Chapter 1

Introductory Chapter: Genome of Material for Combinatorial Design and Prototyping of Alloys

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http://dx.doi.org/10.5772/intechopen.77360

1. Material genome: New paradigm of additive manufacturing

Materials present an integral part of the additive technology (AT). The key task in creation and processing of new materials for the AT is to expand the range of such materials (including through mixing/alloying/modeling of composites), to improve their quality, to increase the additive process stability, reproducibility and reliability, including by using multimaterial powdered systems, while maintaining a low cost of materials, the process of their manufacturing and pre- and/or post-processing.

However, the development of the AT components (i.e., technologies and equipment for the powdered material manufacturing, 3D part synthesis and subsequent post-processing) without a concurrent improvement of the accompanying directions does not allow obtaining the maximum effect. The conventional cycle of the development of new materials for the additive manufacturing (AM) transition needs a revision.

In 2011, the administration of President Obama presented two breakthrough initiatives, "*MGI—Material Genome Initiative for Global Competitiveness*" and "*AMP—Advanced Manufacturing Partnership*," prepared by the USA National Council for Science and Technology [1, 2]. In the AT literature, the second initiative is mostly mentioned. Indeed, the AMP allowed the launch of a number of projects in the USA: America Makes—National Additive Manufacturing Innovation Institute (NAMII); Lightweight and Modern Metals Manufacturing Innovation (LM3I) Institute; Digital Manufacturing and Design Innovation (DMDI) Institute [3–5]. Nevertheless, the MGI initiative is no less significant. In fact, it is a set of tools that implement the iterative concept of the new material development, which allows reducing of the resource intensity (time and cost) of the material science cycle by 50% [1]. The essence of the concept consists of a continuous exchange of information at different stages of the development of new materials, not only within a single subject area (e.g., structural or functional materials), but for all the types of materials (**Figure 1**).

Along with the "America Makes" additive community [3], a self-regulating society has been formed in the United States that consolidates scientists engaged in the development and commercialization of new materials based on the MGI concept [1]. The accumulation of information (Big Data (BD)), presentation of tools for their use and creation of other tools provide a transition from quantity to quality. The principles of open architecture provide the concentration of new ideas in the MGI community. The use of block-chain technologies [6] allows ensuring of the MGI implementation under the BD using, provides the data management, guarantees their reliability and significantly improves quality due to the internal certification of future 3D AM parts.

The traditional cycle of the new material fabrication includes the following stages: (1) development of the material composition; (2) optimization of the material properties; (3) design of products from the material, including manufacturing techniques; (4) testing and certification of the material; (5) commercialization of the material.

The iterative cycle proposed within the framework of the MGI concept allows to combine separate stages in different directions so that to accelerate the achievement of the results (see **Figure 1**). In particular, the information about materials, about the AM processes and optimal regimes for the 3D parts fabrication is subject to association. On the other hand, the spatial and temporal scalability of modern methods of computational materials science should be combined with the experimental results under the searching of optimal AM regimes, that is, should find the experimental confirmation.

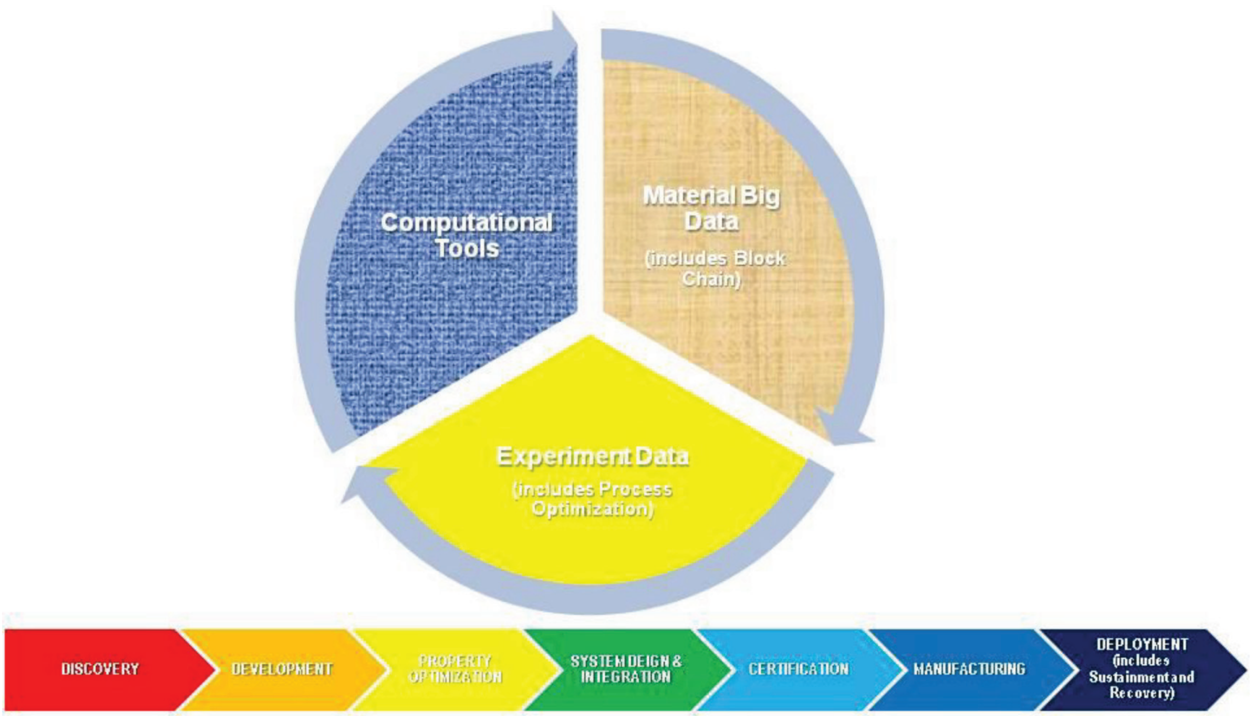

Figure 1. Additive manufacturing via material genome route.

http://dx.doi.org/10.5772/intechopen.77360

The MGI concept emergence became possible due to the advanced achievements in the information technologies (IT) over the past 10 years, namely, due to the cost reduction of the information transmission and storage, increase of the speed of transmission and processing of the information. Priority MGI trends in the AM applications are

- optimization of the development technologies for the complex high-dimensional phase spaces;
- effective methods for the experimental data analysis in order to determine the relationship between properties of different levels (e.g., between microstructure, chemical composition, processing and volume properties);
- fundamental properties of the materials behavior;
- tools for experimental data analyzing and the relationship between the experimental data and predictive modeling;
- revision of theories, modification and updating of the developed models and methods, realization of new experiments, caused by the discrepancy between the theory and new experimental data and modeling.

The MGI approaches erase boundaries between a wide range of materials both in the areas where numerical methods are already in use—structural materials, including composites, and also in the areas where they are still weakly used, for instance for soft materials (oligomers, polymers, 3D inks-jet, powders, wires, etc.).

The essence of the approaches used in MGI can be understood on the basis of the MGI Principal Investigator Meeting projects of the first and second wave conducted in the USA in 2015–2016 [7, 8].

2. MGI in high-performance metals and alloys

The MGI approaches are actively applied both in the development of structural materials and for manufacturing technologies. Depending on the property being modeled, object and process, the following levels are distinguished: atomic, micro, meso- and macrolevels, and the conditional size ranges are <A-nm, nm-μm, μm-mm, >mm, respectively. For each level, certain modeling methods are characteristic.

Atomic modeling is widely used in developing new materials and predicting their features. Here, the numerical molecular dynamics models as well as the density functional theory are used.

At the micro level, the data on the phase stability are determined as the input data for thermodynamic models used to calculate the phase diagrams and crystallization points.

The problems solved by meso-level modeling lie on the border of micro- and macrolevels. There is practically no commercial software for meso-level modeling, still a large number of user subprograms have been developed that extend the resource of standard computing packages. For this, the computational methods are used such as the phase field model, discrete dislocation dynamics, physical plasticity theory, and so on.

At the macrolevel, the problems of mechanics of continua are solved by using the finite elements methods (FEM) and finite differences method (FDM). Recently, an actively developed approach is that involving the creation of structural and multi-physical models based on the FEM [9].

It is obvious that the possibilities for the MGI use should most clearly reveal themselves in the AT, since in fact these technologies are digital manufacturing. The technologies of direct and layerwise laser additive manufacturing (LAM) make it possible to obtain products with directional anisotropy due to their ability to control the laser beam trajectory during fusion and to determine technological parameters such as laser beam diameter, linear energy density and scanning geometry. The 3D part fabrication with the areas differing by their characteristics depending on the local loading conditions becomes possible through the use of technologies of a direct laser deposition (DLD). The ability to design the topology of the macrostructure of the synthesized material is one of the main advantages of the AT in the framework of the concept for generating of smart materials. At the same time, the fused particles arrangement and their size are largely stochastic, thus leading to the material structural heterogeneity and the emergence of defects in the form of residual porosity. In addition, despite the application of the technique of the repeated remelting of the surface layer, the resulting roughness does not meet the engineering requirements. In this connection, there exist the following widespread post-processing methods for the synthesized parts that are divided into two types of technologies—volume effect technologies (hot isostatic pressing (HIP) and surface effect technologies)—that include finishing mechanical (or abrasive) treatment, electrophysical and electrochemical techniques, methods for surface layer modification. A particular attention should be paid here to the methods for predicting of the finished parts properties, taking into account their heterogeneity, as well as to the methods for correction of these properties, for example, by modifying the surface layer of products.

The development and use of the MGI methods in the AT design will improve the predicting accuracy of the material properties and of the surface layer of the parts after modification. The influence on the texture and structure will allow to form the properties of finished parts, not only in the obvious area of the surface layer microhardness increase, but also in providing an enhanced corrosion and erosion resistance; and crack resistance owing to the formation of compression stresses.

The Material Genome Initiative (MGI) offers a paradigm that perfectly matches the AM needs. The MGI is built on the base of the search of specific materials that ensure the generation of different final properties via using different processes. It connects multiple scales, from quantum and atomistic to molecular mechanics and derived potentials, mesoscale (nanometer) methods and, finally, continuum methods. The characteristics and effects of the process play an integral role in the material genome (MG). A similar approach for combining the scales and methods is suitable for the AM. In the AM, the material microstructure can be adapted to the specific requirements and needs, thus providing wide possibilities for the material design.

http://dx.doi.org/10.5772/intechopen.77360

For AT, the problems of certification and safety of the used powder materials and the received 3D products are especially relevant, since these products can work in the important mechanisms of perspective modern cars, aircrafts or missiles. Therefore, the developed approaches for the selection and storage of the data on materials and/or processes are of an extreme necessity. The monitoring of the storage conditions of all the data, codes, and discussions with graphically attached persistent identifiers, along with the low maintenance costs, is fundamental to the continuous and efficient complex operation of the whole platform.

The digital recording of code and data transformations that occur among users of the platform during their cooperative work provides new rich opportunities capable of improving the integration and operational process in all directions (including research, education, authentic knowledge transfer, manufacturing and product life cycle).

3. Combinatorial design of alloys for AM

A wide range of the AM materials and processes requires extensive researches and determination of the "process-structure-properties" relationships. For fabrication of unique structures that do not exist in nature or reproduce its best manifestations (e.g., the parts with a negative coefficient of thermal expansion or optical transmission), of metamaterials, biomimetic structures and surfaces, the problems of using the unique AT resource are of no less interest. Besides, one should also realize the AT applicability for the manufacturing of materials with multilevel hierarchical functionality on nano-, micro- and mesoscales, up to the development of the 3D-printing tools for fabrication of atom-by-atom structures and construction of additive nanofabricators [10].

The 3D combinatorial metallurgical method, called a "*Rapid Alloy Prototyping*" (*RAP*), has been recently proposed by Prof. D. Raabe with coworkers [11] and showed a successful testing on Twinning-Induced Plasticity (TWIP) steels with reduced density [12, 13], high-entropy alloys [14–16], intermetallic alloys [17, 18], high-strength martensitic [19, 20] and high-modulus steels [21]. It includes semicontinuous high-performance fabrication of the 3D parts, their heat treatment, preparation to testing, allowing to synthesize and test up to 45 material parameters within 35 h [11].

The ideas of the LAM use for fabrication of both functional and gradient alloys (FG) have been discussed for a long time [22–24]. However, in the combinatorial design of alloys by the RAP method, the LAM use provides a number of additional advantages.

First, a specific thermal regime is realized throughout the metallurgical process [25, 26]: the temperature-time profile for the samples obtained by LAM methods is rather different from those observed in a typical metallurgical manufacturing. Under layer-by-layer (3D) laser cladding, the powder material is quenched after the melting and crystallized at high speeds due to a rapid heat removal to the substrate. With the overlay of each following layer during the subsequent layers cladding, the consolidated material is repeatedly heated and even melted partially by a laser beam [25, 26]. This means that the materials produced by the LAM are subjected to a series of consecutive short-pulse temperature cycles of a decreasing intensity [25, 27]. Such cyclic heat treatment can also be used for controlling of solid-phase transformations in the material after the cladding. This is favorable for structural steels and super-alloys where the strength, toughness and hardness are ensured by the dispersion hardening also [17].

The second advantage of the LAM use for combinatorial development of high-performance alloys is that a rapid melting and solidification occur locally, within a small volume [25, 26]. This allows working with the materials that are not melting or hardly melting in an ingot, for example, oxide-strengthened alloys, or materials containing components in the amount exceeding the solubility limit in the solid solution. Typical cooling rates for the LAM are from 10^3 to 10^6 K/s [25, 26]. These high cooling speeds lead to a rapid solidification of the melt, creation of a finely dispersed structure that increases plasticity, in contrast to the coarse-grained cast structure obtained by a continuous casting [25, 27]. This proves that the LAM can serve not only as an instrument for combinatorial alloy modeling, but also ensures a qualitative expansion of options for the additive manufacturing (AM).

Third, some LAM methods are "self-adapted" for the RAP, that is, they quickly outline suitable series of applicable compositions, which is explained by the peculiarities of powder metallurgy as a production process [10, 25, 26].

For the RAP purposes, from the whole scope of the AT variety, layer-by-layer selective laser melting (SLM) or laser metal deposition (LMD) techniques can be recommended [28]. The latter is sometimes also referred to as 3D-laser-cladding (or direct metal deposition—DMD) & Laser Engineered Net Shaping (LENS). Thus, all the above said characterizes the LAM as a highly effective technology for the fast study and development of new alloys and the 3D part manufacturing on their basis.

4. Conclusion

The aim of this introductory chapter is to designate for the readers of this monograph the vector of development of these two approaches—the MGI and the newest methodology for rapid alloy prototyping (i.e., accelerated development and testing of new alloys) based on the combination of LAM technologies and methods of combinatorial design. The presentation pursued three goals:

- the first goal was to represent the efficiency of the combination of these two approaches for accelerated manufacturing (i.e., RAP) and study of the alloy versions;
- the second goal was to determine the compositions of the selected composite alloys, providing improved properties in comparison with the existing analogues;
- the third goal was to determine and demonstrate the possibility (in-situ, i.e., on-site) of obtaining metal parts with a pre-specified heterogeneity of microstructure and properties.

The last goal is the most significant for high-performance structural alloys, since the products made of them often must combine a high hardness of the surface layer with a softer and viscous core. The LAM is obviously a technology that is most fitted for a systematic study of all these aspects and provides the possibility of creating complex parts based on digital models using the selected powder compositions. It was noted that:

http://dx.doi.org/10.5772/intechopen.77360

1. The new concept, Material Genome, allows consolidating the efforts aimed to develop such directions as "new materials," "computer technologies for modeling and production of parts" and "additive manufacturing" by providing a single tool that helps to achieve breakthrough results by applying new methods and approaches.
2. The DMD and SLM are suitable for obtaining of 3D samples with a constant or variable composition of the material and can be used for combinatorial design and development of new alloys. The LAM allows the creation of compositionally piecewise-continuous gradient materials and obtainment in situ of new alloys that are not necessarily made from pre-prepared metal powders and is an effective tool for the rapid development of a new alloy. An additional advantage of the DMD in comparison with the SLM in the context of combinatorial metallurgical synthesis is high cladding rates and large dimensions of 3D parts, which are not limited by the dimensions of the synthesis chamber in the SLM installation.
3. Equally important is the possibility to obtain with the aid of the LAM, compositions and microstructures of alloys that are not available for traditional technologies. This principle feature can be used as a goal of combinatorial development of unique alloys for the LAM. It should also be noted that with the DMD, a gradient sample comprising parts from different alloys can be subjected to the HIP (post-treatment) and further research of the alloys that are changing in their composition from the viewpoint of their behavior during the thermo-mechanical treatment.

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