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REVIEW OF THE COMPUTATIONAL APPROACHES TO ADVANCED MATERIALS SIMULATION IN ACCORDANCE WITH MODERN ADVANCED MANUFACTURING TRENDS

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Abstract. In order to be competitive, modern manufacturers have to offer best-in-class products. Superior quality of the product requires introduction of new materials, digital design methods and advanced manufacturing technologies into production process. Special attention is given to numerical simulation as the most time efficient, flexible and cheap method to evaluate the level of optimality and viability of the proposed solution as well as to predict further Product Life-Cycle. Accurate setting of material properties and representation of complex material structure is crucial for product design employing simulation. Commonly, material representation for simulation purpose is based on the analytical relationships that provide approximate data and cannot provide multiscale information about structure. Initiation of Material Genome Initiative (MGI) as well as the study of Big Data and Machine Learning concepts leads to development of new, more accurate and reliable instruments for product design that involve material simulation and optimization of material selection process.
Keywords. Factory of Future (FoF), Material Genome Initiative (MGI), Integrated Computational Materials Engineering (ICME), Computer-Aided Engineering, Big-Data, Machine Learning.

1. Introduction

Nowadays, there is keen interest in development of advanced manufacturing. This interest has been embodied in emergence of some programs and initiatives such as Industry 4.0, Industry + and Advanced Manufacturing Partnership 2.0. Taking into account these trends, a lot of studies are dedicated to automatization and digitalization of manufacturing processes as the key instruments to build the Factories of Future (FoF). The modern computer design systems such as Computer-Aided Design (CAD), Computer-Aided Engineering (CAE) and Computer-Aided Optimization (CAO), improve quality of products and reduce final costs of produced goods. The modern machine tools and equipment have computer numerical control (CNC) that in combination with Computer-Aided Manufacturing (CAM) allows to reduce the time of manufacturing of highly-customized products. Simultaneously the utilization of Internet of Things (IoT) leads to optimization of the whole production process and enables control over the product data and characteristics at all stages of manufacturing.

One more way to improve manufacturing process is to introduce advanced materials. Although, the advanced materials aren't directly related to advanced manufacturing or FoF concepts, the application of this group of resources is often vital to create the designed best-in-class products and implement advanced manufacturing technologies. The importance of materials to key industry sectors and technologies is widely recognized all over the world. For

this reason, there are advanced materials-related strategies in countries that seek to increase the competitiveness of their industry. For example, the US Advanced Manufacturing Strategy that identifies advanced materials as a critical 'cross-cutting technology' R&D priority underpinning advanced manufacturing competitiveness. [1] In fact, most of the advanced manufacturing roadmaps and strategies highlight the important role of advanced materials for novel production technologies such as additive manufacturing (AM) or technologies related to robotics and autonomous systems. [1] For example, successful application of Additive technologies as well as the quality of printed products directly depends on the applied materials. Not only have the advanced materials a significant impact on manufacturing stage but also on such crucial stage as product design where the design characteristics of the product that constitute its global competitiveness are defined and ensured.

The usage of computer-aided techniques at the design stage allows to substantially decrease the cost and production time of the whole manufacturing process. In this case, the first step (Simulation-Based Design) becomes the most expensive part of manufacturing process. However, this expenditure allows to reduce or completely eliminate the subsequent cycles of physical product testing and production changeovers (Fig. 1). Thus, the accurate and reliable simulation models is required. Nowadays, there are a lot of various instruments and methods for calculation of complex structures. However, the key input data for each of them consists of the material properties and the representation of material structure. Taking into account the rapid development of material science, the modern numerical algorithms and approaches for simulation of material characteristics during Simulation-based design stage are of particular interest. The implementation of these methods as an integral part of FoF concept can significantly increase the quality of manufactured goods and provide the manufacturing of "best-in-class" products.

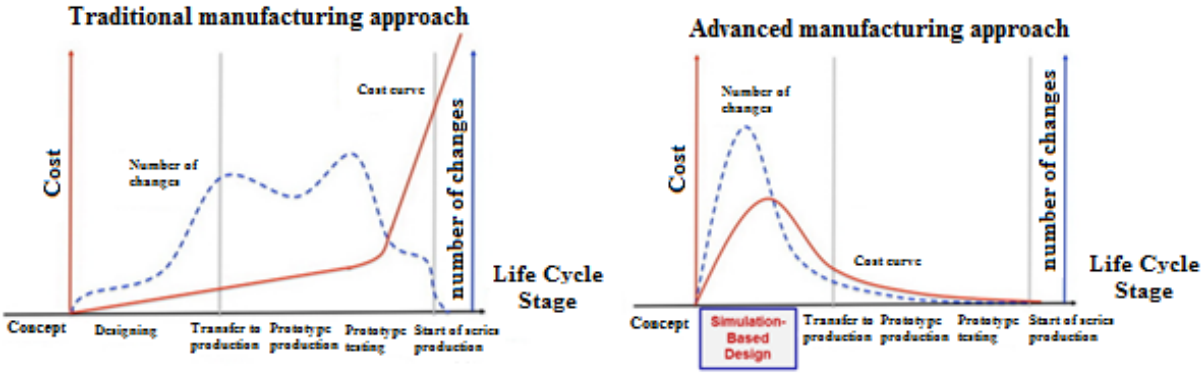

Fig. 1. The impact of computer simulation and design approach on the manufacturing cost[2].

This work provides a review of the most efficient solutions for material simulation and modeling for product design purposes. Fiber-reinforced composite material as the most common and representative advanced material type is discussed in this work. The work is organized as follows. The Section 2 presents a general description of traditional computational simulation of advanced materials using an example of a fiber-reinforced composite materials. The Section 3 provides information about modern approaches based on the combination of experimental and computational instruments, an open data bases as well as several frameworks for integration of various software tools. The Section 4 includes a comparison between traditional and modern approaches and provides general information about usage of Big Data concept for product design purposes.

2. Modelling of material properties in numerical simulation-based design

Substantial development of computing systems as well as the emergence of high-performance computer machines made the computational analysis of composite materials more effective and attractive compared to analytical methods based on solid mechanics. Computational analysis of composite structure and behavior in case of load application is based on the use of numerical integration of the state equations by transforming the system of partial differential equations to a system of linear and linearized algebraic equations with the subsequent solution by means of the mathematical apparatus of the calculus of variations. [3] Nowadays, the finite-element method (FEM) is a commonly used numerical algorithm realized in analytical software applicable for this purpose. The application of FEM as the computational tool is associated with calculation of a significant number of equations and requires high-performance computing resources. However, this method is able to perform calculation of samples with complex geometry and structure. The advantages associated with calculation of complex geometry by usage of linear and linearized equations systems are achievable only through realization of function of the sample partition to the nodes and finite-elements. In case of computing software this partition is realized as meshing step. [3]

The automation sample meshing is realized on the base of mathematical approaches such as Delaunay triangulation and Advancing Front (AF) approaches. [4] Both approaches are widely used to create tetrahedral (tet) mesh. However, there are differences between these methods. AF is based on adding mesh elements starting at the boundaries by inserting one new point or merging different existing points. In this case, the main criteria of adequate triangulation is the intersection absence. The disadvantage of AF method is a very complex analysis of the partition region and surroundings of mesh elements. In that case the Delaunay triangulation is more flexible. For performing this method, the other triangulation methods may be used as the base segmentation. The subsequent algorithm implies checking compliance of base triangulation with Delaunay requirements and further improvement when necessary. In general, the triangulation satisfies Delaunay condition, if none of the given triangulation points fall within the area inside of the circle escribed around any of the built triangles. However, in case of conformity check, the algorithms are based on the theorem that can be formulated as *"Among all possible triangulations, in case of Delaunay triangulation there is the maximum sum of the smallest angles of all built triangles"* The requirement complemented by the theorem provides four analytical instruments for conforming check:

1. Use of the circumscribed circle equation.

The equation of circle circumscribed the triangles built on points (x_1, y_1), (x_2, y_2), (x_3, y_3) can be expressed as: [4]

$$(x^2 + y^2) \cdot a - x \cdot b + y \cdot c - d = 0, \quad (1)$$

where

$$a = \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix}, b = \begin{vmatrix} x_1^2 + y_1^2 & y_1 & 1 \\ x_2^2 + y_2^2 & y_2 & 1 \\ x_3^2 + y_3^2 & y_3 & 1 \end{vmatrix}, c = \begin{vmatrix} x_1^2 + y_1^2 & x_1 & 1 \\ x_2^2 + y_2^2 & x_2 & 1 \\ x_3^2 + y_3^2 & x_3 & 1 \end{vmatrix}, d = \begin{vmatrix} x_1^2 + y_1^2 & x_1 & y_1 \\ x_2^2 + y_2^2 & x_2 & y_2 \\ x_3^2 + y_3^2 & x_3 & y_3 \end{vmatrix}$$

The Delaunay condition is feasible if for any point (x_0, y_0) does not fall into the circle region. This condition can be expressed as:

$$((x_0^2 + y_0^2) \cdot a - x_0 \cdot b + y_0 \cdot c - d) \cdot sgn\, a \geq 0 \quad (2)$$

2. Checking with the previously calculated circumscribed circle.

Use of the circle equation mentioned above, requires a significant number of arithmetic calculations that leads to an increase in computation time. The usage of previously calculated circumscribed circle method allows to overcome this shortcoming. This method is based on the calculation of center (x_c, y_c) and radius r of circumscribed circles for each triangle. [4]

$$x_c = \frac{b}{2a}, \quad (3)$$

$$y_c = \frac{-c}{2a}, \quad (4)$$

$$r^2 = \frac{(b^2+c^2-4ad)}{4a^2}, \quad (5)$$

The Delaunay condition is feasible if the distance from any point (x_0, y_0) to the centre of circle is bigger than radius. [4]

$$(x_0 - x_c)^2 + (y_0 - y_c)^2 \geq r^2 \quad (6)$$

The advantage of this method is the absence of necessity to calculate the parameters of circles for each triangle. The check of Delaunay condition is always performed for pair of triangles, which leads to necessity to calculate the circle just for one of them. That method allows to reduce the amount of calculated circles by 25 - 45% and to reduce the number of arithmetic computations by third.

3. Checking of the sum of the opposite angles.

The primary sources of this method are earlier works [5,6]. According to the authors, the Delaunay condition is feasible if for any point (x_0, y_0) used for area triangulation there is $\alpha + \beta \leq \pi$. (Fig. 2)

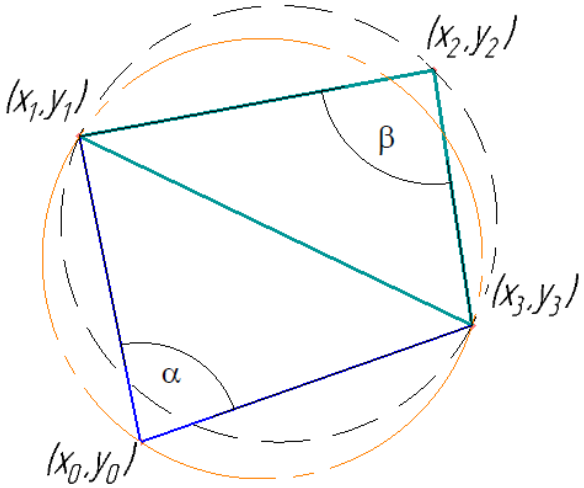

Fig. 2. A check the sum of the opposite angles.

This condition can be expressed as [7]:

$$sin\ \alpha\ \cdot cos\ \beta\ +\ cos\ \alpha \cdot sin\ \beta \geq 0, \quad (7)$$

where

$$cos\ \alpha\ = \frac{(x_0-x_1)(x_0-x_3) + (y_0-y_1)(y_0-y_3)}{\sqrt{(x_0-x_1)^2+(y_0-y_1)^2}\sqrt{(x_0-x_3)^2+(y_0-y_3)^2}} \quad (8)$$

$$cos\ \beta\ = \frac{(x_2-x_1)(x_2-x_3) + (y_2-y_1)(y_2-y_3)}{\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\sqrt{(x_2-x_3)^2+(y_2-y_3)^2}} \quad (9)$$

$$sin\ \alpha\ = \frac{(x_0-x_1)(y_0-y_3) - (x_0-x_3)(y_0-y_1)}{\sqrt{(x_0-x_1)^2+(y_0-y_1)^2}\sqrt{(x_0-x_3)^2+(y_0-y_3)^2}} \quad (10)$$

$$sin\ \beta\ = \frac{(x_2-x_1)(y_2-y_3) - (x_2-x_3)(y_2-y_1)}{\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}\sqrt{(x_2-x_3)^2+(y_2-y_3)^2}} \quad (11)$$

4. Modified check of the sum of the opposite angles.

This method is similar to 'checking of the sum of the opposite angles' method. However, in order to reduce amount of calculation there is a pre-stage that implies partial calculation of equation (7). For this method, the parameters s_α and s_β must be calculated. [4]

$$s_\alpha = (x_0 - x_1)(x_0 - x_3) + (y_0 - y_1)(y_0 - y_3) \quad (12)$$

$$s_\beta = (x_2 - x_1)(x_2 - x_3) + (y_2 - y_1)(y_2 - y_3) \quad (13)$$

According to [7] if parameters s_α and s_β are either positive or equal to 0 then the Delaunay condition will be fulfilled. If the s_α and s_β are both negative then the Delaunay condition will not be fulfilled and triangulation must be improved. The other combinations of these parameter values lead to subsequent calculation by the equation (7). On average, this modified method allows to reduce the number of arithmetic computations by 20 - 40%.

Proposed analytical tools allow to check the correctness of the existing mesh in case of Delaunay triangulation, while the meshing based on Delaunay triangulation is performed by various algorithms such as iterative algorithms, merging algorithms, algorithms for direct construction and two-pass algorithms. Each algorithm is applied for some specific case and is discussed in detail in works [7].

The meshing step is a preparatory stage for subsequent calculations. In general, the existing Computer-aided engineering (CAE) software has solver modules which allows to deal with mechanics, thermomechanics and fluid tasks. In general CAE software is able to provide the following analysis types.

1. Static strength analysis that can provide information about displacement, strain and stress taking place in the sample under mechanical load. The basic equation for this analysis can be expressed as: [7].

$$[K]\{u\} = \{F\}, \quad (14)$$

where $[K]$is the stiffness matrix; $\{u\}$- displacement vector; $\{F\}$- force vector, that can be represented by concentrated forces, temperature loads, pressure and inertia forces.

This type of analysis can be suitable in case of the negligible impact on the structure behavior from action of inertia forces or energy dissipation processes.

2. Dynamic strength analysis can be used for construction study in case of time-dependent load application. The examples of these loads are sudden loads (shocks), cyclic loads (rotation), etc. Analysis of this type of loads is based on equation: [7].

$$[M]\{u''\} + [C]\{u'\} + [K]\{u\} = \{F(t)\}, \quad (15)$$

where $[M]$ - the mass matrix; $[C]$- the damping matrix; $[K]$- the stiffness matrix; $\{u''\}$- the nodal acceleration vector; $\{u'\}$ - the nodal speed vector; $\{u\}$- the vector of nodal displacement; $\{F\}$- the loads vector and *t* is the computation time.

The values of variables $\{u\}$, that at any instant of time satisfy the equilibrium conditions of the system, are the solution of equation (15).

3. Analysis of the construction stability that allows to define the load level that leads to decrease of stability as well as reverse task - the state of construction under applied load can be performed by linear and nonlinear methods. The analytical equation of linear method is [7].

$$([K] - \lambda[S])\{u\} = 0, \quad (16)$$

where $[K]$- the stiffness matrix; $[S]$- the matrix of effective stiffness; λ- scale factor; $\{u\}$- buckling vector.

Nonlinear method is more complex and accurate method:

$$[K]_{i-1}(\{u\}_i - \{u\}_{i-1}) = \{F\} - \{F^{el}\}_{i-1}, \quad (17)$$

where $[K]_{i-1}$ is the stiffness matrix at the previous iteration; $\{u\}_i$, $\{u\}_{i-1}$- the displacement stiffness at the current and previous iteration respectively; $\{F\}$ - the vector of applied loads;

$\{F^{el}\}_{i-1}$- the vector of the elastic forces correspondent to displacements at the previous iteration *(i-1)*.

4. Thermal analysis allows to obtain temperature stress and strain, phase transformations, unsteady temperature conditions, etc. The basic equation for this type of analysis can expressed as: [7].

$$[C]\{T'\} + [K]\{T\} = \{Q\}, \quad (18)$$

where $[C]$ - the matrix of specific heat capacity; $\{T'\}$ - derivative of temperature; $[K]$ - the effective thermal conductivity matrix; $\{T\}$- vector of nodal temperature; $\{Q\}$- the vector of effective heat flux in nodes.

Basic equations of the described analysis contain elements that strongly depend on the properties of construction materials. These parameters are the matrixes of specific heat capacity and effective thermal conductivity for thermal analysis as well as the stiffness matrix for other types of mechanical analysis. For example, stiffness matrix strongly depends on the effective Young's moduli and effective Poisson's ratio. [8]

Traditional bottom-up product design approach involves two simultaneous processes such as design of geometric parameters of product as well as selection of appropriate materials. The information about product functions and conditions of use provides engineers with the information about loading type, concentration and value of stresses that can be used to make an assumption about the required set of material properties. The task of engineers is to choose the material that best meets these requirements. [9]

However, in real application there can be a few materials that allow to fulfill the final product requirements. In this case, the material selection is associated with solution of multi-criteria optimization task. Commonly, material selection charts (Ashby charts) are used to find the most optimal solution. In general, Ashby charts demonstrate material properties plotted against each other on logarithmic scales. Obtained property-space is occupied by each material class and sub-class represented by bubbles that allow to visually compare the combination of properties between various materials. There is a lot of variants of Ashby charts plotted by using combination of about 30 mechanical and thermal properties such as density, Young's moduli, ultimate strength, etc. The example of Young's moduli - density Ashby chart is shown in Fig. 3.

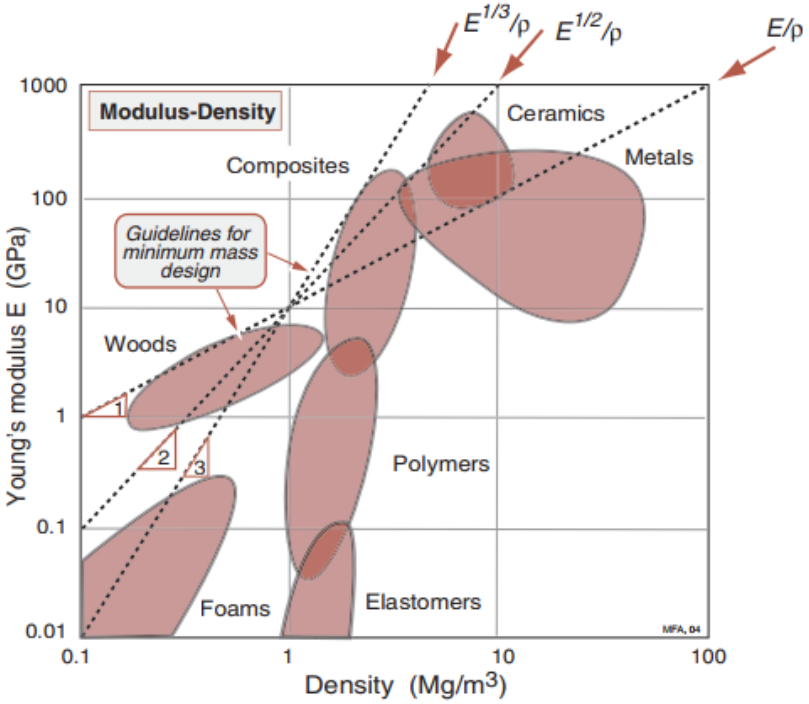

Fig. 3. A schematic Young's moduli - density Ashby chart [10].

In general, the Ashby's method of multi-criteria material selection process involves plotting and usage of material indexes that can be obtained analytically. Basically, the product performance criteria (*P*) are the function of loading requirements (*F*), geometry requirements (*G*) and material properties requirements (*M*). [10]

$$P = f(F, G, M) \tag{19}$$

Needless to say, that material selection is based only on material properties requirements. Thus, there is need to separate variables related with material properties from the others. For example, the performance criteria related with design of light and stiff beam (Fig.4) can be represented by system: [10]

$$\begin{cases} m = A \cdot L \cdot \rho \\ \delta_{max} \geq \frac{C_1 EIF,}{L^3} \end{cases} \tag{20}$$

where L – the length of beam; A – the beam cross-section; ρ - the material density; E – Young's moduli; F – force applied to beam; C_1 – constant that depends on the load distribution; I – the second moment of the area of the section, that can be defined as:

$$I = \frac{A^2}{12} \tag{21}$$

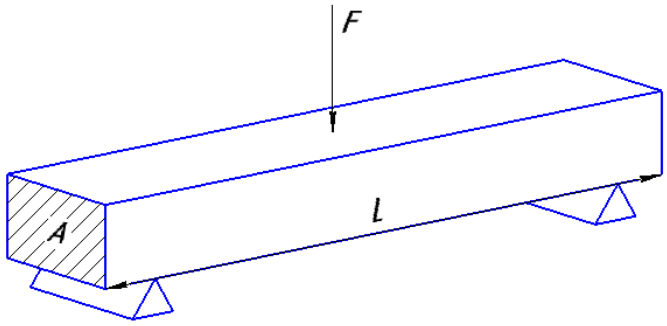

Fig. 4. A beam of square section, loaded in bending [10].

The δ_{max} is the permissible value of bending that must not be exceeded. Taking into account equations 20, 21, the optimization of beam mass can be written as:

$$m \geq \sqrt{\frac{12F}{LC_1\delta_{max}}} \cdot L^3 \cdot \left(\frac{\rho}{E^{\frac{1}{2}}}\right) \tag{22}$$

According to equation 22, material properties requirements can be represented as:

$$f(M) = \left(\frac{\rho}{E^{\frac{1}{2}}}\right) \tag{23}$$

Therefore, the best materials for a light and stiff beam are those with the smallest values of $f(M)$. However, usually engineers invert $f(M)$ in order to obtain material index. For the considered case, the material index is $\sqrt{E}/\rho$. On the Ashby chart, the material index are plotted as a family of straight parallel lines of slope 2 and can be used to find the material with optimal relation of $\sqrt{E}/\rho$ (Fig. 3). The bubbles crossed by the same straight line present materials with the same value of material index. The material that located under or above the material index line have lower or higher value of $\sqrt{E}/\rho$ relation, respectively. According to the Fig. 3, some types of composites, wood and ceramics have the greater value of $\sqrt{E}/\rho$ material index comparing with the metals, polymers and foams. Therefore, in case of presence of composite and metal beams with the same stiffness, the composite beam will be less heavy comparing with the metal one. In works [10], there is description of other material indexes and their applications for engineering tasks.

In order to minimize the search region, the additional limits can be used. Potential materials obtained by the Ashby's method than studied by using supported information in order

to find the best solution. Further, the effective properties of chosen material are used for CAE computation and design confirmation.

The effective properties can be characterized as the averaged material properties of investigated part or whole structure. It is true even in case of analysis of homogeneous materials. The reason is the presence of grains, particles with various dimension and orientation. There is the interaction between these elements that can have influence on the material behavior. However, this interaction can be referred to micro-mechanical investigation. For homogeneous materials the mechanical analysis commonly deals with macro scale that represent level of components and structural parts. The absence of differences in properties on macro scale level allows to avoid the segmentation of calculated structure. On the other hand, the analysis of heterogeneous materials such as composite materials is more complex and requires an investigation on the meso scale (level of composite phases) and micro scale. [11] There are several methods that can be used for property description of composite materials to perform computational analysis.

The most common type of composite materials are plastic materials reinforced by continuous fibers. In fact, this type of composite materials has two types of heterogeneity. The first one is characterized by the presence of two phases such as matrix and reinforcement fibers. The second one represents the heterogeneity provided by layered structure consisting of layers with the certain direction of the fibers ($0^0, 90^0, \pm 45^0$). Commonly for the calculation of the structure behavior and mechanical analysis, only the second type of heterogeneity is taken into account. In these case, the composite material is represented as a number of layers with known properties. [12]

The same approach is commonly used for calculation of lamination composite materials. On the other hand, the structures with fillers represented by spheres, plates, tubes, etc. are commonly exposed to the homogenization process that represents the composite structure as a homogeneous material with effective properties calculated on basis of volume fractions. The study of these composites on the micro scale level is more complex and can be performed when the interaction between matrix and fillers phases must be investigated. [13]

According to [14,15] the minimum set of properties required for computational calculation includes effective Young's modulus along and across of the fibers (E_1, E_2, respectively) (Fig.5); effective shear modulus G_{12}; $\sigma_{1B}^{+}, \sigma_{1B}^{-}$ - ultimate strength under uniaxial tension and compression across the fibers; σ_{12}^{+}- shear strength; μ_{12} - effective Poisson ratio (where the first index shows the direction of load action, while the second - the direction of the relevant transverse deformation), while the μ_{21} can be expressed as [15]:

$$\mu_{21} = \mu_{12}\frac{E_2}{E_1} \tag{24}$$

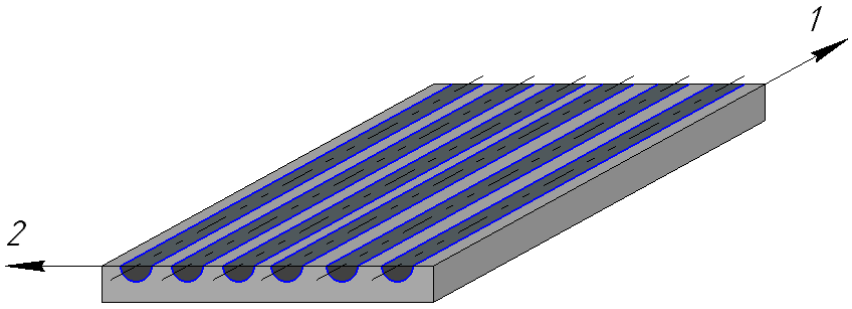

Fig. 5. Cross-section of unidirectional monolayer.

In case of multilayer composite materials reinforced by continuous fibers the set of effective properties must be provided for each layer that is accepted as the homogeneous structure. This process is known as homogenization and is based on the *'Rules of Mixture'* prediction model (ROM). There are several models of ROM. For example, the ROM model

based on the assumption that all components of structure undergo the same deformation in the same direction is known as Voigt-type ROM. [16] Commonly, this model is used for calculation of Young's modulus along fibers (E_1) in case of the load application in direction of fibers.

$$E_1 = \xi_M E_{1M} + \xi_F E_{1F}\ , \tag{25}$$

where ξ_M, ξ_F- the volume fractions of matrix and fiber components, respectively; E_{1M}, E_{1F}- Young's modulus of matrix and fiber components, respectively.

At the same time, the effective shear modulus G_{12} can be calculated by means of Reuss-type ROM based on the equal load distribution among the whole structure.

$$\frac{1}{G_{12}} = \xi_M \frac{1}{G_M} + \xi_F \frac{1}{G_F}, \tag{26}$$

where G_M, G_F- shear modulus of matrix and fiber components, respectively.

Although, this model is accurate for laminate composite materials, in case of matrix based composites Reuss-type ROM cannot provide adequate results. More accurate version of models above is the Reuss–Voigt bounds that provides the upper (Voigt) and lower (Reuss) values of the effective elastic properties.

$$(\xi_M E_{1M}^{-1} + \xi_F E_{1F}^{-1})^{-1} \le E_1 \le \xi_M E_{1M} + \xi_F E_{1F}. \tag{27}$$

In works [16,15,17,18,19], authors demonstrate the usage of Hashin-Shtrikman bounds and Mori-Tanaka methods to calculate the effective elastic properties of two and three phase composites. Moreover, these methods are in line with the test results and can be used for composites with randomly oriented fibers or inclusions of irregular shapes.

In general, other parameters such as mass density, ultimate strength and thermal conductivity of composite materials can be calculated by ROM method.

$$(\frac{\xi_F}{\rho_F} + \frac{\xi_M}{\rho_M})^{-1} \le \rho_{eff} \le \xi_F \rho_F + \xi_M \rho_M, \tag{28}$$

$$(\frac{\xi_F}{\sigma_F} + \frac{\xi_M}{\sigma_M})^{-1} \le \sigma_{1B}^{+} \le \xi_F \sigma_F + \xi_M \sigma_M, \tag{29}$$

where ρ_F, ρ_M – density of fiber and matrix, respectively; σ_F, σ_M – ultimate tensile strength of fiber and matrix, respectively.

The analytical calculation of composite properties provides the range in which the values of effective properties are. For this reason, in case of FEM analysis of composite structure there is a necessity to use the properties obtained from experimental tests in order to increase accuracy of final results.

The obtained effective parameters can be used to describe the elasticity characteristics of the studied construction. The Hooke's law expressed in stiffness form can be used for this purpose. [15]

$$[\sigma] = [K][\varepsilon], \tag{30}$$

where $[\sigma]$ is the matrix of stress arising in the studied structure; $[\varepsilon]$ - the strain matrix of structure; $[K]$- the stiffness matrix.

In case of multilayer composites reinforced with continuous fibers, the stiffness matrix depends on the effective properties of materials as well as geometry of construction. The matrix can be expressed as:

$$[K] = \frac{1}{H}\sum_{i=1}^{n}[k]_i h_i, \tag{31}$$

where H- the thickness of construction; h_i - thickness of i-th layer; $[k]_i$ - the stiffness matrix of i-th layer.

$$[k]_i = [T]_i \left[\bar{k}\right]_i [T]_i^T, \tag{32}$$

where T is the transformation matrix that can be expressed as:

$$[T]_i = \begin{vmatrix} cos^2\theta_i & sin^2\theta_i & -2cos\theta_i \cdot sin\theta_i \\ sin^2\theta_i & cos^2\theta_i & 2cos\theta_i \cdot sin\theta_i \\ cos\theta_i \cdot sin\theta_i & -cos\theta_i \cdot sin\theta_i & cos^2\theta_i - sin^2\theta_i \end{vmatrix} \tag{33}$$

where θ_i- the fiber orientation of i-th layer; $[\bar{k}]_i$ is the stiffness matrix in local coordinates of i-th layer. [15]

$$[\bar{k}]_i = \begin{vmatrix} \frac{E_{1,i}}{1-\mu_{12,i}\mu_{21,i}} & \frac{\mu_{12,i}E_{2,i}}{1-\mu_{12,i}\mu_{21,i}} & 0 \\ \frac{\mu_{21,i}E_{1,i}}{1-\mu_{12,i}\mu_{21,i}} & \frac{E_{2,i}}{1-\mu_{12,i}\mu_{21,i}} & 0 \\ 0 & 0 & G_{12,i} \end{vmatrix}, \quad (34)$$

The obtained stiffness matrix can be used as input data for CAE analysis (eq. 14 -17).

Besides the elastic properties, the solver algorithms must be equipped with the failure criteria that strongly depends on the composite material strength. There are various methods for failure criteria setting. However, the most common method is Tsai-Wu criterion. [15] The simple form of this criterion is equation 35.

$$F_1\sigma_{11} + F_2\sigma_{22} + F_{11}\sigma_{11}^2 + F_{22}\sigma_{22}^2 + F_{33}\sigma_{12}^2 + 2F_{12}\sigma_{11}\sigma_{22} = 1, \quad (35)$$

where

$$F_1 = \frac{1}{\sigma_{1B}^+} + \frac{1}{\sigma_{1B}^-}; \quad F_2 = \frac{1}{\sigma_{2B}^+} + \frac{1}{\sigma_{2B}^-} \quad (36)$$

$$F_{11} = -\frac{1}{\sigma_{1B}^+\sigma_{1B}^-} \quad F_{22} = -\frac{1}{\sigma_{2B}^+\sigma_{2B}^-} \quad F_{33} = -\frac{1}{\sigma_{12B}^2} \quad (37)$$

F_{12} is the coefficient that characterizes the interinfluence of $\sigma_{11}$and σ_{22}. This coefficient can only be determined by experimental measurements. (Fig. 6)

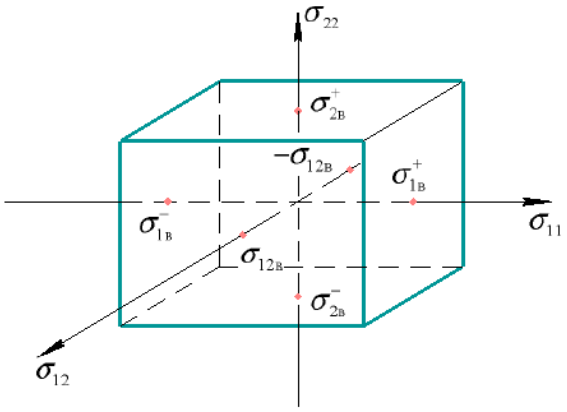

Fig. 6. Surface of maximum stresses.

In these simple forms the Tsai-Wu criterion takes into account only three parameters ($\sigma_{11}, \sigma_{22}, \sigma_{12}$). However, the real numerical calculation deals with stresses in each direction (nine parameters) and coefficients of mutual influence between stresses in plane xy, yz, xz. [15]

$$A + B < 1, \quad (38)$$

where

$$A = -\frac{\sigma_{xx}^2}{\sigma_{xt}^f\sigma_{xc}^f} - \frac{\sigma_{yy}^2}{\sigma_{yt}^f\sigma_{yc}^f} - \frac{\sigma_{zz}^2}{\sigma_{zt}^f\sigma_{zc}^f} + \frac{\sigma_{xy}^2}{\left(\sigma_{xy}^f\right)^2} + \frac{\sigma_{yz}^2}{\left(\sigma_{yz}^f\right)^2} + \frac{\sigma_{xz}^2}{\left(\sigma_{xz}^f\right)^2} + \frac{C_{xy}\sigma_{xx}\sigma_{yy}}{\sqrt{\sigma_{xt}^f\sigma_{xc}^f\sigma_{yt}^f\sigma_{yc}^f}} + \quad (39)$$

$$+ \frac{C_{yz}\sigma_{yy}\sigma_{zz}}{\sqrt{\sigma_{yt}^f\sigma_{yc}^f\sigma_{zt}^f\sigma_{zc}^f}} + \frac{C_{xz}\sigma_{xx}\sigma_{zz}}{\sqrt{\sigma_{xt}^f\sigma_{xc}^f\sigma_{zt}^f\sigma_{zc}^f}},$$

$$B = \left(\frac{1}{\sigma_{xt}^f} + \frac{1}{\sigma_{xc}^f}\right)\sigma_{xx} + \left(\frac{1}{\sigma_{yt}^f} + \frac{1}{\sigma_{yc}^f}\right)\sigma_{yy} + \left(\frac{1}{\sigma_{zt}^f} + \frac{1}{\sigma_{zc}^f}\right)\sigma_{zz}, \quad (40)$$

where $\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{xy}, \sigma_{yz}, \sigma_{xz}$ - stress components in the material coordinate system; $\sigma_{xt}^{f}, \sigma_{yt}^{f}, \sigma_{zt}^{f}$ – failure tensile stress along x, y and z axes in the material coordinate system; $\sigma_{xc}^{f}, \sigma_{xc}^{f}, \sigma_{xc}^{f}$ – failure compressive stress along x, y and z axes in the material coordinate system; $\sigma_{xy}^{f}, \sigma_{yz}^{f}, \sigma_{xz}^{f}$ – failure shear stress in plane xy, yz and xz in the material coordinate system; C_{xy}, C_{yz}, C_{xz} - mutual influence coefficient in plane xy, yz and xz in the material coordinate system.

The inequality fulfillment demonstrates that the construction is able to withstand the applied load. In fact, the value inverse to right part of equation 38 characterizes the safety factor of the tested construction. In addition to the parameters and criteria above, the prediction of the remaining life must be performed by use of the algorithms and models that are able to take into account the material aging during exploitation. [14]

The modern systems for numerical analysis allow to significantly increase the accuracy and quality of the constructions made from composites materials. However, the application of this types of analyses strongly depends on the information about material properties. The mentioned analytical relations and methods used to describe composite properties as well as their structure are not precise enough. They include certain approximation and assumptions. For this reason, the usage of experimental measurements is strongly recommended. However, experimental tools are not always applicable due to the limitations of the composite material theory. Taking into account the duration of the research and development of the new desired material (an average 10 - 20 years), the engineers must look for compromises in the existing materials that deprives the Simulated-based design of one more optimization parameter such as material structure.

3. Genome-Oriented Strategy

Nowadays cost-cutting and time-to-market reduction are relevant ways to gain the competitive advantage in the global market. In order to produce faster and at low cost, it is insufficient to optimize the construction parameters. The deployment of the most suitable materials in the different parts of the construction is a key advantage. For this reason, the Material Genome Initiative (MGI) was initiated in the United States. According to the MGI, ‘the discovery and deployment of advanced material systems is crucial to achieving global competitiveness in the 21st century’. [20] This program or initiative is focused on involvement of computational capabilities and data management in material science and engineering.

The MGI aims to accelerate the advanced materials research and design by creation wide networks and open source platforms involved in advanced material development. The first step to create this type of advanced materials infrastructure is an adoption of rapidly developing computational technologies as well as the development of more efficient algorithms for prediction and modelling of materials’ properties. The involvement of such technologies is crucial for reduction of the time spent on experiments and supplementation of physical experiment data. In addition to the development advanced materials and obtaining information about the structure and related properties, the generated data must be recorded and translated to an open source database. Existence of such open source database allows industry offer new product designs improved by not only an optimization of components by deployment of more suitable materials. [20] An ability to monitor the development of new materials and presence of connection between open source platforms and computer-aided instruments leads to an acceleration of design and improvement of designed constructions.

Thus, the main aim of MGI is an achievement of superiority in advanced material design and implementation by development of new instruments such as digital data platforms and new research and development (R&D) tools. [20]

3.1. R&D computation instruments. Traditionally, material developing is completed by testing. The experimental tools for testing and study of obtained results are expensive and their implementation is time-consuming in comparison with computational instruments. However, in spite of this comparison, the experimental/empirical methods of material study are still used for research and development of advanced materials. The results of computational analysis strongly depend on the quality of calculated models that must include accurate and extensive data about material behavior and properties. For new materials, the physical experimentation is the only possible option to obtaining such accurate set of data. Moreover, the experimental tools are the only possible way to validate calculated results of computer modelling of developed materials. For this reason, the experimental tools cannot be neglected during creation of modern advanced materials infrastructure. The simultaneous use of computational and experimental tools allows to overcome the problems that cannot be solved by using theoretical frameworks. While the experimental tools are able to improve calculation model by incorporating new data, the computational tools can use this improved model to perform analysis of structure, properties and optimization by studying a large set of possible configurations. [20]

The development of novel software that allows to connect the experimental and computational tools is an important step for improvement of Design Stage as the key part of Factory of Future. For this reason, the various research groups and companies are involved in development of this kind of software technologies. One of the example of such software is the Simpleware toolkit. In works [21,22] the usage of this software for characterization of heterogeneous material properties and structures is presented. The methodology is represented by step sequence that involves experimental and computational tools. The first step is usage of scan techniques such as Computed tomography (CT), X-ray Microtomography (micro-CT) [22], and serial sectioning (SEM) for generation of image stack that can be converted from 2D pixels into 3D pixels (voxels) by image processing software. The conversion process is accompanied by segmentation of heterogeneous structure into separate regions (different phases, reinforced particles, defects or porous networks etc.). Typically, the data obtained by scan techniques is presented by regular Cartesian grid of greyscale data that demonstrate the amount of radiation passed through the tested samples. The variation in the shades informs about the changes in material throughput that can be related with difference in materials, phases and structures of the tested sample. [4] Regions segmentation process is based on the presence of this data set and implies determination of various phases in sample structure. Some factors such as noise, poor contrast, and other defects related to the quality of scan techniques can influence on the accuracy of segmentation. [4] The need of accurate results requires the use of thresholding and cropping software techniques. For example, a noise reduction required to eliminate variations of brightness and color information can be performed by using a median filter. The tools such as ‘island removal’ can be used for reassignment of unconnected small areas to the relevant phase, while the ‘smoothing’ algorithms make a deal with the volume and topology of obtained phases. [21]

The segmented 3D image data can be rapidly processed and converted into multi-part meshes by algorithm such as +FE Grid that is the part of Simpleware software or the other finite-element based methods and techniques such as ‘Enhanced Volumetric Marching Cubes’ (EVoMaC). The usage of image-based meshing approach allows to obtain more accurate and complete meshes comparing with CAD-based approaches. The main reason of this is the usage of model segmentation for generation of mesh with different dimension or configuration depending on the size and complexity of local phases. Mostly, this meshing is possible due to the EVoMaC algorithm, that generates hexahedral elements from voxels lying in mask interiors, while the tetrahedral meshing applies to voxels lying close to mask interfaces. [21,4] In case of CAD-based approach, the mesh creation is often accompanied by loss of volume or topology that leads to decrease in model accuracy. Obtained meshed model can be used for calculation

of behavior and properties of tested samples by using existing computational tools mentioned earlier. Typically, the calculation of heterogeneous materials is performed by numerical homogenization. In case of Simpleware, homogenization is carried out by software modules such as +SOLID, +LAPLACE and +FLOW. The work of these modules is based on use of a built-in finite element solvers that allows to calculate and analyze the behavior of a material cuboidal sample in case of boundary conditions. The operability of proposed methodology is demonstrated with studying of advanced materials such as Berea sandstone [23] and Aluminum Matrix Composite with PMMC particles [22].

Without a doubt there are other methods used for converting the 2D scan data to the 3D model. For example, Yiu et al. use the CT image data to generate 3D microstructural model of asphalt mixture. [24,25,26] The study of asphalt mixture structure and properties (shear modulus) by usage of X-ray CT and FEM tools is presented in work [27]. In work [28, 29,30], the X-ray CT is used as the instrument for reconstruction of more detailed "real" model of 3D woven and other types of textile composite materials. In general, the approach proposed to study textile composite material structure is similar to Simpliware methodology, however to classify the material phases there is the database of "training set" that allows to train the program classifier module on the examples. In works [31, 32, 33] the authors perform numerical and experimental studies of delamination process and their prediction for carbon fiber reinforced polymers (CFRP). For this purpose, the Spectral Element Method (SEM) is applied to support numerical analysis as well as Scanning Laser Doppler Vibrometry (SLDV) is related with experimental research.

In fact, the experimental tools can be used not only for initial data obtaining but also to confirm the correctness of the calculated model and the predicted behavior of structure. For example, nanoindentation techniques can be used to measure mechanical properties in a pattern at nanoscale. [34] In work [35], the technique for collection of Acoustic Emission data is applied to validate the numerical prediction of L-flange behavior under quasi-static load conditions. However, the application of this technique provides a small amount of data for numerical model validation. In fact, AE is the audio records that include sequence of sound spikes with regard to time. These spikes cannot be used to identify the area of fracture or the magnitude of deformation. However, the obtained data can be compared to numerical results in terms of moments of deformation and fracture occurrence. In fact, strength testing allows to provide more information that can be used for validation. [36]

Nowadays, there is a large number of instruments and methods of empirical investigation that can be used for improvement of numerical algorithms. This approach allows to obtain highly-accurate data that further can be used to design the high-quality constructions as well as to create platform for material R&D. However, the undeniable advantage of systems such as Simpleware software compared to using various separate tools is a quick data transferring and usage of data format transparent for all software modules. The involvement of existing methods and improvement of performance in digital research and design trends is possible due to development of data representation standards as well as various frameworks provided interaction between different experimental and numerical instruments.

The development of such frameworks is mentioned in work [35]. In order to numerically predict L-flange behavior under quasi-static load conditions the authors involve a variety of tools such as COMPRO software, Abaqus Simulation and Autodesk Helius PFA softwares. In this work, the model of composite structure is performed by means of COMPRO software that are able to provide additional information about the structure behavior during processing as well as to predict the deformation and to calculate residual stresses. Partly on the base of this model, the model of L-flange mechanical properties such as the ply-level strength is calculated by means of Abaqus Simulation software. The data obtained from these tools and design steps is transferred into the final step carried out by means of Autodesk Helius PFA software. It is

the powerful instrument of progressive FE analysis that allows to perform more advanced multiple failure analysis of composite structures. Each of these software instruments can be applied separately for providing high-quality results with subsequent analytical calculation or replaced by other numerical tools. However, the main aim of the proposed calculation method is the combination of their advantage in order to obtain fast and accurate results and construction behavior prediction. Such integration and data communication is provided by usage of commercially available ModelCenter software package. The advantage of this software is an ability to interface with other standalone applications and to automate the data transfer process by integration of applications outputs into a system model. In fact, the proposed in the work [35] framework covers the stages from composite material preparation to testing of construction made from this material. The complex calculation of these stages involves material study on various scale levels such as micro, meso and macro scales. Although this approach requires considerable computing power, but the obtained results allow to understand the links between material creation process, material structure, material properties and behaviors as well as properties of final construction. This approach is known as Integrated Computational Materials Engineering (ICME). [35, 37]

3.2. Integrated Computational Materials Engineering (ICME) approach as an efficient design instrument for FoF concept. In general, the ICME approach aim is to provide all stakeholders with a relevant tool for designing materials for targeted performance requirements. [37] Moreover, this approach is a disruptive technology. In order to satisfy the product requirements, the design of micro- and mesostructure of materials can be performed instead of the traditional material selection. This replacement allows to provide the Simulated-based design with one more optimization parameter such as material structure that allows to design best-in-class products with the reduction of time to market parameter.

The improvement of design process by use of ICME approach instead of traditional methods, some basic aspects of which is described in Section 2, can be explained by level of input data. Both approaches are based on the top-down design process in which the function and requirements of final product are target functions used for creation and optimization of product construction. For traditional approach the target functions define the necessary geometry and properties of construction that leads to use of materials with strictly required mechanical, thermal or electrical properties. In case of traditional approach, the designer's work with material is limited by selection of more appropriate materials among the existing options. This selection is based on compromises, which means sacrificing some characteristics for the sake of taking more important ones. In this case, the ideal design solution can be rarely obtained due to the time-consuming nature of the process as well as lack of suitable materials.

The ICME approach ignores material selection step. In fact, required material properties obtained on the macroscope investigation level are used as the input data for meso-, macro- and sometimes nanoscope level design. Requirements of mechanical, thermal and electrical properties are used as the basis for calculation and design of material structure as well as the processing of this materials. For example, such sequence of processing-structure-properties investigations is mentioned in work [38] as the integration of Moldflow and Moldex3D software for characterization of structure and fiber orientation obtained during processing and NX Nastran or Ansys Workbench software to analysis of the properties and behavior of obtained material structure. The involvement of micro- and mesoscale investigation into design process makes the ICME similar to another approach that is commonly associated with properties and behavior prediction. This prediction approach is the bottom-up process that deals with atomic structure. The key process is combinatory search of more optimal atomic configuration that provides the required properties. The examples of such approach is CALculation PHAse Diagram (CALPHAD) method [39,40,41] and Universal Structure Predictor: Evolutionary Xtallography [42, 43] as well as several other methods [44,45].

However, such combinatorial methods deal only with atomic structure while ignoring the morphology of multiple phases and interphase strength. This concentration on atomic structure and properties such as atomic bonding cannot guarantee the multiscale investigation to meet the final product requirements. For this reason, this prediction approach is commonly used for study of new materials in material science, chemistry and physics researches, while the ICME can be integrated into the design process for competitive products. [37]

In fact, the ICME approach combines the top-down and bottom-up methods in order to provide the multiscale product design. The data about product functions and characteristics as well as the information about material genome that includes relationship between microstructure and desirable properties is important information for investigation by this approach. According to [37] the realization of such multiscale approach faces a number of problems such as:

- creation of relations between polyphase microstructures and the properties of construction behavior by considering their behavior at all scales;
- description and determination of responses in higher scales behavior to variations and changes in structure or mechanisms in lower scales;
- description of relations between microstructure and applied processing technology as well as the environment and impurities;
- involvement of the physics and chemistry knowledge into design process and combine them with engineering methods.

The last but not least problem is description of microstructure by means of mathematical and digital methods. In work [46], the microstructure is presented as the key factor that links the different scales during investigations. The authors describe three important types of microstructure representation. The more approximate type is statistical representation that involves statistical tools and instruments. However, the data obtained using these tools cannot provide the highly resolved information for accurate multiscale design valuation. Commonly this type of microstructure representation deals with average value of microstructure parameters such as grain size, aspect ratio, etc. This information as the statistical model of material microstructure is entered into materials equations on the process scale in order to estimate material properties for other scales calculations. On the other hand, there are two more complex types such as Spatial and Numerical representations. In general, any spatial descriptions are based on the use of scalars, vectors and tensors. In order to use numerical algorithms for their calculation and characterization, they must be represented by data arrays with dimension corresponding to the amount of objects/features in the microstructure. Besides the description of objects/features positions, the scalars, vectors and tensors represent concentration fields for individual chemical elements, stress-strain fields and others parameters that allow to describe and take into account various changes in the structure. The Spatial representation method may be based on experimental approach using data from empiric studies (CT, SEM, etc.) or on simulation approach that involves phase-field and crystal plasticity FEM computation algorithms. In addition, the Spatial representation method may use the synthetic approach that use neither experimental nor simulation tools. In fact, this approach involves algorithms that create artificially microstructure design on basis of statistical representation. The third representation method (Numerical) is based on use of voxel type numerical representation and calculation of microstructure. Commonly this method is more suitable for subsequent FEM approaches. More comprehensive description of representation methods is presented in works [47,48, 49].

The described above principles of ICME approach are illustrated in various works. For example, in work [50] the multiscale design is applied to create the car door assembly from fiber reinforced composite material. The main aim is to achieve the best mass-strength ratio. For this purpose, the optimization of composite geometries is performed. The design of door

assembly as well as behavior simulation in case of load applications is performed in ABAQUS software. The assembly components are designed by the use of failure criterion Tsai-Wu and stiffness based deflection criteria. In this case, the preliminary calculation is performed by the use of isotropic material in order to obtain the stress contours and stiffness requirements that can be used for composite structure optimization. For this purpose, a repetitive unit cell model (RUC) is generated by the open source TexGen software. The obtained RUC microstructural models have various structure architectures such as plain, woven and 3D textile weaves. These models are virtually tested with regard to required stiffness parameters generated on the macroscale level until the optimal parameters such as matrix and fiber materials, fibers orientation are obtained. The automatization of ICME approach and data transfer between divided instruments and simulation modules are achieved by a framework based on TCS PREMAP software platform. [50]

In work [38], authors propose a novel framework for FRP parts design that besides traditional CAD/CAE modules includes Computer-Aided Conceptual Design (CACD) tools. According to the authors, the main application of CACD is searching for optimal structure, fiber orientation and distribution in polymer matrix taking into account the minimum fiber consumption requirement. The main object for data representation and transfer between various steps is the heterogeneous feature model (HFM) proposed by the authors. HFM fully describes the fiber-reinforced composite details during design and optimization process and is thoroughly described in work [38]. In general, the HFM is based on structure and material optimization results and is further supplemented by detailed design from CAD modules and processing simulation data from Injection molding CAE tools. The obtained model can be sent to part-scale simulation powered by CAE software. Depended on the obtained results the structure and material optimization can be repeated and the process continues until the optimal solution is obtained.

3.3. Digital Data. Nowadays, it is crucial not just to develop the new materials but also to provide the results of study to all concerned participants of advanced material innovation process. This set of data may significantly help the product designer in choosing the material with certain parameters and properties. [20] For this reason the MGI and ICME are based on creation of open databases that contain significant amount of existing material knowledge. The modern material scientists and engineers have access to the information about advanced materials, materials' structures and properties as well as the information about development of new materials more suitable for their purpose. The existing material databases are represented by Total Materia, Material Data Facility [51], the Material Commons [52], the Material Project [53], the Harvard Clean Energy Project [54], Inorganic Crystal Structure Database [55], the Open Quantum Materials Database [56] and the Cambridge Structural Databases [57].

The main goal of such instruments development is serving the needs of the growing advanced materials research community and providing it with the powerful tools for its work. In fact, the presented databases differ from the usual understanding of this therm. Modern material data bases are not resources with the lists of existing materials and their properties, but cloud platforms for communication and data exchange between participants of the material research and development process.

For example, the Material Commons is a cloud platform and information repository with computation and experimental results, research publications, storing experience and analytic of the current material science state. Moreover, the Material Commons includes abstracts and description of a data models for material processing-structure-property relationships that can be used for ICME design.

Material Data Facility, like the previous platform, is focused on providing wide range of information. This platform makes raw and derived data available in order to provide a more detailed information about methodology of studies and obtained results. The platform creators

believe that the data accompanying research such as models codes, protocols and experimental conditions are of particular interest to use in similar studies or real applications. Thus, Material Data Facility platform provides simplified access to this type of data.

The platforms such as the Materials Projects and the Harvard Clean Energy Project are open-source analytical tools. Such platforms allow performing numerical calculation to define the properties of compounds, to validate the obtained results and make them available to wide auditory. On the other hand, the databases, such as Total Materia, are a source of significant amount of material properties and characteristics that can be exported into numerical software to perform accurate simulation and analysis of designed products. Moreover, such platforms provide information about materials' structures and can determine the material utilizing the chemical composition obtained with the help of spectrometry, which can be useful for re-engineering purposes.

Modern platforms for generation of material data and sharing of research data contribute to the material science growth and advanced material development. The wide range of existing databases provides information that can be useful for various branches of materials study. Moreover, existing data platforms can be integrated into the work processes that use numerical software, which allows to increase quality of obtained results in product design. The combination of ICME approach and open source material databases allows designing and manufacturing highly competitive products with lower costs. These principles are similar to the idea of Factories of Future. For this reason, the implementation of ICME approach supported by open material data bases in the real production process is an important step towards realization of FoF concept.

4. New strategy

As mentioned before the traditional process of product design involves the selection of more appropriate material on the macroscopic level. [12] The described process may be schematically represented as in the Fig. 7.

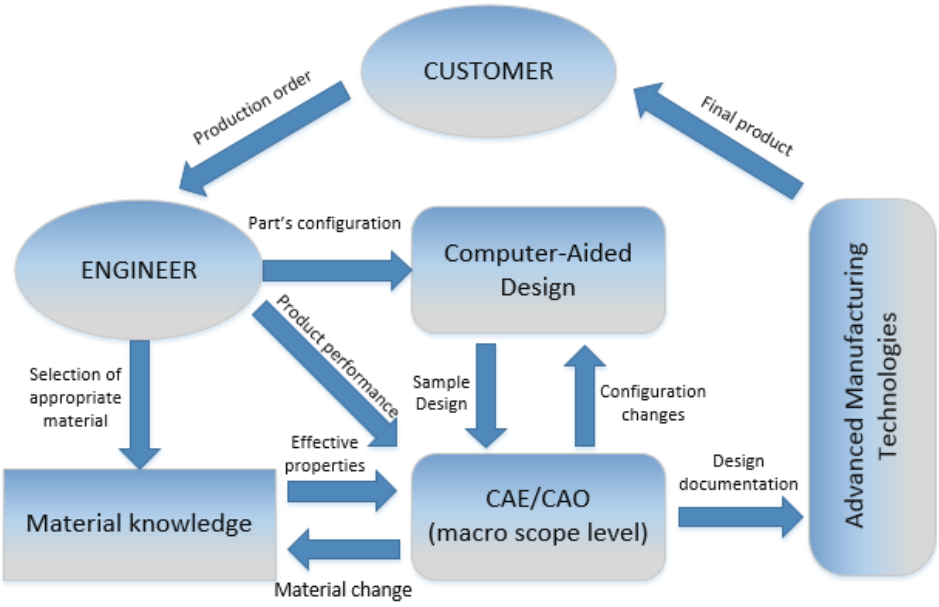

Fig. 7. The traditional process of product design.

An engineer obtains the information about the final product characteristics. Based on this information, engineers create the 3D concept of constructions, prepare calculation models for numerical simulation and optimization as well as set material properties. In this case, the material properties are the effective properties analytically evaluated with no regard to the

microstructure as well as the processing of the materials. This approximate data can be used for product simulation-based design. However, there is less optimization parameters that prevent the creation of the most optimal design. In addition, the lack of information about the microstructure and quality of material processing leads to reduction in accuracy of the product life-cycle prediction.

The ICME approach allows for expanding the boundaries of material selection step. The proposed approach of production design involves study and selection of material parameters on each scope level (macro, meso, micro, nano) in order to maximize product optimization and to take into account all structure and processing features that may influence on the product performance. In the ICME approach the cornerstone is the processing - structure - property - performance (PSPP) relationship. The movement from right to the left (top-down design approach) allows finding many possible variants of material structures that match to the one set of product requirements (performance). The top-down approach is concerned with a study of one-to-many relationships that provide the array of available variants. The bottom-up design is undertaken to take the available variant and due to calculation and simulation to find the most optimal solution. The ICME design approach is a resource intensive method that requires a lot of material science data and involves various numerical and experimental instruments. In order to provide collaboration and data transfer between various tools, the framework connected to open material data bases is used. Nowadays, there is no universal framework for ICME product design. However, according to Section 3 the ICME approach may be illustrated by the scheme presented on the Figure 8.

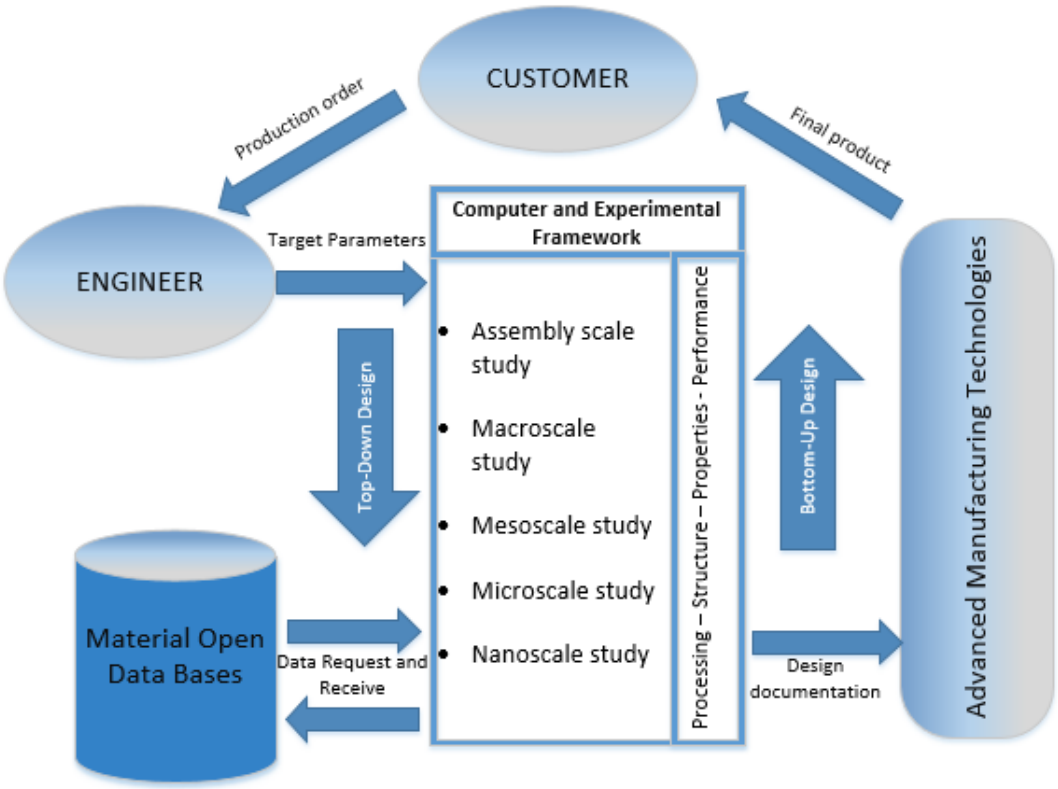

Fig. 8. A schematic representation of ICME approach.

However, the combination of experimental and numerical instruments proposed by ICME approach also has some limitations. Both of these instruments are based on theoretical knowledge that is represented in algorithms and analytical relations. Although, the MGI leads to the accelerated development of material science, it is quite difficult to represent PSPP

relationships by computational models and algorithms. It is particularly true for advanced materials, PSPP relationships for which can even be unknown. For this reason, the intelligent and high-performance analyzing algorithm for accurate prediction of material performance is required. Considering the existence of open data bases with colossal amount of material information, the Big Data concept can be mentioned as one of the possible ways to improve design approach. In general, the big volume of valid information from various sources that is being updated with high velocity can be characterized as Big Data. The various algorithms and methods such as Machine Learning, Deep learning, etc. can be used for processing of such open resources and creation of prediction models involved into product design.

In general, the Machine learning as the method for automation creation of prediction model use algorithm that iteratively compares the feature relations from available data in order to find hidden insights non-obvious in terms of the existing theory. According to [58] the basic idea of using machine learning methods for design process is to automate the analyzing and mapping of the nonlinear relationships between the processing-structure-properties-performance features by extracting knowledge from existing empirical data. The result of this method utilization is the model that can be applied for current product design as well as for dealing with the similar design orders in the future.

According to work [59], obtaining of prediction model requires the setting of “goal”, “sample” and “algorithm”. The term “sample” implies the presence of significant volume of available information such as experimental data, protocols, computation results, etc. provided by open source material data bases. In fact, the sample preparation is the first basic step for machine learning method. (Fig. 9) The preparation involves data cleaning from noise and incomplete elements as well as reduction of the amount of inadequate information. In addition, the sample preparation involves feature engineering step that provide some simple physical basis for extraction of main structural and chemical trends to provide fast and accurate material performance prediction. [59]

Fig. 9. Basic steps of Machine Learning approach.

The well-prepared sample is the input information for the second basic step - “model building”. The core of this method is the algorithm used for data learning and prediction model generation. For these purpose, the “algorithm” is set of operations with input information that performed under control of “goal” parameters, that may be illustrated by scheme presented in Fig. 10. The “goal” is the target characteristics that must be achieved and used for study of the provided “sample”. The most commonly used algorithms for machine learning is Naive Bayes [60], Logistic regression [61] as well as Linear regression [62], Support vector machine [63], Logistic model tree [64] and Artificial neural networks [65]. The selection of appropriate algorithm is based on the task of prediction and target parameters. In case numerical target parameter such as fatigue strength, etc., the algorithms based on the regression methods is more effective. The target parameters represented by categorical information involves usage of classification techniques and relevant algorithms. In general, the commonly used algorithms are Artificial neural networks (ANN) and Support vector machine (SVM) as the algorithms capable to use both regression and classification techniques.

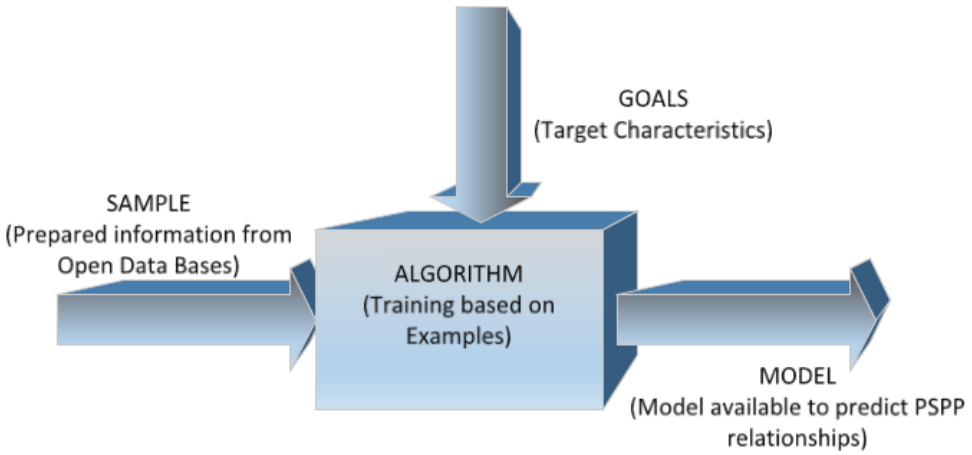

Fig. 10. Principle of Model building step.

The process of model building is similar to training by using existing examples. However, the obtained model with mapping function and set of various approximation coefficients, might be able to deal only with the data that was used during the training and be unsuitable for work with previously unseen data. In this case, the model cannot be considered as valid and cannot be used for purposes of product design. The obtained model must be evaluated. Commonly for this purpose the information obtained from data bases is divided into training set used for sample preparation and testing data set. Testing data sets are proposed to the obtained prediction models obtained in order to validate the model suitability. There are various methods of test sets preparation. In general, the initial amount of data is partitioned in proportion of 2/3 to training data and 1/3 to test data (Hold-out method). In case of cross-validation method, the initial data can be divided into *k* mutually exclusive subsets of the same size and the *(k-1)* sets is the training data set.

Results obtained during evaluation tests allow for evaluating the quality and accuracy of the created prediction model that is vital for their implementation into product design process. According to [60, 59], the model error is represented by the mean absolute percent error (MAPE), the root mean square error (RMSE) and the correlation coefficient (R^2).

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|y'_i - y_i|}{y_i}, \tag{41}$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y'_i - y_i)^2}, \tag{42}$$

$$R^2 = \frac{\left[\sum_{i=1}^{n}(y_i-\bar{y})(y'_i-\overline{y'})\right]^2}{\sum_{i-1}^{n}(y_i-\bar{y})^2\cdot\sum_{i-1}^{n}(y'_i-\overline{y'})^2}, \tag{43}$$

where y_i and y'_i are the original values from SAMPLE and the predicted value by using of obtained model, respectively; $\bar{y}$ and $\overline{y'}$ are the averages of the original and predicted values, respectively. [59]

The example of use of Machine Learning and Big Data concepts can be found in work [66]. The authors propose the framework for determining material genome of granular minerals. The proposed framework uses the mineral databases as the source of granular material genome information. The genome of granular materials represents the “parent rocks”, weathering process as well as the mineral composition and structure. The available instruments for genome

study are experimental tools such as scanning electron microscopy (SEM), transmission electron microscopy (TEM), Energy-dispersive X-ray (EDX), etc. According to work [66], these techniques make it possible to link mineral composition with the shape, texture and other morphological characteristics of particles. However, performing these experimental investigations is time consuming. More reasonable approach is to use open data base that can be filled by researches related to this area of material science. The information about minerals presented in data base must involve reference number, mineral, chemical composition, crystal structure information, typical grain size, etc. In addition, the mechanical properties obtained from laboratory experiments and transferred to multiple scales by means of computer simulation approach must be sent to this data base. Significant volume of information accumulated in mineral data base can be considered as a Big Data. The authors, proposed to use algorithms for Big Data processing in order to define relationships between genome and mechanical properties of granular materials. The obtained prediction model can allow for developing materials with required properties as well as reducing the timeline from discovery to implementation of granular materials.

These works among the others [67, 68, 69, 70] show the significance of the role of Big Data and Machine Learning methods for development of new materials. On the other hand, there is a limited number of works that connect the Big Data concept with product design. However, according to [58], Machine Learning is capable of providing model that can be used for both the direct (bottom-up) and for the reverse (top-down) prediction of materials PSPP relationships. This feature is similar to the ICME multiscale design concept that allows making assumption that Big Data and Machine Learning concepts can be used for product design based on ICME approach. The schematic representation of this idea may be represented by Fig. 11.

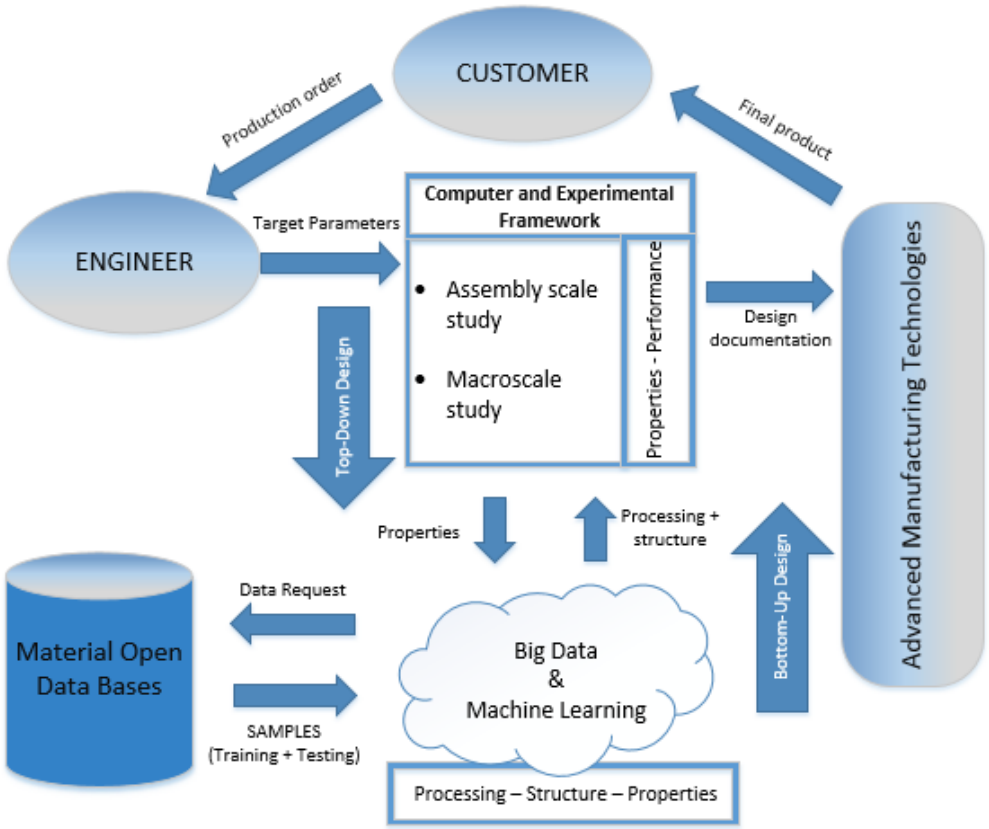

Fig. 11. Product design based on ICME and Machine Learning approaches.

Theoretically, the usage of Machine Learning can automate the design process on the nano-, micro- and mesoscale levels by providing prediction models taking the input information

about material properties giving the best structural and processing solutions without involving the additional tools into this optimization process. The simulation of product performance based on the material properties and working conditions is still performed by CAE/CAO macroscale systems under engineers' control. Study of properties-performance relationships by traditional algorithms provides the optimization criteria for prediction model building by the means of Machine Learning. Although, Machine Learning is able to accelerate the process of choosing the optimal material processing and structure solutions, their usage is associated with some limitations. For example, preparation of significant amount of unstructured data and their further analysis require for utilization of high-performance computation resources that might be unavailable. Moreover, the creation of prediction models for specific product design purpose takes time and can be more complex comparing with the existing computer or experimental measurement instruments. However, when developed, such models can be used for design of similar products in future. Thus, the communication environment and open libraries or data bases that publish prepared prediction models are critical for such product design approach. (Fig. 11)

In addition, the implementation of Big Data analysis into the product design process allows for development of digital product models with more information comprehensively characterizing the designed objects. In case of the computer and experimental investigation the obtained information is limited by existing theoretical knowledge while the Big Data analysis can provide links that can be unknown for material science but have significant influence on final product quality. Thus, the implementation of Big Data analysis and Machine Learning approach can be significant push for improvement of Product Life-Cycle management as well as for creation of best-in-class products that is the goal of FoF concept.

5. Conclusions

In this work, the review of advanced material representation approaches for product design purpose is presented. The basic information about traditional approaches in simulation of fiber-reinforced composites structure as well as calculation algorithms for analyzing of details made from composite materials are described to illustrate the influence of the accuracy of material data on the quality of prediction of final product performance. In general, the effective properties of composite materials are used for product simulation. Considering the results obtained by the use of the analytical methods as average values for components properties, the effective parameters of composite materials for numerical simulation can be used as an approximate evaluation of the designed products. Thus, the development of more complex frameworks and related computing tools is required for improving Product Life-Cycle management and creation of best-in-class products. Some solutions developed within the Material Genome Initiative (MGI) are represented in this work. Key solutions are related to combination of experimental and computer aided R&D methods as well as the creation of communication environment for cooperation and sharing of generated material science data. The creation of such open material data bases contributes to accumulation of huge amount of experimental and simulation data that can provide comprehensive information about processing-structure-properties-performance relationships for advanced materials. That information lays the foundation for effective product design and simulation. The implementation of Big Data analysis utilizing Machine Learning algorithms in ICME approach allows to automate of material structure optimization and provides engineers with powerful tools for the most efficient optimization of designed product available.

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References

[1] C. Featherston, E. O'Sullivan, *A review of international public sector strategies and roadmaps: A case study in Advanced Materials. A report for Government Office of Science & the Department for Business, Innovation & Skills* (Center for Science Technology and Innovation, Institute for Manufacturing, University of Cambridge, Cambridge, 2014).
[2] https://www.cimdata.com/de/resources/complimentary-reports-research/commentaries/item/3345-design-with-confidence-commentary/3345-design-with-confidence-commentary
[3] A.G. Kotov, *CAD of products from composite materials. Modeling of the processes of deformation and destruction by the ANSYS software* (Publishing house of Perm. state. tech. university, Permian, 2008). (in Russian).
[4] P. G. Young, T. B. H. Beresford-West, S. R. L. Coward, B. Notarberardino, B. Walker, A. Abdul-Aziz // *Philosophical Transactions of the Royal Society A* **366** (2008) 3155.
[5] L. Guibas, J. Stolfi // *ACM Transactions on Graphics* **4(2)** (1985) 74.
[6] C. Lawson, *Software for C^1 Surface Interpolation.* In: Mathematical Software III (Academic Press, NY, 1977) 161.
[7] A.V. Skvortsov, *Delaunay triangulation and its application* (Tomsk University Publishing House, Tomsk, 2002). (in Russian).
[8] S. A. Berggren, D. Lukkassen, A. Meidell, L. Simula // *Applications of Mathematics* **48(2)** (2003) 87.
[9] D. R. H. Jones, M. Ashby, *Engineering Materials 1. An Introduction to Properties, Applications and Design.* 3rd Edition (Butterworth-Heinemann, Oxford, 2005).
[10] M. Ashby, *Material Selection in Mechanical Design.* 3rd Edition (Butterworth-Heinemann, Oxford, 2005).
[11] H. Pettermann, *Continuum Mechanics Modeling of Composite Materials* (Technischen Universitat Wien, Vein, 2003).
[12] Z. Hashin // *Journal of Applied Mechanics* **50(3)** (1983) 481.
[13] Xiaowei Ouyang, Guang Ye, Klaas van Breugel // *Construction and Building Materials* **135** (2017) 538.
[14] C.P. Sturrock, E.F. Begley, *Computerization and Networking of Materials Databases: Fourth Volume* (ASTM International, 1995).
[15] Yu.V. Skvortsov, S.V. Glushkov, A.I. Khromov, *Modeling of composite structural elements and analysis of their destruction in CAE-systems MSC. Patran-Nastran and ANSYS* (Samara, 2012). (in Russian).
[16] H. E. Pettermann, H. J. Bohm, J. Alcala // *Metallurgical and Materials Transactions A* **33(10)** (2002) 3187.
[17] Carmen Calvo-Jurado, William J. Parnell // *Journal of Computational and Applied Mathematics* **318** (2017) 354.
[18] Inch-Long Ngo, S. V. Prabhakar Vattikuti, Chan Byon // *International Journal of Heat and Mass Transfer* **114** (2017) 727.
[19] Yasser Zare // *Polymer Testing* **51** (2016) 69.
[20] John P. Holdren *Materials Genome Initiative for Global Competitiveness* (Executive office of the president national science and technology council, Washington D.C., 2011).
[21] Yach Agarwal, Wojciech Smigaj, Philippe G. Young, Ross Cotton, Patrick Tompsett // *Materials Today: Processings* **4** (2017) 1860.
[22] I. G. Watson, P. D. Lee, R. J. Dashwood, P. Young // *Metallurgical and Materials Transactions A* **37(3)** 551.

[23] R. Cotton, P. Tompsett, W. Smigaj, K. Genc, P. G. Young, In: *NAFEMS World Congress* (21 – 24 June, San Diego, CA, 2015).
[24] T. You, R. Abu Al-Rub, E. Masad, D. Little // *Transportation Research Record: Journal of the Transportation Research Board* **2373** (2013) 63.
[25] T. You, R. K. Abu Al-Rub, M. K. Darabi, E. A. Masad, D. N. Little // *Construction and Building Materials* **28(1)** (2012) 531.
[26] T. You, R. K. Abu Al-Rub, E. A. Masad, E. Kassem, D. N. Little // *Journal of Materials in Civil Engineering* **26(4)** (2014) 607.
[27] E. Coleri, J. T. Harvey, K. Yang, J. M. Boone // *Construction and Building Materials* **30** (2012) 783.
[28] Yang Liu, Ilya Straumit, Dmytro Vasiukov, Stepan V. Lomov, Stephane Panier // *Composite Structure* **179** (2017) 568.
[29] N. Naouar, E. Vidal-Sallé, J. Schneider, E. Marie, P. Boisse // *Composite Structure* **116** (2014) 156.
[30] Ilya Straumit, Stepan V. Lomov, Martine Wevers // *Composites Part A: Applied Science and Manufacturing* **69** (2015) 150.
[31] T. Wandowski, P. Kudela, P. Malinowski, W. Ostachowicz // *Health Monitoring of Structure and Biological Systems* **9805** (2016).
[32] C. Willberg, S. Koch, G. Mook, J. Pohl, U. Gabbert // *Smart Materials and Structures* **21(7)** (2012).
[33] P. Kudela, T. Wandowski, P. Malinowski, W. Ostachowicz // *Optics and Lasers in Engineering* **99** (2017) 46.
[34] O. L. Warren, T. J. Wyrobek // *Measurement Science and Technology* **16(1)** (2004) 100.
[35] Joshua S. Dustin, Richard Dalgarno, Matt Hockemeyer, *Lessons Learned from the Development of a Structural Finite Element Progressive Failure Simulation for Integration into the ICM2 Framework* (AIAA SciTech, San Diego, 2016).
[36] Karthik RM, Bhaskar Patham, Swaroop Kavi, Virupakshappa Lakkonavar, Jayaraj Radhakrishnan // *Materials & Design* **89** (2016) 727.
[37] Jitesh H. Panchal, Surya R. Kalidindi, David L. McDowell // *Computer-Aided Design* **45(1)** (2013) 4.
[38] Jikai Liu, Yongsheng Ma, Junyu Fu, Kajsa Duke // *Advances in Engineering Software* **87** (2015) 13.
[39] Yong-Jie Hu, Yi Wang, Samad A. Firdosy, Kurt E. Star, Jean-Pierre Fleurial, Vilupanur A. Ravi, Zi-Kui Liu // *Calphad* **59** (2017) 207.
[40] Zi-Kui Liu // *Journal of Phase Equilibria and Diffusion* **30** (2009) 517.
[41] Mehdi Hosseinifar, Dmitri V Malakhov // *Journal of Alloys and Compounds* **505(2)** (2010) 459.
[42] Andriy O. Lyakhov, Artem R. Oganov, Harold T. Stokes, Qiang Zhu // *Computer Physics Communications* **184(4)** (2013) 1172.
[43] Maribel Núñez-Valdez, Zahed Allahyari, Tao Fan, Artem R. Oganov // *Computer Physics Communications* **222** (2018) 152.
[44] Geoffroy Hautier, Chris Fischer, Virginie Ehrlacher, Anubhav Jain, Gerbrand Ceder // *Inorganic Chemistry* **50(2)** (2011) 656.
[45] S. V. Dudiy, A. Zunger // *Physical Review Letters* **97(4)** (2006).
[46] G. J. Schmitz, H. Farivar, U. Prahl // *Integrating Materials and Manufacturing Innovation* **6(1)** (2017) 127.
[47] Georg J. Schmitz, Ulrich Prahl, *Handbook of Software Solutions for ICME* (Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2016).
[48] A. Reid, S. Langer and S. Keshavarz, *OOF: Flexible finite element modeling for materials science* (2nd International Workshop on Software Solutions for ICME, Barcelona, 2016).

[49] A. S. Bhadauria, C. Agelet de Saracibar, M. Chiumenti, M. Cervera, *A new approach to interoperability using HDF5* (2nd International Workshop on Software Solutions for ICME, Barcelona, 2016).
[50] Azeez Shaik, Yagnik Kalariya, Rizwan Pathan, Amit Salvi, *ICME Based Hierarchical Design Using Composite Materials for Automotive Structures.* In: Proceedings of the 4th World Congress on Integrated Computational Materials Engineering (ICME 2017) (2017) 33.
[51] B. Blaiszik, K. Chard, J. Pruyne, R. Ananthakrishnan, S. Tuecke, I. Foster // *JOM* **68(8)** (2016) 2045.
[52] Brian Puchala, Glenn Tarcea, Emmanuelle A. Marquis, Margaret Hedstrom, H. V. Jagadish, John E. Allison // *JOM* **68(8)** 2035.
[53] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek // *Apl. Materials* **1(1)** (2013) 011002.
[54] J. Hachmann, R.Olivaresamaya, S. Atahanevrenk, C. Amadorbedolla, R. S. Sanchezcarrera, A. Goldparker // *The Journal of Physical Chemistry Letters* **2(17)** (2011) 2241.
[55] A. Belsky, M. Hellenbrandt, V. L. Karen, P. Luksch // *Acta Crystalloqr B* **58** (2002) 364.
[56] S. Kirklin, J. E. Saal, B. Meredig, A. Thompson, J. W. Doak, M. Aykol // *npj Computational Materials* **1** (2015) 15010.
[57] F. H. Allen // *Acta Crystalloqr B* **58** (2002) 380.
[58] Ankit Agrawal, Alok Choudhary // *APL Materials* **4** (2016) 053208.
[59] Yue Liu, Tianlu Zhao, Wangwei Ju, Siqi Shi // *Jiurnal of Materiomics* **3(3)** (2017) 159.
[60] George H. John, Pat Langley, In: *Proceedings of the Eleventh Conference on Uncertainty in Artificial Intelligence* (1995) 338.
[61] D. Hosmer, S. Lemeshow, *Applied Logistic Regression* (John Wiley and Sons, Inc., 1989).
[62] Allen L. Edwards, *An Introduction to Linear Regression and Correlation (Series of Books in Psychology)* (W. H. Freeman and Comp., San Francisco, 1976).
[63] V. N. Vapnik, *The Nature of Statistical Learning Theory* (Springer, 1995).
[64] Niels Landwehr, Mark Hall, Eibe Frank // *Machine Learning* **59(1-2)** (2005) 161.
[65] C. Bishop, *Neural Networks for Pattern Recognition* (Oxford University Press, 1995).
[66] Wenjuan Sun, Wenjing Xue, Yinning Zhang, Linbing Wang // *International Journal of Pavement Research and Technology* (2017). (in Print).
[67] ViníciusVeloso de Melo, WolfgangBanzhaf // *Neurocomputing* **246** (2017) 25.
[68] Zhen Liu, Yifan Li, Diwei Shi, Yaolin Guo, Mian Li, Xiaobing Zhou, Qing Huang, Shiyu Du // *Scripta Materialia* **143** (2018) 129.
[69] Ashley A. White // *MRS Bulletin* **38(8)** (2013) 594.
[70] Sergei V. Kalinin, Bobby G. Sumpter, Richard K. Archibald // *Nature Materials* **14** (2015) 973.