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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.