SOME NOTES ON THE OPTI MIZATION OF CHEMICAL COMPOSITION IN THE F IELD OF MATERIAL SCI ENCE

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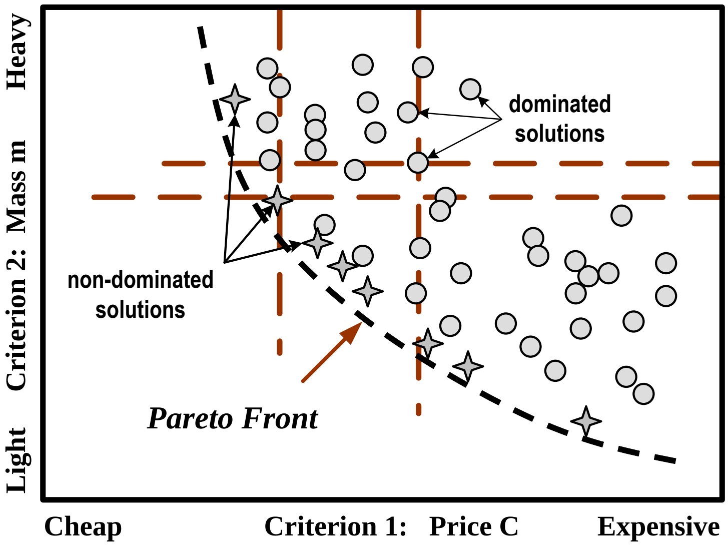
Efficiency and effective solutions are a frequent theme in literature and in our practice. Many research teams worldwide work and strive to offer innovative solutions. These important human activities can not take place without optimization. Materials science, in which I work is a source of optimization problems. This is dictated by the object which it explores.

The set of material properties is dependent on the chemical composition and also on the processing technology. This set includes strength and plastic indicators that are inherently contradictory. This determines the specificity of the optimization problems that are solved in the field of materials science. These problems are of multicriteria nature the solutions of which seek strategies to satisfy the experts, designers, technologists and users.

Since the second half of the 19th century compromise solutions are visualized in the plane in the same way together with effective, unbetterable and non-dominated solutions determined by Pareto fronts.



I present such graphic interpretation in this sense to your attention. In recent years, the University of Cambridge includes this curve in the course of materials science; along the axes / the ordinates / we have the weight and the cost of the possible alternatives. Various solutions compete on the basis of reliable and lightweight materials at lower prices. In the case when considering just these two criteria of the product and it is not possible to reduce its mass, then it is not possible to decrease the production cost, too.

Today I will use this curve to describe the concept of our research. Rational doping, determining the amount and the type of different alloying elements directly affects the price of fusing and the strength of the alloy. The higher strength of the alloys is a condition to reduce the carrying section of the piece / product thus reducing its mass. The smaller mass in the [context of the] automotive industry means less fuel and less pollution. From this point of view we have the relevant problem of the composition and to the contradiction between the mass and the cost is added another contradiction: the one between the strength and the ductility. The solutions of this concept lead to the creation of tools for a whole class of problems in the field of materials science. My explanation is that this class of problems is fundamental because it serves directly the subject of materials science, namely the formalized relationship between the composition and the properties of alloys.

The design stage is inconceivable without the choice of the material. In this respect, I happened to mention the University of Cambridge because there was elaborated the best to-date software for the selection of material. This tool has exceptional benefits; besides the choice on the various criteria, the material is evaluated by type, size of the load and the shape of the product. Considerable attention has been paid to the classification of all types of engineering materials discussed on various features / criteria. Various competing agents are indicated for which different assessments are made. The only bottleneck in this achievement is that the software may indicate materials just and only from the database that requires continuous expansion.

What is presented and what is done in the research which today is the object of our discussion? Using the information from an existing database algorithms, methods and software are developed to improve controlled properties by Pareto optimization. This can be done at the level of chemical composition and due processing; the result will be a representative of the class with better controlled characteristics. With these procedures it is possible to identify solutions which, when tested in practice to fill a variety of databases. In this regard, this research can be treated as a pilot one applied to the class of magnesium alloys. The developed and demonstrated in the research procedures, and the included criteria, too are independent of the used database.

I present the multicriteria model for analysis of tasks in the field of materials science. Performing the specialty of this kind of "black box" the concept may be implemented by two mechanisms: the regression models and the neural networks. It consists in the creation of sufficiently reliable software tools with which to determine the chemical composition and the technological parameters of the system that provide pre-set requirements for strength and ductility.

It states that when modeling the material properties of iron-based materials, as a function of the chemical composition it is possible to determine effective solutions by defining a multicriteria problem for the complex of characteristics defined by the decision maker. The arrangement of these effective solutions depending on their composition and / or the energy consumption leads to the formulation of an innovative solution.

` It has been demonstrated that it is possible to research theoretically, using the capabilities of modern computer hardware and software, the impact of various alloying elements on the value of the final properties of the product using artificial neural networks for approximations and genetic algorithms for optimization.

It has been demonstrated that there is an ability to improve the properties of a representative of a certain class of magnesium alloys via a multicriteria procedure for determining the amount of alloying elements in the alloys based on the Taguchi method, providing quality for a pair of parameters. Thus the alloy composition is refined.