THE PECULIARITIES OF THE METALLURGICAL DESIGN DEVELOPED THROUGH PROJECT MANAGEMENT PRINCIPLES

Prof.Tontchev N.[1], Assoc. Prof. Dimitrov D.[1] Prof. Hai Hao[2]
[1]«Todor Kableshtov» Higher School of Transport, Sofia, Bulgaria
[2]Dalian University of Technology (DUT): 大连理工大学

Abstract. *The tools for statistical expert evaluation of the influence of alloy composition elements on pre-selected quality indicators are described in order to improve the mechanical properties of the products through the prism of project management. Through the defined approach, it is possible to define a composition providing relatively best meanings of the values of the selected mechanical indices.*

KEY WORDS. SIMULATION, ANN, MODELING, OPTIMIZATION, METALLURGICAL DESIGN.

1. Introduction

At the design stage, the material selection process reflects a whole strand of material science. The traditional alloy development strategy consists of producing multiple samples with varying composition and variations in chemical composition and processing mode to define an alloy with better properties [1]. This approach, known as "trial-error" leads to high experimental costs [2]. In most cases, experimental research may be difficult, too long and unacceptably expensive. An alternative effective approach is the use of previous experience data processed into a statistical model based on a large amount of data associated with composition, processing and properties. Compared to physical models, the advantage of statistical models lies in their ability to obtain complex informative in a peculiar and effective way even when there are no well-established physical theories and models [3], [4].

We develop a system of methods for modeling the properties and optimization of the composition of different alloys. This paper attempts to point to a number of examples with the formulations of which, from various daughter projects, it is possible to develop further and improve the original idea developed in [7]. The formulated task stems directly from the subject of material science and it is already implemented for alloys of iron [7], titanium [9] and magnesium [9] base. In this regard, the graphical visualization of the basic problems of the material science – the basis of the projects for research of the relationship between properties and structure – is depicted in Fig. 1.

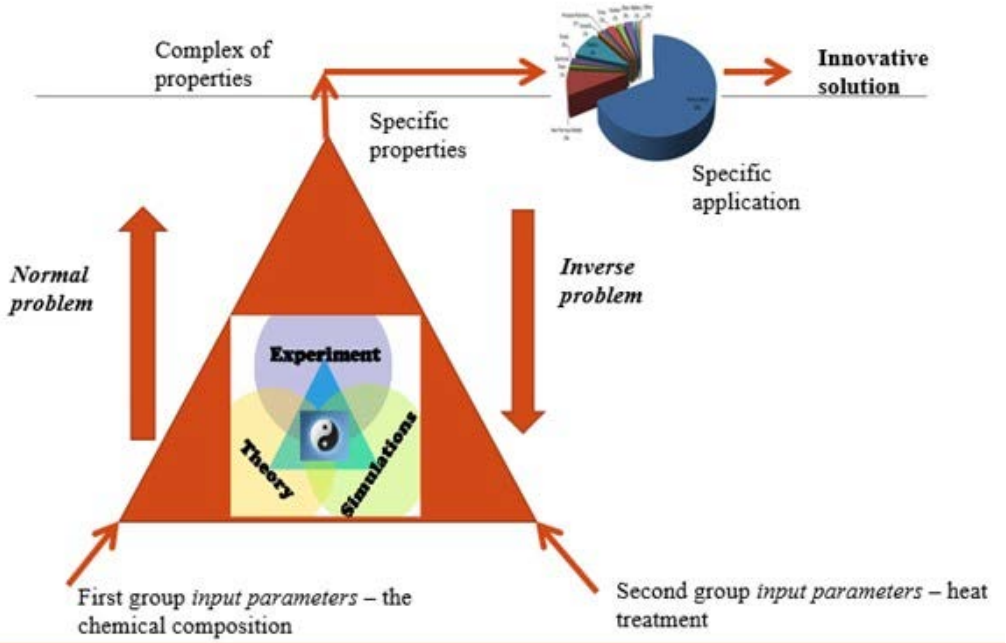

Fig.1. *Relationship between the elements of the problems and the projects from material science.*

The number of all parameters in the project is determined by the sum of the two sets of parameters (the parameters for the type, the number and the quantity of the alloying elements and the parameters of thermal, physical or mechanical impact).

The right task examines the impact of these parameters to synthesize new materials and in the inverse task and a defined and known application or characteristic values of the exploitation behavior, a rational type of material is determined with its composition and processing parameters.

The numeric metallurgical design is not only designing in the base of allying elements by type, number and quantities but also taking into account their synergistic effect. It is necessary to select such a synergistic effect by a combination of elements in which the more expensive elements are in smaller quantities. Along with the accomplishment of this task, the metallurgical design has to fulfill the desired compromise between the properties of the product, depending on the processing parameters. These several groups of parameters should form the overall processing and composition parameters. The complexity of the so formulated problem lies in the large

number of input parameters and in the fact circumstance that the chemical composition participates implicitly via the synergistic effect in the system "composition – processing – structure – properties – price.

Alloy composition design and optimization of process parameters are directly related to resolving the trade-off between measured values relative to defined selected quality indicators for a set of materials in a surveyed group or class.

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2. Classification of Material-Science Projects

The pursuit of strengthening in defining the specific purpose of a project in the field of material science is associated with its uniqueness. In this subject area, in the development of projects arising from the main task and also from "studying the relationship between the influence of chemical composition and heat treatment on mechanical properties in order to search for new applications", the projects have a unique effect because – as a result of the optimization – a new innovative solution is usually obtained (Fig.1).

The specificity of these tasks is associated with a certain complex of properties, which analyzes several criteria (different qualitative indicators, which are most often contradictory in character), and the optimization of which determines solutions that are inherently effective. This goal is defined in the literature as the SMART goal, and the meaning of this abbreviation is described and explained in more detail in the table below.

Table 1. *Defining the SMART-goal abbreviation*

S	**S**pecific
M	**M**easurable
A	**A**chievable
R	**R**ealistic
T	**T**imed

The specificity of such projects is a consequence of the subject matter of the material science from which the basic relationship "structure-properties" derives. For the definition of qualitative indicators (most often mechanical characteristics) there are standardized methodologies that guarantee a measurable quality result. Many examples from our previous experience prove that the objectives of such a project are achievable. They depend on the database used, and the result of the project is to apply authoring methods that can determine chemical compositions outside the database to exceed the mechanical performance of the database. In this sense, the purpose of the project is realistic.

Determining the project over time depends on the volume of tasks set such as the size and the number of research quantities, and the organization of the implementation of the key activities. The main focus of this organization is at the stage of experimental testing of the prescribed compositions, which are determined by the application of the methodology as optimal.

Since the process of formulating the goal is not an easy process, there are projects that start with an undefined purpose. There is a certain categorization in this sense, which is presented in Fig. 2. It – besides an established or unsettled SMART goal – has also been implemented through known and unknown methods and technologies that will be implemented during the implementation of the project.

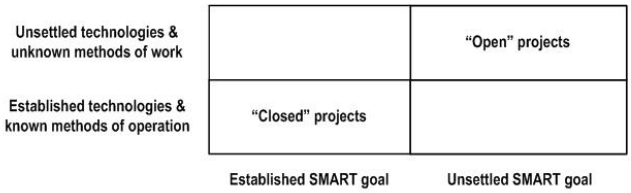

Fig.2. *Classification of projects for clarified goals and used technologies*

"Closed" projects are standard and routine projects. They are most likely to be successful and their performance is associated with the least risk. However, in any organization there is a "narrow" place, shaped as a project where the goal is difficult to be determined and the technology for its solution is unknown.

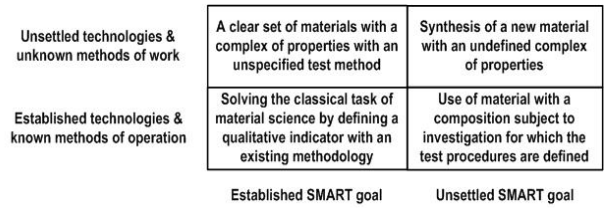

Fig.3. *Specifying the classification from Fig.1 for projects in the field of material science*

In this sense, the project team has never solved such problems, and these projects are called "open" because the issue is open to both the goal and the technologies and methods to be used. The organization balances its activity by accepting to develop both "open" and "closed" projects. "Closed" projects are implemented in a short-term perspective, but similar projects are also being implemented by competitors so they are not very lucrative.

Fig.3 presents a specific application of the above Classification for Material Science projects to elucidate the structure-property relationship in order to provide a more rational application.

In the discovered project of the type described, there is a partial requirement for the material group and the conditions for the operational work in which the workpiece/product will work are known. If it is on a metal base, it is possible to apply a solution theoretically developed by the cited project, consisting of the following:

The existing system of numerical methods, by means of which it is possible to determine optimal thermal processing compositions and parameters, associated with a pre-search complex of properties. Various iterations, specifying shape and size, are performed with CAD / CAE system calculations. The search object in the project does not appear in the CAD system database. The calculations are performed with the material closest to the research class. On the basis of the strength calculations the complex of properties is determined. If there is no standardized test in the **set** of properties, a methodology is developed and experimental research is performed. Project calculations provide optimal formulations for the desired complex of properties. These compositions are validated as being appropriate after an experimental check. Following the verification, the database can be supplemented with the newly defined compositions.

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calculations are performed with the material closest to the research class. On the basis of the strength calculations the complex of properties is determined. If there is no standardized test in the set of properties, a methodology is developed and experimental research is performed. Project calculations provide optimal formulations for the desired complex of properties. These compositions are validated as being appropriate after an experimental check. Following the check, the database with the newly defined compilations can be added.

The Project Life Cycle is related to the full set of stages (phases) of the project, the definition and number of which define the technology of production and the control needs of the organizations involved in the project.

"Open" and "closed" projects differ in their lifecycle approaches. Each project is fragmented in steps. Defining the lifecycle of the "closed project" bears the name "waterfall", because the tasks are done in a top-down sequence and it resembles a cascade of water.

The example of the "closed" project authorizing the classical task "chemical composition – property" according to an approved methodology of the tested indicator is defined by the following phases of the "waterfall" life cycle:

1.Start the project.

2. Collecting existing experience, described by experimental data, expressing the relationship between the different chemical elements of the alloy and the

3.Data processing to obtain a regression [model] or neuronal model.

4. A single-criterion optimization of the derived model, resulting in a composition, guaranteeing an optimal value of the studied property.

5.Experimental examination of the theoretically determined composition.

6.Final of the project with a specified optimal chemical composition.

The definition of the waterfall life cycle model is related to the definition of the main project parameters (content, time, price cost and thus it determines the start of the project. Planning takes place for each project, and some of the phases can be run in parallel. The model is effective when it has a high degree of certainty.

However, the algorithm for "open" projects is [somewhat] different. The first necessary condition is to take steps to clarify the goals and technologies under which these projects will be implemented. However, this condition is not always possible to fulfill in conditions of great uncertainty and a constantly changing external environment. In this case, the "waterfall" life cycle ceases to work. If it is applied, time and resources may be lost and when the project finishes, it can be ascertained that the results obtained are not needed by our applicant.

For open projects where there is a large uncertainty, an iterative life cycle model is being developed. This model involves breaking the content of the project into small iterations. The end of each iteration is controlled by the applicant who has a feedback on the execution of the corresponding intermediate state. Then work continues and begins the next iteration, which in a certain sense is another mini project at the end of which a feedback from our applicant is expected again.

The result of the last stage may be unsatisfactory, which means it is possible to go back [with] a step back before proceeding with the new iteration. After a certain number of iterations, the applicant is fully satisfied with the outcome and this determines the end of the project. This result is ensured at all stages of the project. The end of the project was unknown and it was determined in the course of the work. The great advantage of the iterative approach is to work with a large variability in the external environment.

The iterations ensure the improvement of the resulting product in the course of the project. Planning is performed only for the upcoming iteration. The disadvantage of the iterative approach is that re-expenditures are incurred for the individual iterations of the project itself. The team performs planned actions, some of which the applicant in the process of work may not accept, as a result, and then go another way.

The example of an iteration from the defined in Fig. 2 "open" project is limited to the following:

1. Sequential gradual clarification of the influence of individual elements of the chemical composition on the investigated properties. Determining the synergistic effect of the specified elements and selecting a combination that contains smaller quantities of costly elements. This synergistic effect should relate to the properties of the entire explored complex.

This example is typical for the application of the iterative life cycle, because the simulation uses the idea of a "trial-error" method to elucidate the effect of a combination of individual elements on a sought-after complex of properties.

3. Tools Used to Implement Material Science Projects

In the process of a numerical experiment, the solutions determining the predictive potential of the regression and neural models in the multi-criteria optimization of a number of properties are compared in varying the percentage of the alloying elements or the processing parameters.

The recommended tools are looking for and finding convergent and compromising solutions in the presence of diversity and heterogeneity of the output data. This is also done for the contradiction of the requirements to the designed objects. The influence and the interaction between the alloying elements and their synergistic effect related to the properties of the alloys and in particular their strength and performance properties are monitored.

The methodology of the research project consists of the following stages:

- Preliminary statistical analysis of the research data with visualization of the dependencies between observed quantities. This includes the determination of the basic (descriptive) statistical characteristics, the presence of a correlation of the parameters of the experimental studies.
- Simplification of the dependencies between the participating in the alloy chemical elements and its mechanical properties using neural models.

The most important task at this stage is to find an opportunity to find a possible relation between the independent parameters and the dependent characteristics in the experimental research. The statistical analysis allows determine the uncorrelated input parameters from the experiment that can be used to construct a regression model – the percentage of elements in the composition of the alloy under consideration. The limited number of observations sometimes does not make it possible to draw conclusions on the statistical distribution of the observed variables.

Then with these problems with the construction of the statistical models, approximating the influence of the predictors on the values of the result quantities, most often of Rm and A, there is a need to seek the modeling of the studied relationships with other means. To solve the specific problem, the most commonly used approach is the use of neuronal models of the "multilayer perceptron" (MMP) type. This approach is not a novelty, but it proves to be too effective in cases where classical statistical methods do not work. It allows for the compilation of approximation models in cases where the relations between the

observed values are considerably more complex and sometimes implicit.

In general, neural models are not related to statistical techniques, but they are regarded as self-contained outcomes of machine learning. However, many authors note the computational similarity of these models with the methods of statistical analysis. It is possible to use the Automatic Neural Network of the popular statistic package Statistica. It enables an experiment with more than 2000 models for each of the approximate searches, the selection being made according to the value of the correlation coefficients between the observed and the calculated result values (respectively for the learning, the test and the validation sets).

The analysis of the results of the approximation with the fixed neuronal models can be supplemented by a sensitivity analysis. The latter shows the relative importance of the predictors in the formation of the values of the resultant variables. There is a significant influence of the predictor is if its value is greater than 1.

Following these statistical techniques, it is recommendable to use a Pareto front, which is an established traditional method in multi-criteria research. It makes it possible to assess the appropriateness and the expected effect of combining different preferences regarding the significance of the physico-mechanical parameters of the material, such as the tensile strength Rm and the relative elongation A. The classical formulation of the task of building a set of non-dominated solutions for the multi-criteria selection has the following appearance:

- Basic optimization task - presented in the following form:

$$\max(f_1(x), f_2(x),..., f_m(x)), \quad (1)$$

where:

$f_1(x), f_2(x),..., f_m(x)$ are the private optimization criteria (physico-mechanical characteristics of the material);

$$x \in D \subset R^n, m \le 2, x = (x_1, x_2,..., x) \quad (2)$$

are the conditions defining the decision domain D of the solution vector $x=(x_1,x_2, \ldots, x_n)$. In the specific problem the definition area is set in the form of interval limits:

$$D: x_k \in [l_k, h_k] \subset R, \ k = 1,.., n, \quad (3)$$

where l_k and h_k are respectively the lower and upper bounds of the change interval of each of the arguments (percentage of the chemical element in the material)

- The relation of dominance between a pair of solutions $x^{(1)}$ and $x^{(2)}$ ($x^{(1)} \prec x^{(2)}$) - is expressed as follows:

$$\forall i = 1,..., m \ \ f_i(x^{(1)}) \ge f_i(x^{(2)}),$$
$$\exists j = 1,..., m \ \ f_j(x^{(1)}) > f_j(x^{(2)}). \quad (4)$$

The dominance of $x^{(1)}$ versus $x^{(2)}$ exists when at least one of the criteria has strict inequality (with the indicated orientation) for the two alternative solutions, and for the other criteria is in effect non-steady inequality (or at least equality) .

The Pareto- optimal set is a set of solutions $P^* \subset D$ that are not dominated by any element of the D set. The Pereto-front can be graphically displayed in the space of the considered criteria $f_i(x)$.

The implementation of this experimental-computational approach requires the preliminary ~~study~~ research of the experimental data in order to obtain approximating quantitative relation~~ships~~ between them and subsequently to include the established dependencies in a suitable optimization algorithm.

The steps involved in conducting the research are as follows:

- Creation of approximation models linking the parameters of the alloy composition with the resulting physico-mechanical parameters;
- Selection of a suitable algorithm for building a Pareto front;
- Incorporating the aproximation models into the algorithm and realization as a programming tool.

All numerical approaches for the metallurgical design are set out in [7]

4. Conclusion

An approach has been described to offer a realistic opportunity to significantly reduce the cost and time to predict chemical concentrations for multiple properties of a class of alloys and technological processes so that under new conditions these materials have better properties. The obtained results from our previous research have shown that the proposed methodology can be fully used to determine the essential relations between the extreme values of the mechanical parameters of the investigated alloys.

Any addition to the experimental measurement database would allow the software model to be refined and further refine the results. The proposed approach and established dependencies can be used in engineering practice.

References:

1. Campbell C.E., G.B. Olson, “System design of high performance stainless steels I, Conceptual and computational design”, Journal of Computer-Aided Materials Design 2001, 7:145-17
2. Vitos L., P.A. Korzhavyi and B. Johansson, "Stainless steel optimization from quantum mechanical calculations", Nature Materials 2003, 2:25-28
3. Jones, J. , MacKay, D. J. C., "Neural Network Modeling of the Mechanical Properties of Nickel Base Superalloys", 8th Int. Symposium on Superalloys, Seven Springs, PA, eds. R. D. Kissinger et al., published by TMS, 1996, pp. 417-424.
4. Fujii, MacKay, D. J. C. and Bhadeshia, H. K. D. H., "Bayesian neural Network Analysis of Fatigue Crack Growth Rate in Nickel-Base Superalloys”, ISIJ International, Vol. 36, 1996, pp. 1373-1382.
5. Borst R. de, “Challenges in computational materials science: Multiple scales, multi-physics and evolving discontinuities”, Computational Materials Science 2008, 43:1-15
6. Fischer C.C, K.J. Tibbetts, D. Morgan and G. Cedar, "Predicting crystal structure by merging data mining with quantum mechanics", Nature Materials 2006, 5:641-646
7. Tontchev N. Materials science, Effective solution and technological variants. Lamber, 2014.
8. Razmov T., D. Dimitrov , Laboratory Exercise and Course Design on "Project Management" - Third Edition, Todor Kableshkov University of Technology, 2012.
9. https://www.researchgate.net/profile/N_Tontchev/contributions