Editorial

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A great number of material brands available nowadays offer new innovative possibilities in design, manufacturing and implementation of products. Manufacturing is the transformation of raw materials into products from the raw materials in various processes, using various machines and in operations organised according to a well-prepared plan. Therefore, the manufacturing process consists in a proper use of resources like: materials, energy, capital and people. Nowadays, manufacturing is a complex activity uniting people working in various professions and carrying out miscellaneous jobs using diverse machines, equipment and tools, automated to a great extent, including computers and robots, The goal of manufacturing is always to satisfy market needs of customers, according to a company strategy or an organisation being engaged in manufacturing, employing available possibilities and equipment. The technical aspect of this effort pertains to the engineering design of products.

Engineering design is connected with determining the shape of a product and its elements, the selection of materials from which they are to be made and the selection of relevant technological processes. The designed product has to meet the characteristics pertaining fully to its functionality, and also requirements connected with its shape and dimensional tolerances; moreover, the design has to include the set of materials used, manufacturing methods and other necessary information. Then engineering design of a product is not a separate activity and is to merge in itself three equally important and indivisible elements, that is, structural design (goal is to work out the shape and geometrical features of products satisfying human needs), technological design (enabling to impose the required geometrical features and properties to the particular product elements, and also to ensure their correct mating after assembly, accounting for the production volume, its automation level and computer assistance, and also ensuring

the lowest possible costs of the product), and material design (for the selection of the required physical and chemical, as well as technological properties, ensuring the expected life-time of a product or its elements).

Functional properties of the product are thus obtained only when right material is used, manufactured in a properly selected technological process, imparting both the required shape and other geometrical features, including dimensional tolerances of particular elements, making the final assembly of the product possible and also forming the required material structure, ensuring the expected mechanical, physical and chemical properties of the product. The determination of dependencies among the structure, technological processes and functional properties as well as materials selection and technological properties forming their structure and properties for employment in complex manufacturing systems feature the core interest of materials science and engineering. In the light of the presented information it is clear that in order to achieve common aims the cooperation between specialists from various fields is necessary. It is expected that such multithematic cooperation will bring synergic effects, which cannot be expected earlier.

An essential determinant of the manufacturing processes' development, giving consideration to economical and ecological conditions, is an integration in the area of advanced design and manufacturing of the up-to-date products and consumer goods, deciding the improvement of the quality of life and welfare of the societies, which encompasses the development of design methodology and connected with it newer and newer designs developed using the Computer Aided Design (CAD) methods, the development of new technologies and manufacturing processes, of technology design methodology, contemporary production organisation, operational management and quality driven management along with the Computer Aided Manufacturing (CAM), and also the development of materials engineering methodology, the development of entirely new engineering materials with the required better and better functional properties, with the pro-ecological values and minimised energy consumption along with the development of the computer based materials science and methodology of Computer Aided Materials Design (CAMD). The strategic importance of engineering materials for the future development of civilisation poses essential requirements in that area, and the cooperation with the specialists of other branches in order to achieve synergic effects and the short half-obsolescence period of knowledge in materials science, materials engineering and materials processing technology areas call for methodical and dynamical studies as well as research and development activities, along with the coordinated and systematic efforts for upgrading the general knowledge level of the engineering cadres of various special fields for fast transfer of that knowledge to the product engineering design practice and their spheres of their manufacturing and use.

There is no doubt that it is the very important role of materials selection and design in the design and manufacturing processes of new, needed products, having the highest attainable quality and performance at the optimum and reasonably set, possibly lowest cost level. The vision of the future and evaluating the development trends of various fields of activity and manufacturing processes based on visions proposed by eminent bodies consisting of scientists and futurologists is connected with forecasts pertaining to the development of various engineering materials. Nearly all of the forecasted projects will require the relevant manufacturing technologies and above all – relevant materials. Many of these materials are already available nowadays, some of them should be developed soon according to the outlined requirements. It is good to realise that many

venturous projects will be made possible if those new materials are made. The future successes connected with the introduction of better and better products into the market, satisfying the needs of the steadily growing requirements of the societies, are connected closely with the development and the implementation of new generation of engineering materials, which can be used, for manufacturing those newly expected products. The process of implementing the new materials is connected with improving the existing materials or with taking into account the contemporary achievements connected with the outworking of the new compounds, structure and ensuring the new properties.

The contemporary knowledge in the area of materials science and engineering and further investigations of many phenomena, among others, electric, magnetic, optical, mechanical, thermal ones, taking into account the mutual interactions among external factors, material structure and theory pertaining to the fundamentals of those phenomena, after using modern mathematical modelling methods, and also in using the artificial intelligence tools and other computer assistance methods along with the advanced analytical techniques and testing methods explaining materials' behaviour, especially in their nanometric and atomic scales, and in the exceptionally short time periods of femtoseconds (10–15 sec) make it possible to adjust properties of materials, including nanomaterials, biomaterials and biomimetic materials to requirements posed by their practical use. The introduction of the new generations of materials and the propagation of products with the expected properties that can be made from those materials, calls for coming to know the materials behaviour, as substances for manufacturing the new products, from their atomic/nanostructure scale, through their microstructure, up to the macroscopic one, using the advanced analytical methods and computer modelling. This strategy calls for the improvement of the conventional materials manufactured and used on a large scale, like steel or non-ferrous metals alloys, and also of the new functional materials used in smaller and smaller smart devices.

The scope of interests of materials science and engineering is unusually broad today – from metal alloys through ceramic, carbon, polymer to composite materials. Traditional materials and technologies including structural, engineering and tool ones and those which because of structure and application, for example, for work in elevated temperature or cryogenic conditions and in the corrosion environment called so far special ones although to a bigger extent interests of those concerning functional materials, for example, designed for electronics and optoelectronics, smart and adaptive, biomimetic materials including classic and also nanostructural ones and connected with nanotechnologies. The target of materials science and engineering is an investigation of the effect of their structure in various scales (electron, crystalline, micro and macro) on properties of materials. A great number of material brands available nowadays offer new innovative possibilities in design, manufacturing and implementing of products. These issues deal both with synthesis and processing of materials, their chemical composition and microstructure, phenomena and properties and connected with them the analytical and research techniques, behaviour of materials in exploitation conditions and materials design and prediction of their durability and lifetime.

The end of the 20th century has demonstrated that achievements of materials science and engineering are usually an outcome of the significant integration among various branches of science, which resulted in consequences in making the 21st century materials science and engineering an interdisciplinary area developed on the crossroads of many pure science disciplines, mostly of the solid-state physics, chemistry, mathematics and process engineering, but also mechanics and mechanical engineering, ecology, economy,

management and applied computer science, and even biology and medicine, taking advantage of achievements of those scientific disciplines to propose materials with the most advantageous set of properties and suiting higher and higher requirements posed to products and goods used by people in the best way, under conditions of fierce market competition and with high requirements concerning quality, reliability, lifetime and price. Materials science and engineering as a discipline of science develops significantly intensively nowadays and in its development and yet in a few other avangarde disciplines of science the biggest chances are seen in contemporary civilisational progress. Giving people access to products and consumer goods deciding directly the level and the quality of living, the information interchange, the education level, quality and potential of health service and many other aspects of the environment in which we live, features the profoundly humanistic mission awaiting the engineers' societies, in which the materials issues play a key role in establishing and upgrading the economical conditions of quality of living and thus decide directly possibilities of the raise of the level of societies' life.

One should estimate, in particular, that the further progress of civilisation connected with introducing new products with the required high functional properties, will be – to a great extent, synthesis conditions, exploitation conditions and the material waste disposal method in its after-service phase as well as the price-dependant issues connected with obtaining the material, its transforming into a product, the product itself and also costs of the disposal of the industrial waste and scrap as well as the modelling of all processes and properties connected with materials, feature the fundamentals of the dynamically developing computational materials science. During millenniums and also yet during 20th century materials were chosen and worked out by a process of trial and error as a matter of fact not guaranteeing an optimal solution because of a set of criteria and at the same time time-consuming and expensive one. At present the great emphasis is put on the development of methods of modelling of structure and materials properties and interrelations between them, conditions of manufacturing, processing and exploitation and the type of material and its chemical composition. Classic mathematical models, not only for statistical or even numerical ones are used, for example, using finite element method or boundary elements method and also the full set of artificial intelligence ones with neural networks, genetic algorithms or expert systems are used.

These methods are basis for intense development of computational materials science as a new scientific specialisation in the field of materials science and engineering being intensively developing materials design, not requiring usually such a range of experimental works as traditional methods and very often leading to experimental verification of calculations or predictions made in the virtual computer reality. Employing the fundamental principles of physics and chemistry pertaining to the state and properties of the condensed matter, the theory of materials is used for modelling the structure and properties of the real engineering materials and for designing and forecasting the new materials and devices with improved practical usability. The modern theory of materials science and engineering and modelling specific for the computational materials science is used for the development of new materials. Various models are employed in computational materials science, depending on scale and also possibilities of using the engineering materials modelling, their synthesis, structure, properties and phenomena. The experimental verification enables to check the computer simulation in various scales and using the artificial intelligence methods, for employing the new

materials. The introduction of new materials and the improvement of the properties of materials manufactured to date also calls for working out and implementing the new synthesis and processing methods.

Computational surface engineering, enables the selection and design of technological processes ensuring the best possible exploitation properties of surfaces of constructional, tool and functional elements made of classic engineering materials, and many times of advanced materials, without the necessity of repeating complex and expensive researches and experiments connected with the improvement of surface layers properties of structural or functional elements, and also tools created from them, develops analogically.

All issues mentioned were in the orbit of interests of the *International Journal of Computational Materials Science and Surface Engineering*. Our Journal has ambitions and at the same time hopes to accompany and document these development in both fields that is computational materials science and computational surface engineering. I think that it will attract to it the broad group of both the Authors and Readers. I do count on the promotion of these achievements in many countries of the world by the presence of the Journal in scientific and national libraries and the activity of broad multinational Editorial Board and also Fellows of the World Academy of Materials and Manufacturing Engineering and organisers of important international scientific conferences which will take advantage of the possibility of the publication of proceedings of those conferences or the best selected papers just in that Journal.

Directing to the Readers' hands the second issue of the *International Journal of Computational Materials Science and Surface Engineering*, I am convinced that it fulfils the requirements of both the Authors and Readers since the former issue dated January 2007 will ensure urgent entry of the journal to the group of the ones indexed by Thomson Institute in Philadelphia, USA. Together with the group of the closest coworkers I will make all the efforts to do it. I also hope that it will meet the acceptance of both the Authors and Readers because without them no journal can exist and if it exists, it is just for them. I would like to invite you to actively cooperate and cocreate the Journal on which we do count as the editorial team. I am convinced that we will not be disappointed and thanks to our common activeness it will happen in the nearest future.