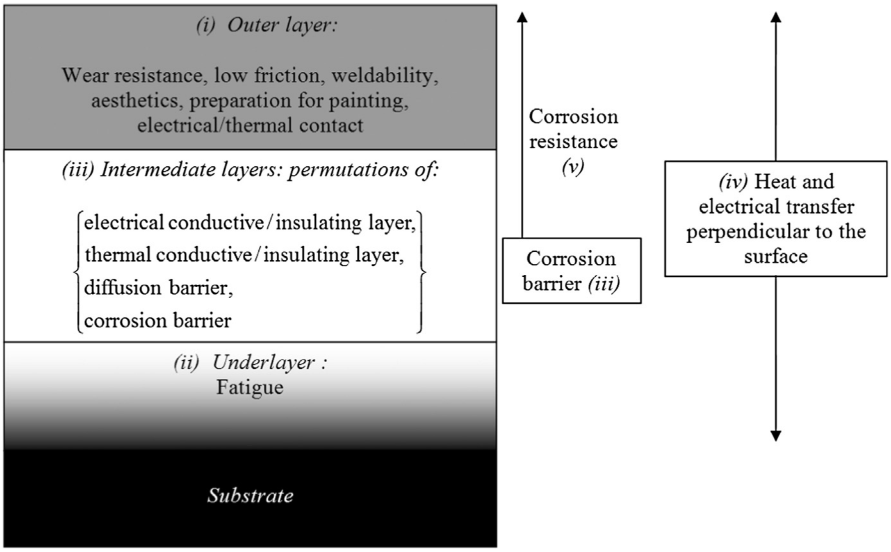

Fig. 2. Generic multi-treatment architecture.

(v) Total thickness (i.e., the sum of the minimum thicknesses of the individual layers given in τ) is superior to the maximum desired by the user, if expressed.
(vi) Other practical constraints expressed by the user are not met by at least one layer: the medical compatibility, topological considerations (size of the component, complexity of the shape, presence of holes) or the way the substrate should be handled (fragile, necessity to perform a treatment on a limited area or on site).

9. *Ranking and output*: solutions are ranked according to the number of necessary treatments or the number of necessary contractors and printed using "/" as a separator.

2.6. Implementation

Present programme is the complete reengineering of a previous expert system, where the present stacking rules were not implemented yet [33]. Briefly, it is composed of the following components:

- A table "τ", similar to Tables 1 and 2, extended to 46 treatments.
- A database search algorithm, described in Section 2.5.

To better focus on the selection process, and to make the system easy to improve within the community of surface engineering, the programme is written in Matlab, while the tables are written in Excel (Fig. 3). It is run for three examples that are detailed in the next section.

3. Results

3.1. Example 1: automobile body corrosion protection

An automobile body has to be protected against corrosion and is generally painted for aesthetic purpose. The system is questioned for a treatment that improves seawater corrosion resistance and aesthetic properties, for a thin substrate in ordinary steel, with a typical length of 4 meters, facing up to 60 °C in use. Architecture (1) simplifies to:

$$\eta = S/C \tag{4}$$

σ contains 75 solutions. Some of them clearly need the intervention of more than two workshops and are not presented. In this application, the last layer is particularly important in terms of colours and solutions that finish by aluminium anodizing, TiN obtained by PVD, bronze or brass, black chromium and chromate do not give all the desired flexibility. Only the most convenient ones are given below:

```
σ =

Organic (Painting) //CrN (PVD) //SUBSTRATE
Organic (Painting) //Zinc phosphate (Chemical conversion) //Zn (Electroplating) //SUBSTRATE
Organic (Painting) //TiN (PVD) //SUBSTRATE
Organic (Painting) //Si3N4 (PVD) //SUBSTRATE
Organic (Painting) //PTFE (PVD) //SUBSTRATE
Organic (Painting) //NiCrAlY (after high temp. exposure) (Thermal spray) //SUBSTRATE
Organic (Painting) //Ni-P (Electroless plating) //SUBSTRATE
Organic (Painting) //Ni (decorative) (Electroplating) //SUBSTRATE
Organic (Painting) //Ni (technical) (Electroplating) //SUBSTRATE
Organic (Painting) //Cr (black) (Electroplating) //SUBSTRATE
Organic (Painting) //Cr (hard) (Electroplating) //SUBSTRATE
Organic (Painting) //Zinc chromate (Chemical conversion) //Zn (Electroplating) //SUBSTRATE
Anodizing (Al, phosp. acid) (Electrochemical conversion) //Al (PVD) //SUBSTRATE
TiN (PVD) //SUBSTRATE
Bronze or brass (Thermal spray) //NiCrAlY (after high temp. exposure) (Thermal spray)//SUBSTRATE
Cr (black) (Electroplating) //SUBSTRATE
Zinc chromate (Chemical conversion) //Zn (Electroplating) //SUBSTRATE
Aluminium chromate (Chemical conversion) //Al (PVD) //SUBSTRATE  (Electroplating) //SUBSTRATE
Aluminium chromate (Chemical conversion) //Al (Thermal spray) //SUBSTRATE
```
(5)

Some of these remaining candidates implying PVD coatings are likely to fulfill the desired functions. However, they are challenged by more affordable solutions, consisting of painting onto phosphated zinc. Nickel and chromium obtained by wet processes are also proposed as underlayers for painting, but the adhesion of painting is less clear in these cases. To conclude this example, the algorithm is successful in finding reasonable

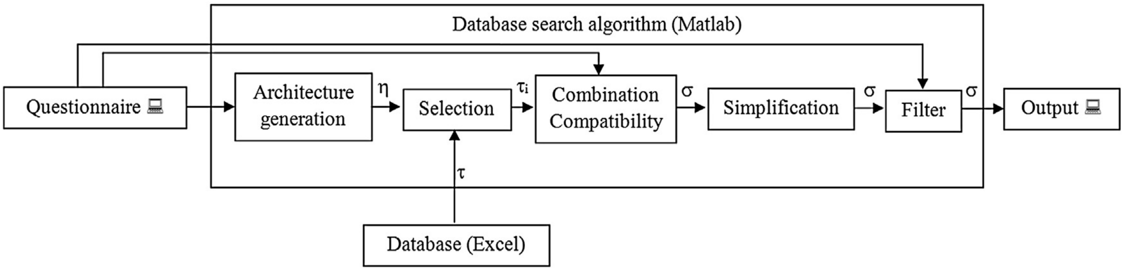

Fig. 3. Algorithm architecture.

solutions. However, more complex demands (on the final color) or constraints (on the available workshops) are necessary to help the user in the final choice.

3.2. Example 2: electrical packaging

Several electric and electronic applications are covered by present algorithm. Let us consider packaging aimed at containing electronic devices that need protection against electromagnetic fields. Such an electromagnetic shielding can be obtained using one electrically conductive layer to conduct electrons parallel to the surface. Since it does not need any connexion to another electrical circuit, it is not mandatory to put that function as a top coat.

Zhitomirsky et al. [34] proposed to design such an electromagnetic shield with the additional function of wear resistance. Imposing high hardness and at least one electrically conductive layer, one gets, for a thin polymeric substrate of maximum 50 cm length and a maximum allowed temperature of 80 °C in use and 250 °C during treatment:

$$\eta = S/E. \tag{6}$$

And 32 solutions, among which the following that can mostly be processed inside one single workshop:

σ =
CrN (PVD) //Cu (PVD) //SUBSTRATE
CrN (PVD) //Au or Ag (PVD) //SUBSTRATE
CrN (PVD) //Al (PVD) //SUBSTRATE
CeO2 (PVD) //Cu (PVD) //SUBSTRATE
CeO2 (PVD) //Au or Ag (PVD) //SUBSTRATE
CeO2 (PVD) //Al (PVD) //SUBSTRATE
TiC (PVD) //Cu (PVD) //SUBSTRATE
TiC (PVD) //Au or Ag (PVD) //SUBSTRATE
TiC (PVD) //Al (PVD) //SUBSTRATE
TiN (PVD) //Cu (PVD) //SUBSTRATE
TiN (PVD) //Au or Ag (PVD) //SUBSTRATE
TiN (PVD) //Al (PVD) //SUBSTRATE
ZrN (PVD) //Cu (PVD) //SUBSTRATE
ZrN (PVD) //Au or Ag (PVD) //SUBSTRATE
ZrN (PVD) //Al (PVD) //SUBSTRATE
Ni-P (Electroless plating) //Cu (Electroplating) //Ni-P (Electroless plating) //SUBSTRATE
Ni (technical) (Electroplating) //Cu (Electroplating) //Ni-P (Electroless plating) //SUBSTRATE
Cr (hard) (Electroplating) //Cu (Electroplating) //Ni-P (Electroless plating) //SUBSTRATE (7)

Various combinations of wear resistant PVD coatings and conductive PVD coatings are proposed, in agreement with Zhitomirsky's work. Using wet processes, wear resistance can be obtained using nickel or chromium coatings, while copper can provide the component with electrical conductivity. However, a nickel underlayer is needed to improve adhesion, reason why triple treatments are proposed. Assuming that the electrical conductivity of nickel coatings is sufficient would lead to single nickel plating, with the limitation that nickel is prone to tarnishing.

3.3. Example 3: mould for aluminium die casting: thermal fatigue

Moulds and other devices used to process components in aluminium or other light metals are exposed to aggressive conditions that include corrosion by molten metal and thermal fatigue. Thermal fatigue consists of the fast and repeated exposure of one side of the substrate, typically hot work tool steel in this example, generating repeated thermal stress and mechanical fatigue. The phenomenon is aggravated by higher temperatures that reduce mechanical resistance.

Thermal fatigue can be solved in two different ways: by treating the substrate specifically for fatigue resistance or by adding a thermally insulating layer. Substrate is made of hot work tool steel. Maximum component size is 1 m and maximum long term service temperature is 700 °C.

The possible architectures are:

$$\eta = C/H \text{ or } H/C \text{ or } C/F. \tag{8}$$

21 solutions reduce fatigue and 32 reduce thermal shocks. Solutions involving thermal spray and PVD technologies were rejected due to the fact that workshops are generally not specialised in both. A first group of solutions consists of “duplex” treatments, consisting of a corrosion resistant PVD coating onto a nitriding treatment:

$$\begin{array}{l}\sigma = \\ \mathrm{CrN(PVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \mathrm{CeO2(PVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \mathrm{TiN(PVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \mathrm{Si3N4(PVD)//N(Diffusion(nitriding))//SUBSTRATE.}\end{array} \tag{9}$$

Such solutions were extensively studied in literature, especially in the cases of TiN [35–37] and CrN [38–41](Fig. 4). They are extremely convenient, because plasma nitriding can be performed inside PVD chambers before nitride coatings. The following group of solutions follows the same family of architectures:

$$\sigma = \begin{array}{l} \text{B(Diffusion(boriding))//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{NiCrAlY(after high temp. exposure)(Thermal spray)//N(Diffusion (nitriding))//SUBSTRATE} \\ \text{NiCrAlY(after high temp. exposure)(Thermal spray)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{NiCrAlY(after high temp. exposure)(Thermal spray)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{NiCrAlY(after high } \textit{temp}\text{. exposure)(Thermal spray)//Ni–Cr–B–Si alloys(Thermal spray)//SUBSTRATE .} \end{array} \qquad (10)$$

The first solution assumes that thermally sprayed chromium steel improves fatigue resistance, and that boriding can be performed on such a treatment. The other solutions assume that in oxidizing conditions, NiCrAlY coatings are covered by an alumina layer that resists molten metal. The relevance of these architectures is uncertain since there is no feedback in literature.

By coating corrosion protection treatments with insulating coatings, one gets (again, combinations of PVD and thermal spray were removed):

$$\sigma = \begin{array}{l} \text{ZrO2(porous)(Thermal spray)//NiCrAlY(porous)(Thermal spray)//B(Diffusion (boriding))//SUBSTRATE} \\ \text{ZrO2(porous)(Thermalspray)//NiCrAlY(after high temp. exposure)(Thermal spray)//SUBSTRATE} \\ \text{Alumina(tech.)(Thermal spray)//B(Diffusion(boriding))//SUBSTRATE} \\ \text{Alumina(tech.)(Thermal spray)//NiCrAlY(after high temp. exposure)(Thermal spray)//SUBSTRATE} \\ \text{CeO2(PVD)//B(Diffusion(boriding))//SUBSTRATE} \\ \text{CeO2(PVD)//CrN(PVD)//SUBSTRATE} \\ \text{CeO2(PVD)//TiN(PVD)//SUBSTRATE} \\ \text{CeO2(PVD)//Si3N4(PVD)//SUBSTRATE} \\ \text{CeO2(PVD)//SUBSTRATE.} \end{array} \qquad (11)$$

Solutions involving CeO_2 PVD coating as a thermal barrier are limited by the fact that PVD generally produces thin coatings that will be suitable only in particular situations. It will fail to mitigate thermal stress in massive substrates. Consequently, to discriminate between thin and thick thermal barriers, advanced rankings should be applied to every new case of thermal flows and geometry. Last solution is valid if the morphology of CeO_2 allows both functions that are somewhat contradictory: corrosion protection needs dense coatings, while thermal barrier do not. The first solution was studied in our previous work for thermal fatigue [42]. A close variant of solution "CeO_2 (PVD)//TiN (PVD)" was studied in [43](Fig. 5).

By permuting thermal protection and corrosion protection, one also gets:

$$\sigma = \begin{array}{l} \text{CrN(PVD)//CeO2(PVD)//SUBSTRATE} \\ \text{TiN(PVD)//CeO2(PVD)//SUBSTRATE} \\ \text{Si3N4(PVD)//CeO2(PVD)//SUBSTRATE} \\ \text{NiCrAlY(after high temp. exposure)(Thermal spray)//ZrO2(porous)(Thermal spray)//NiCrAlY(porous)(Thermal spray)//SUBSTRATE} \\ \text{NiCrAlY(after high temp. exposure)(Thermal spray)//Alumina(tech.)(Thermal spray)//SUBSTRATE.} \end{array} \qquad (12)$$

Again, these solutions do not seem to have been proposed yet, but are quite close to some solutions from Eq. (11).

3.4. Example 4: gears designed for wear resistance

Gears are a frequent study case for wear resistance and generally must fulfil complex requirements of sufficient hardness, as well as low friction coefficient. Very hard coatings are sometimes suggested, but their best performance cannot be exploited, due to the collapse of the substrate. The

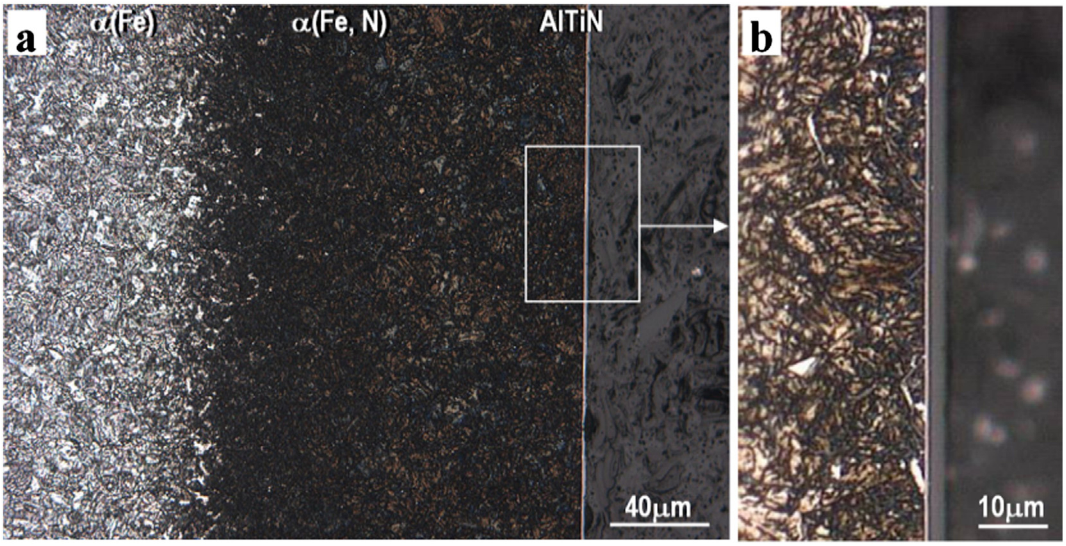

Fig. 4. optical micrograph cross section of a duplex system consisting of plasma nitriding and thin PVD coating [41].
Courtesy of Prof. Y. Birol.

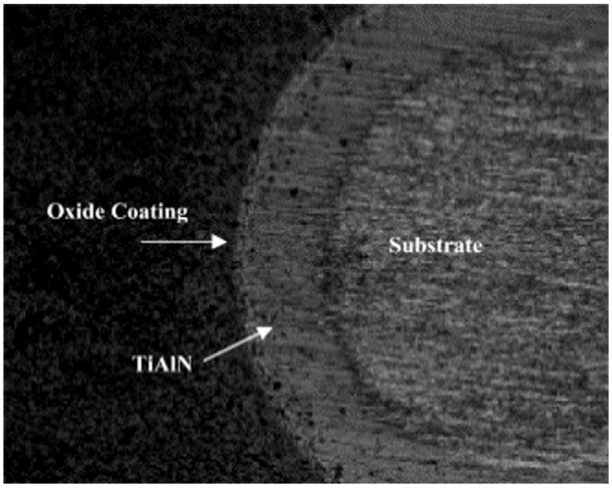

Fig. 5. Multilayer coating consisting of a rare earth insulating oxide and a nitride underlayer [43].
Courtesy of Prof. R. Shivpuri.

repeated character of the load implies the use of a treatment aimed at increasing the substrate load capacity.

The illustrated query is therefore the following: a combination of treatments on steel able to provide with low friction coefficient, high hardness and fatigue resistance. Maximum temperature during treatment is set high and the maximum dimension of the component is ~0.1 m. The proposed generic architecture is:

$$\eta = S/F, \tag{13}$$

where "S" brings low friction coefficient and high hardness in one single layer. 41 solutions are proposed. A first group is composed of the combination of a structural modification of the substrate, covered by a thin hard coating with good friction properties:

$$\begin{array}{l} \quad\sigma = \\ \text{DLC(CVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \text{TiN(PVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \text{TiC(PVD)//N(Diffusion(nitriding))//SUBSTRATE} \\ \text{Ni–P(Electroless plating)//N(Diffusion(nitriding))//SUBSTRATE} \\ \text{Cr(hard)(Electroplating)//Compressive stress(Mech. treat.)//SUBSTRATE} \\ \text{Ni–P(Electroless plating)//Compressive stress(Mech. treat.)//SUBSTRATE} \\ \text{TiN(PVD)//Compressive stress(Mech. treat.)//SUBSTRATE} \\ \text{Ni(technical)(Electroplating)//Compressive stress(Mech. treat.)//SUBSTRATE.} \end{array} \tag{14}$$

Nitriding and shot peening are often proposed as a single treatment for the gear problem [44], but are not proposed alone in this set of solutions, since they are not listed as fulfilling the low friction required in present paper. DLC deposited onto nitrided steel is however studied yet for similar problems [45](Fig. 6). Ni–P coatings are also proposed, but to fulfill the wear resistance condition, they need to be customized using adequate heat treatment. A second group of solutions is composed of at least one thermal spray coating of higher thickness, which implies additional cautions regarding dimensional tolerance. Some examples are:

$$\begin{array}{l} \text{Ni–Cr–B–Si alloys(Thermal spray)//SUBSTRATE} \\ \text{Alumina(tech.)(Thermal spray)//Bronze or brass (Thermal spray)//SUBSTRATE} \\ \text{Cermets(Thermal spray)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{Metallic carbides(SiC)(Thermal spray)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{Alumina(tech.)(Thermal spray)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{Cermets(Thermal spray)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{Metallic carbides(SiC)(Thermal spray)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{DLC(CVD)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{TiC(PVD)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{TiN(PVD)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{Cr(hard)(Electroplating)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{Ni(technical)(Electroplating)//Bronze or brass(Thermal spray)//SUBSTRATE} \\ \text{DLC(CVD)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{TiC(PVD)//Cr steel(Thermal spray)//SUBSTRATE} \\ \text{TiN(PVD)//Cr steel(Thermal spray)//SUBSTRATE.} \end{array} \tag{15}$$

The first solution of Eq. (15) is rather simple and is justified by the fact that Ni–Cr–B–Si coatings own the three required properties at the same time. It was proposed yet for similar problems, but as functionally graded layer combined with WC [46,47]. The other solutions consist of a top coat that combines low friction and high hardness, and a bond coat that provides the surface with fatigue loading resistance. Some of the other proposed solutions (not shown) combine three treatments or are likely to be very complex to implement in practice, like diffusion treatment onto thermally sprayed coating.

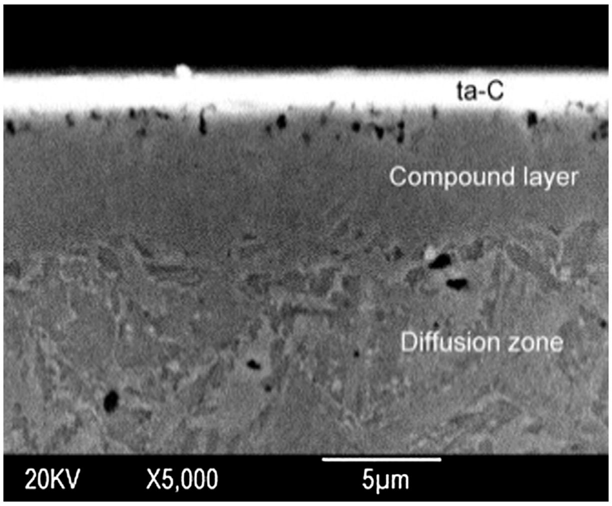

Fig. 6. Duplex treatment consisting of amorphous carbon (ta-C) and nitriding layer (here with precipitation of iron nitride), to increase the load carrying capacity of steel and reduce friction [45]. Courtesy of Prof. B Podgornik.

4. Discussion

Previous examples show that existing practices for multiple surface treatments are particular cases of proposed algorithm that is moreover able to propose alternatives. However, the number of solutions is relatively high: an increase of the database size would make complex to sort the solutions manually. For instance, sequences implying thermal spray, PVD and again thermal spray are of little practical interest due to costly transfers between plants. For a bigger database, they might be automatically eliminated by regrouping processes into typical workshops where they are likely to be present simultaneously, and by counting for each solution how many workshops are visited.

However, more advanced filters would be useful. In example 1, the common solution consisting of phosphating a zinc layer does not seem to be the simplest one, except for workshops equipped with zinc coating and painting facilities at the same time while titanium nitride obtained by PVD technology seems to be a better solution. More precise questions should be asked, i.e., in this case, about the need to finely tune the colours of the car, to select one of these options. Another way of solving the problem would be a fast cost or environmental assessment. This is more complex in terms of data collection, since the cost of surface treatments strongly depends on practical parameters like the size of series or the availability of equipment, and since it should be rigorously expressed per unit of service (i.e. increasing the substrate lifetime of 1 year) instead of surface area. A last solution would be that the used fills in his/her own database, reduced to his usual subcontractors. This would automatically lead him/her to a short list of easily available treatments.

In example 3, and even after afore mentioned sorting, the proposed treatments cannot be assessed in a trivial way. Regarding thermal fatigue, performance indexes must account for time and space characteristics of every problem and should be applied via separate modelling tools, in a second step, using results from present work.

While developing the database, care should be given in order to avoid factorial multiplication of close sequences. In above examples, we avoided to split PVD into magnetron sputtering, evaporation, … , or to split CrN into all the existing doped CrN coatings. Such a multiplication leads to a factorial increase of the number of solutions that current filters are not able to discriminate. Nevertheless, in order to promote a specific family of processes, say thermal spray, and to compare it with other families, it would be acceptable to increase the number of processes (here, flame spray, HVOF, …) or variants of them (thick and thin coatings listed with distinct attributes) and to add adequate filters able to discriminate between these particular technologies.

To ensure completion of the database, simplification was necessary for functions and attributes. For instance, adding specific corrosion modes, like corrosion by sulphurs, would generate problems to find data for the attributes of all the additions and subsequent gaps in the database. Similarly extreme differentiation between substrates would not add much to the system. Most attributes must be expressed as Booleans, since available metrics do not easily compare treatments, especially regarding wear and corrosion.

5. Conclusion

A database search algorithm aimed at selecting not only materials and processes, but also combinations of them to meet several incompatible functions, was developed, using surface treatment technologies as an example. This tool is not limited to a family of technologies or applications. It can be tailored to account for an increased number of possible queries.

Logics relies on the generation of an architecture of functions, based on the users queries and the selection of individual layers based on mostly Boolean attributes listed in a database. Filters that usually discriminate surface treatments with each other are also implemented. Classical multilayer designs could be efficiently found by questioning the system that should be completed by elaborated ranking tools:

- A physical one, that would need numerical data and physical laws that do not exist yet, for instance, to predict and compare wear rates for new multilayers, based on single layers attributes.
- A practical one, with data on available contractors and approximate costs.

This work offers the following perspectives:

- Creating similar heuristics for similar problems, like the selection of multiple shaping processes, or the selection of individual materials for complex walls in civil engineering.
- Multiplying covered functions, like the resistance to particular wear modes (erosion, fretting, …) or corrosion modes (use of sacrificial layers) that often impose constraints on more than one treatment.

In the latter case, the constitution of a web-based interface would make it possible not only to inform basic users about their needs in surface treatments, but also to question the most advanced ones to collect feedbacks on the solutions proposed in the database, as well as to further extend it towards additional cases. An interface asking their opinion or personal experience, typically about new corrosion modes or the compatibility between layers, would help completing the database.

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