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Establishment of the Most Effective Methods of Obtaining Nanosize Magnesium Oxide

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The relevance of the research is based on the development of nanometallurgy, which is an adequate response to the growing demand and expansion of the fields of application of nanoparticles of metallic oxides. Scientific and engineering thought is constantly searching for solutions to optimise and modernise the production of target nanosize metallic oxides that leads to the establishment of a significant scientific and informational landscape, which currently does not provide an unambiguous answer regarding the single methodology for obtaining the target product (in this case, nanosize magnesium oxide) that requires additional research and appropriate analytical conclusions. Therefore, the purpose of this study is to determine the technological method of manufacturing nanosize magnesium oxide, which has the most effective and competitive indicators, as well as to check the possibility of using digital modelling tools to optimise production processes in nanometallurgy. To achieve the formulated goal, the methods of digital modelling of the magnesium-oxide nanolattice and corresponding analytical conclusions and proposals are used in the current research. The study establishes that, among the seven typical methods of obtaining nanosize magnesium oxide (combustion in solution, co-precipitation, sol–gel, hydrothermal synthesis, solvothermal synthesis, sol–gel using microwaves, green synthesis), the most effective for the industrial production of the target nanomaterial are sol–gel and coprecipitation. The technological method of green synthesis of nanopar-

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ticles of metallic oxides (including nano-MgO) is also relevant, which is more ecological with competitive industrial and technological indicators of the production process. The conclusions obtained during the analysis of chronotaxometric schemes, which are the result of a bibliometric analysis of scientific studies and publications on the leading scientometric resources, indicate an increase in the variability of possible areas of use and production of metallic oxides in nanoforms, which indicates the dynamic and extensive stage of development of nanometallurgy. Digital modelling of the desired magnesium-oxide nanolattice helps to optimise the technological process and can be involved in the industrial field of nanometallurgy as a design stage. The practical value of the study is to obtain a correlative systematisation of various technologies for obtaining magnesium-oxide nanoparticles and to assess the impact of the design and modelling stage on the development of nanometallurgy in general.

Key words: nanometallurgy, sol–gel, hydrothermal synthesis, manufacturing, microwaves.

Актуальність дослідження ґрунтується на розвитку нанометалурґії, яка є адекватною відповіддю на зростаючий попит і розширення сфер застосування наночастинок оксидів металів. Наукова й інженерна думка здійснює постійний пошук рішень для оптимізації та модернізації виробництва цільових нанорозмірних оксидів металів, що приводить до створення значного науково-інформаційного ландшафту, який наразі не дає однозначної відповіді щодо єдиної методології одержання цільового продукту (в даному випадку нанорозмірного оксиду Маґнію), що потребує додаткових досліджень і відповідних аналітичних висновків. Тому метою даного дослідження є визначення технологічного методу виготовлення нанорозмірного оксиду Маґнію, який має найбільш ефективні та конкурентоспроможні показники, а також перевірка можливости використання інструментів чисельного моделювання для оптимізації виробничих процесів у нанометалурґії. Для досягнення сформульованої мети в даному дослідженні використано методи чисельного моделювання маґнійово-оксидної наноґратниці та відповідні аналітичні висновки та пропозиції. У результаті дослідження встановлено, що серед сімох типових методів одержання нанорозмірного оксиду Маґнію (спалювання в розчині, співосадження, золь–ґель, гідротермальна синтеза, сольвотермічна синтеза, золь–ґель за допомогою мікрохвиль, зелена синтеза) найбільш ефективними для промислового виробництва цільового наноматеріялу є золь–ґель і копреципітація. Актуальним є також технологічний метод зеленої синтези наночастинок оксидів металів (у тому числі нано-MgO), який є більш екологічним за конкурентоспроможних промислово-технологічних показників виробничого процесу. Висновки, одержані під час аналізи хронотаксометричних схем, які є результатом бібліометричної аналізи наукових досліджень і публікацій на провідних наукометричних ресурсах, свідчать про збільшення варіятивности можливих сфер використання й одержання оксидів металів у наноформах, що свідчить про динамічний та екстенсивний етап розвитку нанометалурґії. Чисельне моделювання бажаної маґнійово-оксидної наноґратниці допомагає оптимізувати технологічний процес і може бути задіяне в промисловій сфері нанометa-

лурґії як етап проєктування. Практична цінність дослідження полягає в одержанні кореляційної систематизації різних технологій одержання магнійово-оксидних наночастинок та оцінці впливу етапу проєктування та моделювання на розвиток нанометалурґії в цілому.

Ключові слова: нанометалурґія, золь–ґель, гідротермальна синтеза, виробництво, мікрохвилі.

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1. INTRODUCTION

The research vector for determining effective technologies for producing metal nanooxides is updated by the trend dynamic growth of the field of nanometallurgy, as evidenced by the relevant industry statistics: according to Custom Market Insight, the volume of global demand for consumption of nanomaterials in the form of metal oxides according to the results of 2022 is estimated at 1.11 billion USD [1]. The same indicator is expected to increase by 2 billion USD by 2030. The total compound annual growth rate (CAGR) is 7.53%. Similar, but somewhat more optimistic indicators of the CAGR are provided by specialised organisations (for marketing assessment of markets) Reports and data [2], Industry ARC [3], and Data Intelo [4], which estimate the growth dynamics of the global nanometallurgy market at the level of 9.2–9.4% of the CAGR. Estimates of Custom Market Insight [1] and Data Intelo [4] regarding the qualitative structure of demand for metal oxide nanometres coincide:

- proportion of aluminium oxide is the highest – 35%;
- proportion of titanium dioxide – 22%;
- proportion of copper oxide – 16%;
- proportion of magnesium oxide – 14%;
- proportion of zinc oxide – 9%;
- proportion of other metal oxides – 4%.

Similarly, the estimates of these marketing and analytical companies regarding the global industry structure of the consumer market coincide: the share of electronics and optics is the largest – 38%, the share of medicine and hygiene products – 26%, the share of the paint and varnish industry – 14%, the share of the energy industry – 12%, other industries – 10%. Custom Market Insight provides a wider and more detailed range of consumer structures for nanometallurgy products, which, in addition to the above categories, includes the automotive, ceramic and glass industries [1].

The target product of the current study is nano-MgO; so, the marketing dynamics of this nanomaterial will be considered in detail. As noted in Mordor Intelligence, according to the results of 2022, the global consumption market for nanoscale magnesium oxide is estimated at 155.4 million USD (which correlates with Custom Market Insight [1] and Data Intelo [4] estimates), and the CAGR is expected to reach 7% by 2028-2030 (which is a somewhat restrained estimate compared to Reports and Data [2] and Data Intelo [4], but correlates with industry-wide nanometallurgy statistics provided in the marketing research at Custom Market Insight [1]) [5]. Mordor Intelligence also notes the industry structure of magnesium-nanooxide consumers, which differs from the above for the general field of nanometallurgy by including such consumers as the production of refractory materials, the aerospace industry, and the oil refining industry [5]. Thus, market and marketing dynamics and corresponding specific indicators indicate the unconditional development of the nanometallurgy industry, in particular, the sector of nanoscale magnesium oxide, which actually proves the relevance and expediency of research to find solutions to optimise, modernise, and increase the economic attractiveness of the target nanomaterial production system.

Recent studies, the results of which are reported by F. Nisa *et al.* [6] (on the use of nano-MgO biosynthesis technology), M. Kotresh *et al.* [7] (on the temperature regimes of production of nanosize magnesium oxide), Z. Rajabimashhadi *et al.* [8] (on the use of hydrothermal methods for the production of magnesium oxide nanoparticles) in the review parts contain generalisations about the existence of a fairly wide range of technological methods for the production and synthesis of the target nanomaterial, which mostly bear signs of laboratory-scale production and do not form ideas about the generalised optimised technology for the production of nanosize magnesium oxide for industry (except for individual proposals in the form of publications by F. Mirza and H. Makwana [9], in which the co-precipitation method is preferred). Also noteworthy are the studies by J. Veronica *et al.* [10] (which favours the sol–gel method), S. Abinaya *et al.* [11] (which favours the green synthesis method), which in general do not form a stable and consistent vector of commitment to any one prevailing method of producing the target nanoproduct).

Therefore, the appropriate basis of scientific problems is formed, according to which it is necessary to perform a correlative and systematic comparison of existing technologies for the production and synthesis of nano-MgO and determine the most optimised and adaptive production and technological method for industrial and economically attractive applications. Therefore, the purpose of the current study is to establish, based on the results of comparative analysis, the most adapted method for the production of magnesium oxide nanoparticles within the framework of the nanometallurgy paradigm, followed by the proposals and recommendations for the potential development of the latter, and to test in detail the hypothesis of the potential applicability of modern digital software tools for optimising technological processes in the production of metal oxide nanoparticles.

2. MATERIALS AND METHODS

Firstly, the method of median analysis was used to form the basis of scientific problems. This method facilitated the development an appropriate factual background, conceptual and taxonometric structure, and allowed establishing the latest achievements of the nanometallurgy sector under study. In particular, it was possible to obtain up-to-date data on the characteristics of the studied nanomaterial (in comparison with the full-size (macrosize) equivalent), data on the areas of application of the target nanoproduct with an appropriate assessment of the industry impact, and data on the establishment of the classification of laboratory methods for the production of nanoscale magnesium oxide, which became the basis for the latest iteration of the study – an analytical solution to the goal.

Secondly, as the next iteration, the method of generalising the relevant scientometric landscape in the current chronometric horizon (over the past five years) was applied, which determined the general trends and vectors of interest in the dynamics of scientific and engineering thought in the development of technology for the production of nanoscale magnesium oxide and confirm (or refute) the results of the first iteration of the study. The logical conclusion of the previous iterations of the search and generalisation of the existing scientometric landscape and the basis of scientific problems was the correlation and systematic analysis of the classification of laboratory and production methods for the production of magnesium nanooxide with the definition of the most effective technological methods adapted to the industrial scale.

The empirical part of the study consisted of testing the influence of digital programme modelling methods of nanostructures on the technological sequence of production of the target product. That is, in this case, the nano-MgO modelling method was used. Among the software tools used for modelling and forecasting design nanomaterials are BIOVIA Materials Studio [12], Integrated Scientific Computing and Information Technologies [13], Synopsys 14, Informer Technologies [15], Furious Atoms [16], CoNTub [17], Atelgraphics SL [18], Exabyte Inc. [19], JCMwave [20], LAMMPS [21], which allow for full-fledged modelling of nanostructures of various chemical elements, which are subsequently subjected to the corresponding calculated spectrum with a wide range of variability, which leads to an optimal resulting nanogrid, both individual metal oxides (including nano-MgO) and composite structures.

Most of these software products were designed for nanotube design, but BIOVIA Materials Studio [12] has the greatest variability in compositing various structures and chemical compositions, so this software is used as the basis for creating a digital programme model of nanoscale magnesium oxide. The resulting model allows including design stages in the production technology of nanometallurgy, which can potentially reduce the load on laboratory research and diagnostic stages, thereby increasing the economic attractiveness of the industry under study.

Thus, based on analytical iterations No. 1 and No. 2, the most adapted nano-MgO production method for industrial applications was established, and with the help of empirical iteration No. 3, the potential possibility of using modern digital software tools to optimise the technology of metal nanoparticle production was tested.

3. RESULTS

The characteristics of magnesium oxide in the nanoform were investigated by M. Rajab *et al.* [22], J. Hornak *et al.* [23, 24], J. Chen [25], S. Vijayakumar *et al.* [26]. J. Hornak *et al.* [23, 24]. The researchers put forward the idea that nanoscale magnesium oxide does not differ in chemical composition and molecular structure from natural full-size magnesium metal oxide, namely, the MgO lattice with the lattice parameter 4.21, and consists of Mg^{2+} and O^{2-} ions, which are connected by an ionic bond by configuration $1s^2 2s^2 p^6 3s^2$ (Mg) and $1s^2 2s^2 p^4$(O) (without filling the d-orbital) and consist of two crossed lattices (grids) that are shifted relative to each other by 0.5 diagonals of the body. These data are confirmed empirically in the study by F. Mirza and H. Makwana using energy-dispersive x-ray spectroscopy [9]. Similar results are provided by S. Vijayakumar *et al.* [26]. According to the results of energy-dispersive x-ray spectroscopy, the percentage of magnesium and oxygen is close to the stoichiometric ratio, and the chemical purity of the nanoscale oxide under study is confirmed.

F. Mirza and H. Makwana [9] and M. Rajab *et al.* [22] also note other differences between nano-MgO and full-size MgO, including, in particular, a high value of the band gap parameter (7.3–7.8 eV); a high value of the volume resistance parameter of 1.017 Ohm·m (which is the maximum value for nanoscale metal oxides that are currently widely used); high thermodynamic stability due to low heat capacity and high melting point (2850°C), that obtained a response in the use of the studied material in the production of refractories; low permittivity (9.8) used for creating insulation materials; low distortion of the refractive index.

These advantages of nanoscale magnesium oxide distinguish it not only from the full-size form of MgO oxide, but also from other widely used metal nanooxides. For example, nano-MgO is an excellent transition layer for growing thin-film materials for various purposes [26].

F. Mirza and H. Makwana [9], M. Rajab *et al.* [22], J. Hornak *et al.* [23, 24], J. Chen [25], S. Vijayakumar *et al.* [26] note that nano-MgO is characterised by peaks of the 2θ angle values on the crystal lattice diffraction pattern (obtained by x-ray diffraction method): 36.8°, 42.9°, 62.2°, 74.6°, and 78.6°, which are identified as the corresponding values of the lattice areas of nanoscale magnesium oxide (111), (200), (220), (311), and (222). In addition, F. Mirza and H. Makwana [9] and J. Hornak [24] highlight the possibility of identifying the structure of magnesium nanooxide using the Fourier transform infrared spectroscopy method, the image of which is characterised by corresponding peaks with physicochemical decoding of the constituent elements and their interaction at the molecular level.

As noted by J. Hornak [23, 24] and S. Vijayakumar *et al.* [26], to determine the characteristics of nano-MgO, it is also advisable to use the method of ultraviolet-visible spectroscopy, in particular, to establish a quantitative characteristic of the band gap energy parameter, and similar results can be obtained using the photoluminescence method. Temperature–frequency graphs are also used to interpret the thermal stability and relative permittivity of nanoscale magnesium oxide, illustrating the effect of the temperature regime on the dielectric properties of the metallic magnesium oxide nanoform, which is a consequence of the influence of weakly bound water molecules on the surface of the material.

Visualisation of magnesium oxide nanoformations is obtained by F. Mirza and H. Makwana using scanning electron microscopy [9]. According to the results of scanning electron microscopy, nanoscale formations are synthesised with a minimum size of 14 nm, while structuring into agglomeration clusters. Data obtained by the researchers and the frequency of formation of classes of magnesium oxide nanoparticles by size characteristic were confirmed by J. Chen [25]. However, one of the main features of MgO nanoparticles (NPs) is its high antibacterial activity, which is confirmed by numerous studies, among which the papers by A. Khan *et al.* [27], J. Maji *et al.* [28], N. Baniasadi *et al.* [29], B. Das *et al.* [30], L. Cai *et al.* [31]. However, this property is more clearly confirmed and illustrated in the study by N. Y. Nguyen *et al.* [32]. The researcher was able to record the alleged destruction of the membrane of bacterial microorganisms.

Thus, considering the relatively and objectively distinguishing characteristics of the magnesium oxide nanoform among other metal nanooxides, industries and sectors have now been formed where the use of the nanomaterial under study is a priority, and sometimes there is no alternative.

Based on the obtained data of multilocal information search against the background of the scientometric landscape in relation to the areas of application of nanoscale magnesium oxide, it was found that the

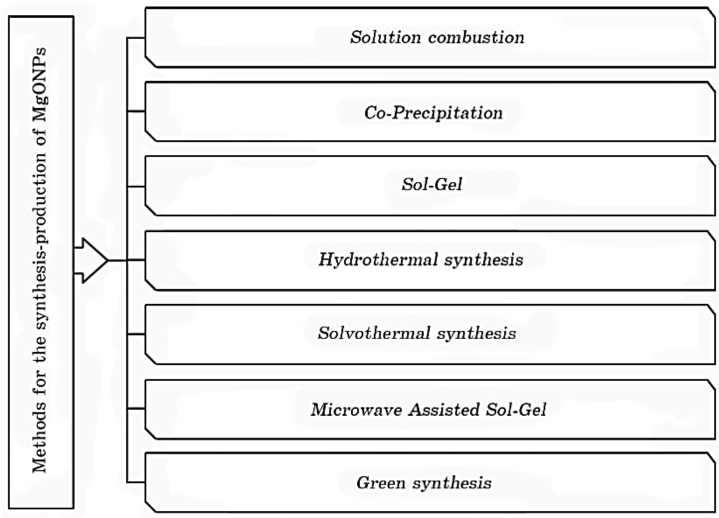


Fig. 1. System of existing methods of synthesis and production of MgO NPs [22–26].

range of use of the nanomaterial under study is quite wide: from medical applications to nanometallurgy, which correlates with the data of marketing studies by Custom Market Insight [1], Data Intelo [4], and Mordor Intelligence [5]. Currently, there are about seven methods of MgO NPs synthesis and production, which have a fairly wide range of technological features (Fig. 1).

The characteristics of each method of synthesis and production of magnesium nanooxide are given in order to establish the characteristic technological features of the implementation of the process under study. Using the results of review and empirical studies by F. Mirza and H. Makwana [9], M. Rajab *et al.* [22], J. Hornak *et al.* [23, 24], J. Chen [25], S. Vijayakumar *et al.* [26], in order to establish an optimal and economically feasible method for the synthesis and production of magnesium oxide nanoparticles (among the methods described in Fig. 1), the median (due to the existence of a significant number of relevant studies, the results of which vary slightly) technological, and operational parameters will be compared (Tables 1 and 2).

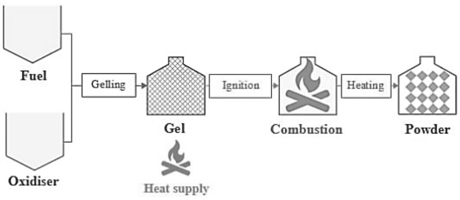
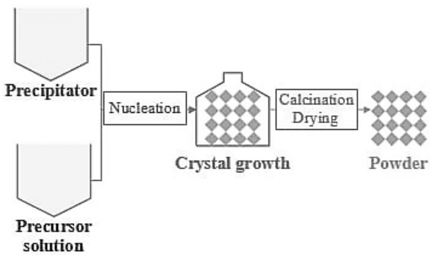
According to the above comparison, the smallest particles of magnesium nanooxide can be obtained by combustion in solution, co-precipitation, and green synthesis.

Other technological and operational parameters for the compared methods of synthesis of nanoscale magnesium oxide in comparison (with the exception of the composition of reagents and the reagent medium) correlate. Therefore, using the data from Table 2, it is possible to establish the necessary synthesis technology depending on the target product: for medical purposes, it is advisable to use smaller nanoparticles, and for industry, larger ones.

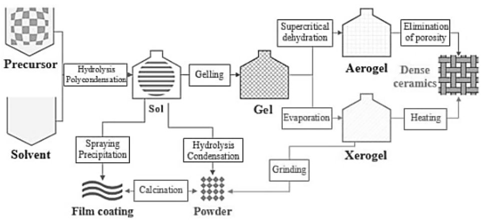
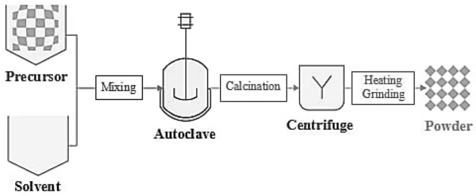
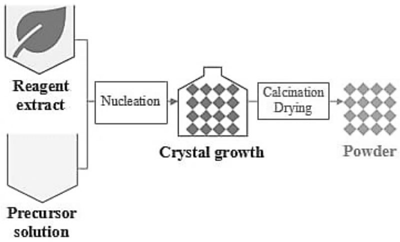
The current study focuses on efficient and cost-effective methods for synthesising MgO NPs, which have a high level of adaptation to production on an industrial scale. According to the nano-MgO production technology (Table 1), for the industrial production of nanoscale magnesium oxide, it is advisable to use sol–gel synthesis technology. Moreover, the study by J. Veronica *et al.* provides an economic substantiation for the industrial use of the MgO NPs sol–gel synthesis method, which uses Arabian gum as a raw material [10]. The performance of the industrial plant for the production of nanoscale magnesium oxide using sol–gel technology:

- cycle capacity – 1.425 kg of nano-MgO;
- monthly capacity – 35.625 kg of nano-MgO;

TABLE 1. Characteristics of methods for synthesis and production of nanoscale magnesium oxide [22–26].

Graphical representation of the process	Brief description of the technology
	Burning in solution. Low-cost widely used method. Two technological approaches are used: self-propagating synthesis and volumetric combustion synthesis. The methodology of the first one provides for the mechanism of spontaneous redox endothermic reactions between the oxidiser and the fuel, which are mixed at the molecular level in the corresponding solution with the gradual establishment of the target product in the solid aggregate state [33]. The second technological approach involves external heat supply to the entire volume of the reagent solution.
	Co-deposition. This method is based o the precipitation phenomenon, and als involves the technology of liquid-phas synthesis or steam-phase synthesis. S dium hydroxide is mainly used as a pr cipitator. The method is based on tl principles of homogenisation of precip tation reactions, which includes tw consecutive processes: nucleation an growth of nanoparticle crystals [34].

Continuation of TABLE 1.

Graphical representation of the process	Brief description of the technology
	Sol–gel and sol–gel using microwave exposure. This method is based on the use of an inorganic precursor and an organic solvent: metal alkoxides combine with a solvent and reagents to form a homogeneous solution [35]. This solution is gradually converted to a colloidal suspension (sol) and eventually polycondensated into integrated structures (gel), which is converted later to aerogel and xerogel (which is established by a certain drying method).
	Hydrothermal synthesis and solvothermal synthesis. This method involves the use of an autoclave in the technological process, where the precursor and solvent are mixed under the influence of high temperature and pressure, forming the target product as a result. Due to the physical conditions of conducting a set of reactions, nanomaterials with high crystallinity are obtained, significantly higher than other methods for obtaining nanoparticles [36]. In the case of non-aqueous solvents, the method is considered solvothermal, and in the case of using water as a solvent, it is considered hydrothermal.
	Green synthesis. This method does not require the creation of critical parameters of the reaction medium and the involvement of toxic substances [37]. Various organic materials (plant extracts, bacterial cultures, enzymes, vitamins) can be used as non-toxic synthesis reagents. Distilled (twice) water is used as the extraction medium.

- annual capacity – 427.5 kg of nano-MgO.

These indicators are quite competitive. In addition, the economic substantiation indicates a reasonable payback period for the installation of an industrial sol–gel synthesis plant (up to 3 years) and poten-

TABLE 2. Comparison of median technological and operational parameters of methods for synthesis and production of nanoscale magnesium oxide [38].

Synthesis-production method	Reagent	Reagent medium	Reaction nature and parameters, °C	Temperature exposure (calcination) parameters, °C	Duration of temperature exposure (calcination) hours	Size of obtained MgO NPs nanoparticles
Burning in solution	Oxidiser: $Mg(NO_3)_2$	Fuel: NH_2CONH_2	Burning at 100°C	500	2	22
Co-depositio	Precursor: $Mg(NO_3)_2$	Precipitator: NaOH	Reaction at 20°C	550	4	16
Sol–gel and sol–gel using microwave exposure	Precursor: $Mg(OCH_3)_2$, $Mg(NO_3)_2$	Solvent: CH_3OH, C_7H_8	Gel drying at 200°C	600	5	50
Hydro-thermal synthesis and solvo-thermal synthesis	Precursor: $Mg(NO_3)_2$	Solvent: NaOH	Autoclave mixing at a temperature of 180°C	400	2	50
Green synthesis	Precursor solution: $Mg(NO_3)_2$	Reagent extract: plant extracts, bacterial cultures, enzymes, vitamins	Crystal growth reaction at 90 °C	400	4	22

tial high profitability.

The next step in the study of synthesis technology is an empirical test of the hypothesis about the possibility of optimising the target industrial algorithm by means of digital programme modelling. When establishing the methodological basis of the current study, it is noted that now there is a fairly wide range of digital software tools for modelling nanogrids of various materials, including metal oxides, but the most optimal nanomodelling is performed by BIOVIA Materials Studio [12].

Using the internal repository of chemical structures, BIOVIA Materials Studio identified a prototype model of nanoscale magnesium oxide with MgO [12]. Next, the corresponding model molecular structure was obtained, consisting of 27 magnesium and oxygen atoms, which are stirred at an angle of 90° (2·45°) with a bond size of 4.2112 (2·2.1056) and with the corresponding symmetry (*Fm*–3*m* group (OH-5)), which actually proves the crystallinity of the structure and corre-

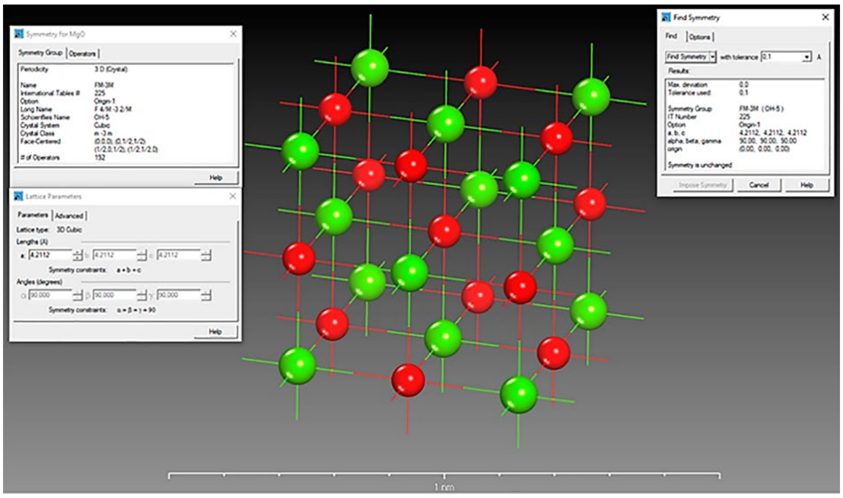


Fig. 2. Magnesium-oxide nanogrid model.

lates with empirical observations.

Using the CASTEP Tools in BIOVIA Materials Studio [12], the energy structure of the MgO NPs model nanogrid was obtained: a discrete energy structure, a nanogrid bond density structure, and a simulation of energy-molecular dynamics. CASTEP Tools also allows obtaining the values of elastic constants for the simulated magnesium oxide nanostructure with correlation using the Voigt, Royce, and Hill methods. According to the calculated data for nano-MgO, the universal anisotropy index is 0.11021, the median speed of sound in the nanostructure is 6547.20857 m/s, the Debye elastic temperature is 925.75893 K, the compressibility is 0.0068 1/hPA, and the generalised volume mod-

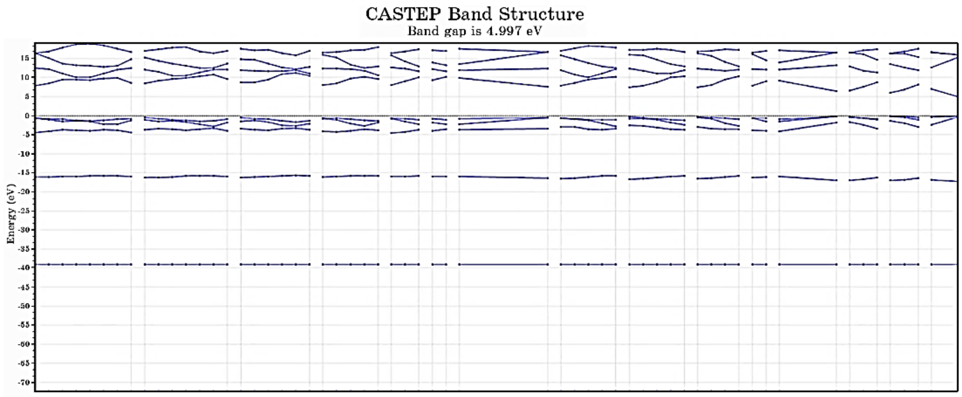


Fig. 3. Discrete energy structure of the magnesium-nanooxide model [12].

ulus is 147.01725±2.01 hPA (Figs. 2–4, Table 3).

The simulation results allow visualising the actual dimensions of the

TABLE 3. Elastic constants for polycrystalline material (hPa) [12].

Parameter	Methods		
	Voigt	Royce	Hill
Volume module	147.01725	147.01725	147.01725
Shear modulus (*Lame Mu*)	129.05727	126.27386	127.66556
Lame lambda	60.97907	62.83468	61.90687
Young's modulus	299.52658	294.50445	297.02166
Poisson's ratio	0.16044	0.16613	0.16328
Hardness (relative to titanium 2012)	23.76759	2379104	24.27706

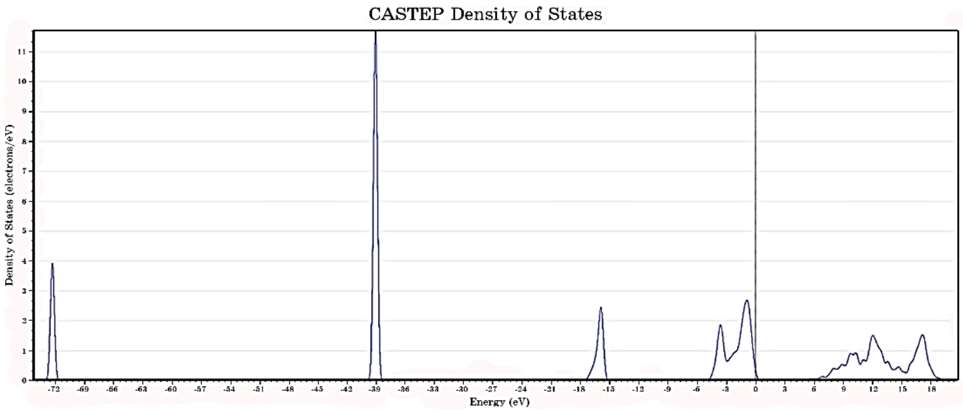


Fig. 4. Structure of the energy-bond density of MgO nanoformations [12].

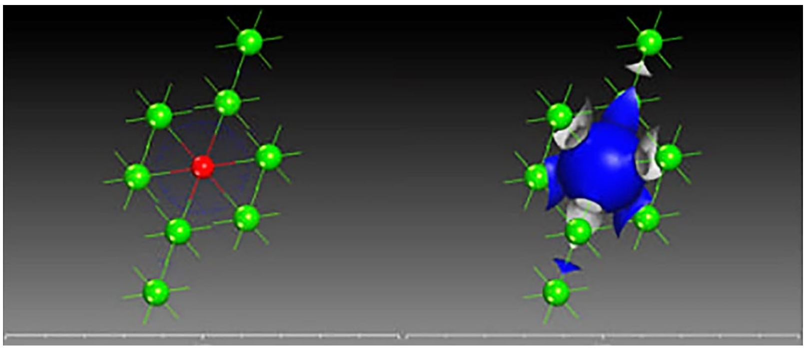


Fig. 5. Creation of a dimensional model of a MgO nanostructure [12].

magnesium oxide nanostructure (Fig. 5).

The Forcite module integrated into BIOVIA Materials Studio also provides analysis of the radial-distribution function (RDF), concentration distribution, x-ray intensity distribution (and scattering), velocity-distribution profile, pressure-distribution profile, density-field distribution in the form of model visualisation (Figs. 6–11).

The GULP Tools module integrated in BIOVIA Materials Studio allows obtaining the optical characteristic of the nanomaterial under study, the phonon dispersion characteristic, and the powder distribution of magnesium-oxide nanoparticles (Figs. 12–15).

BIOVIA Materials Studio also allows modelling (and corresponding calculations) for hybrid composites doped with magnesium oxide na-

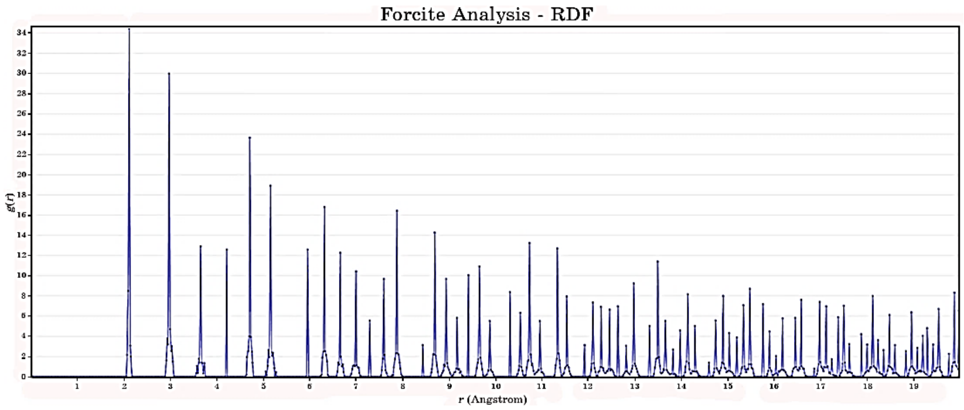


Fig. 6. Analysis of the radial-distribution function of the nanogrid of the MgO NPs model [12].

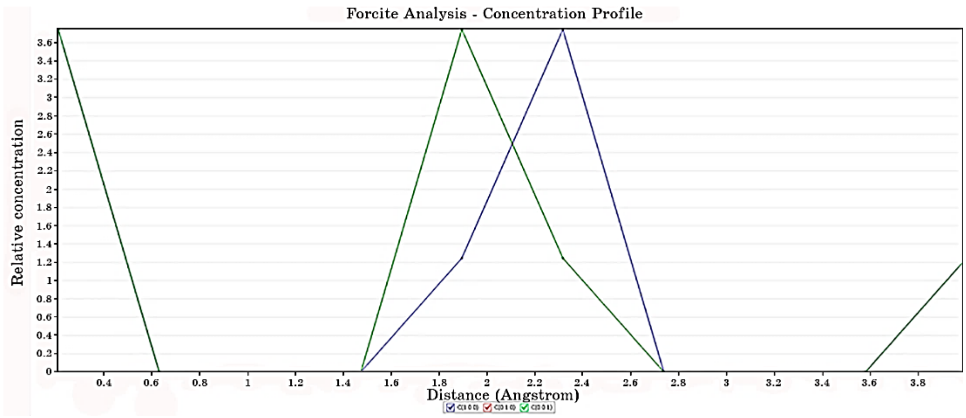


Fig. 7. Analysis of the concentration distribution of nano-MgO [12].

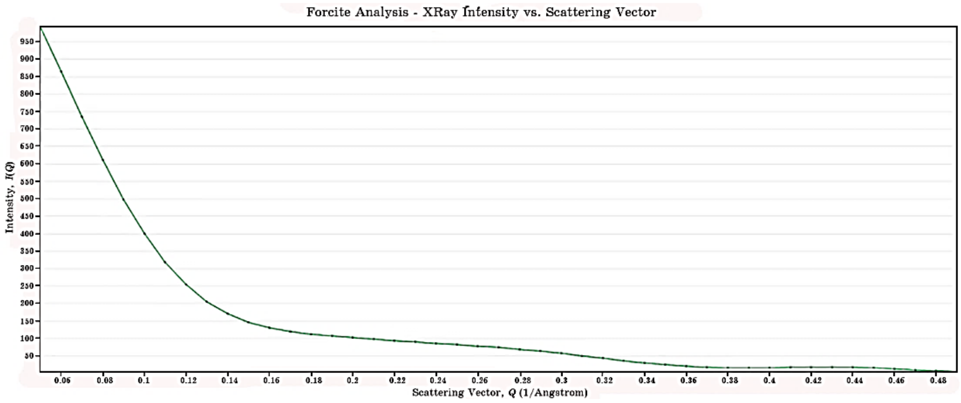


Fig. 8. Analysis of the results of modelling the x-ray intensity distribution (and scattering) in a magnesium-oxide nanostructure [12].

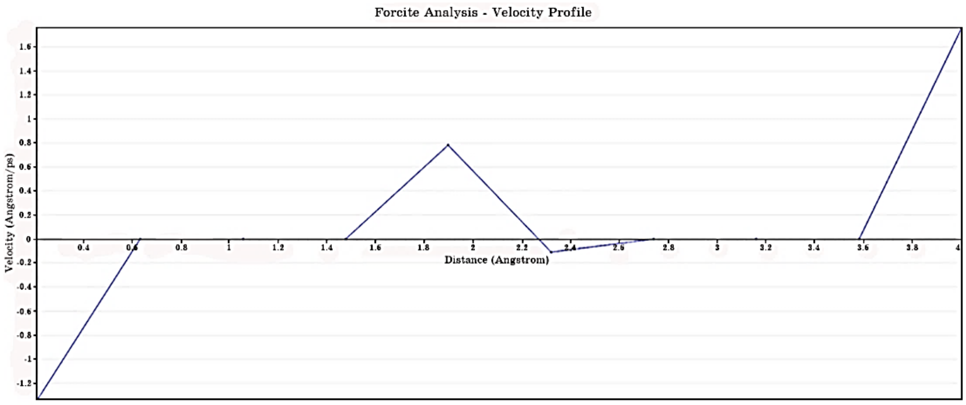


Fig. 9. Velocity distribution profile in magnesium-oxide nanogrid [12].

noparticles.

Thus, considering the facts of correlation of digital model characteristics of magnesium nanocomposites and corresponding empirical observations (obtained in laboratory conditions with the involvement of appropriate specialised equipment), the hypothesis about the feasibility of using BIOVIA Materials Studio as a solution to the design stage of creating various nanocomposites within the framework of the concept of nanometallurgy is confirmed [12].

4. DISCUSSION

This paper contains the results of studies of methods of synthesis and

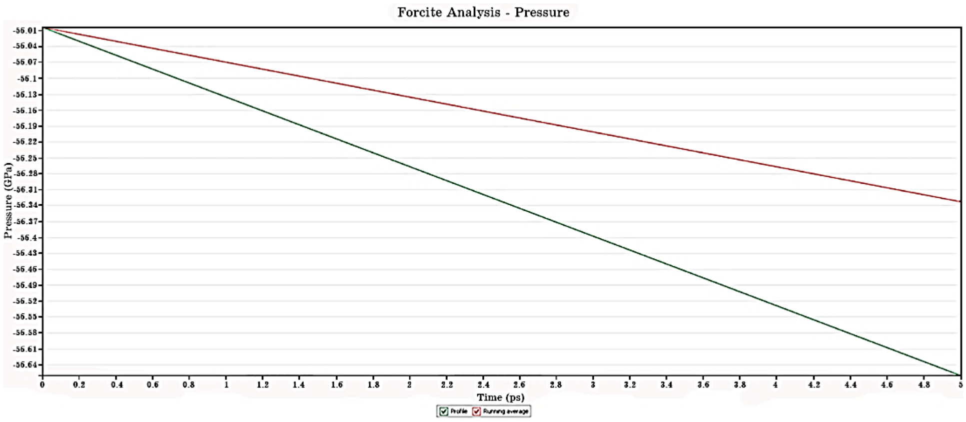


Fig. 10. Pressure distribution profile in magnesium-oxide nanostructure [12].

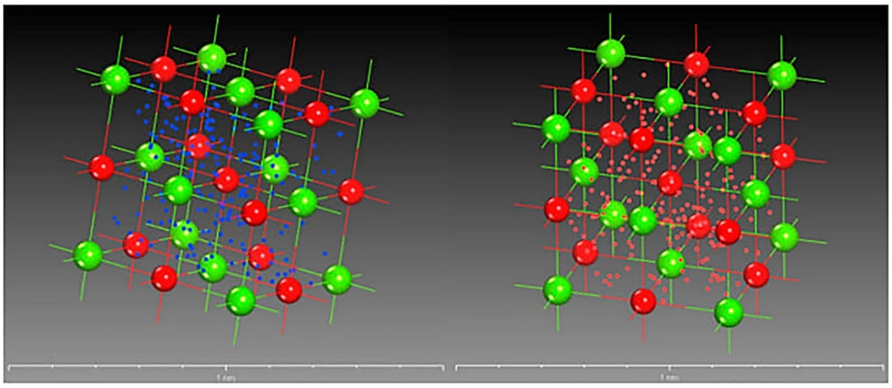


Fig. 11. Visualisation of the density-field distribution (shown as dots) obtained by modelling magnesium nanooxide [12].

production of nanoscale magnesium oxide, provided by several iterations (multilocal information search, bibliometric analysis and modelling using appropriate digital software tools) and contains more in-depth data on similar studies given in publications by F. Mirza and H. Makwana [9], M. Rajab *et al.* [22], J. Hornak *et al.* [23, 24], J. Chen [25], S. Vijayakumar *et al.* [26].

In the first iteration (multilocal information search), data on the properties of magnesium nanooxide are systematised, which contain a complete set of empirical data obtained in various studies to date and contain more generalisations, in particular, due to the correlated analysis of the results obtained by F. Mirza and H. Makwana [9] and J. Hornak *et al.* [23, 24] on the results of the FTIR study of target nanostructures, the results of the XRD study of nanocrystals of the

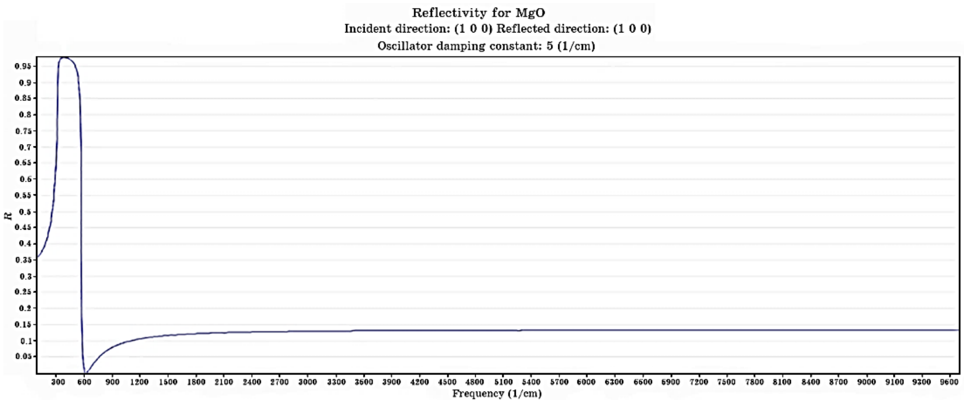


Fig. 12. Analysis of optical properties of MgO nanostructure [12].

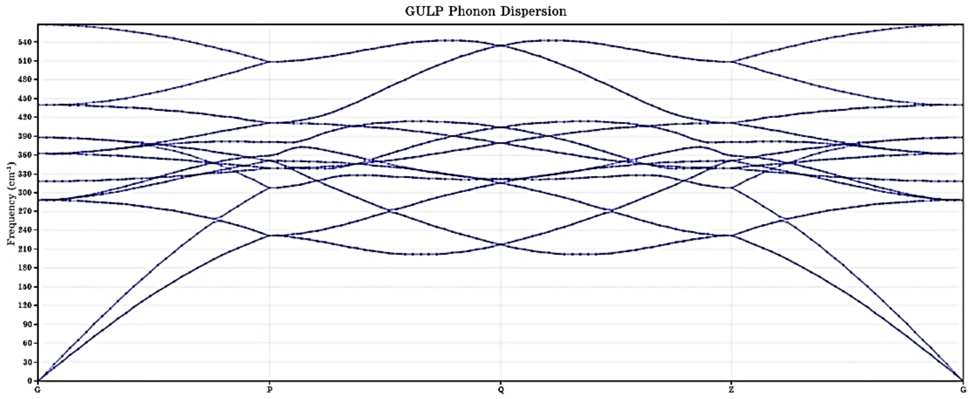


Fig. 13. Phonon dispersion of nano-MgO [12].

magnesium oxide and the physical and electronic structure of nano-magnesium oxide.

Moreover, expanding the range of the research vector with the papers by A. Khan *et al.* [27], J. Maji *et al.* [28], N. Baniasadi *et al.* [29], B. Das *et al.* [30], L. Cai *et al.* [31] and, in particular, N.Y. Nguyen *et al.* [32] allowed creating a more complete picture of the properties of the target nanostructure, forming cross-branch bonds and transitions for the latter (due to the detected antibacterial activity). The applied approach established the median physicochemical and specific properties of the nanostructure under study, which allows creating appropriate verification information array of values that can be referenced when applying subsequent iterations in the current study.

Furthermore, using multilocal information search, the systematisation of the areas of application of the studied nanomaterial was performed, which revealed the following characteristic areas and areas of

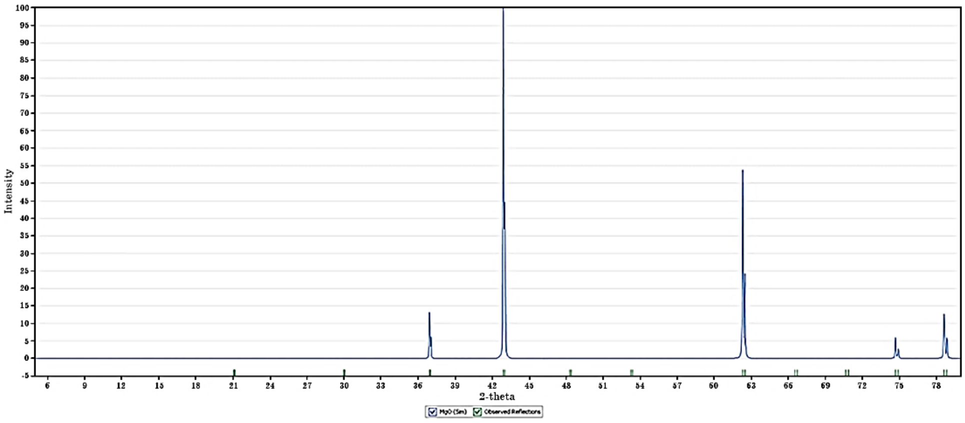


Fig. 14. Distribution of magnesium-oxide nanoparticle powder [12].

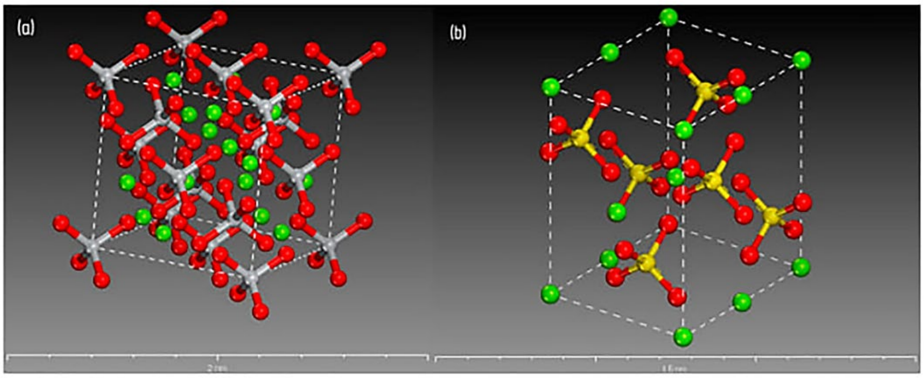


Fig. 15. Examples of hybrid nanocomposites based on titanium (a) and silicon (b) doped with magnesium-oxide nanoparticles [12].

application:
- prosthetics;
- medicines;
- oil and gas production;
- electronics;
- communication tools;
- engineering life support systems;
- food industry;
- construction;
- agronomy and powder metallurgy, in particular, nanometallurgy.

The obtained data correlate with marketing studies by Custom Market Insights [1], Data Intelo [4], and Mordor Intelligence [5]; however, it provides an appropriate scientific basis for the mechanism of application of magnesium nanooxide for selected industries by bringing relevant scientific papers from the profile scientometric landscape.

Similarly, multilocal information search tools established existing methods of MgO NPs synthesis and production, and updated relevant empirical data by forming a median information technology array, which was not used by F. Mirza and H. Makwana [9], M. Rajab *et al.* [22], J. Hornak *et al.* [23].

Based on the generalisation of technological and empirical data obtained in the analysis of relevant studies, an assumption is made about the possibility of obtaining an optimised for industrial use and economically substantiated technological method of synthesis and production in the form of sol–gel synthesis, which was not only observed in papers by A. Nandiyanto *et al.* [39], J. Zhao *et al.* [40], S. Liu *et al.* [41], but also received an implementation with a corresponding feasibility study by J. Veronica *et al.* [10] (the obtained competitive productivity of the nano-MgO synthesis plant for sol–gel technology was 427.5 kg per year, with a probable economic payback of three years, which gives reason to consider this method economically justified and profitable).

The hypotheses of the first iteration (multilocal information search) were confirmed by means of bibliometric analysis (the second iteration of the study).

In particular, when analysing chronotaxonometric schemes built on the basis of relevant scientometric information (relevant publications in the current search scope), it was found that the sol–gel synthesis method has the greatest weight of scientific opinion on the assessment and study of methods for synthesising the nanomaterial under study. It was also found that the green synthesis method is a promising method for the production of magnesium oxide nanoparticles, which is expected to implement fully the eco-friendly concept in the field of nanometallurgy. A special feature of this method of synthesis of metal oxide nanoparticles (including magnesium oxide) is the use of various organic materials (plant extracts, bacterial cultures, enzymes, and vitamins) as a reagent medium, without involving toxic compounds in the technological process. Thus, compliance with the main goal of the study, namely, obtaining data on the optimal technology for obtaining nanoscale magnesium oxide, was confirmed, while in two iterations (information and search, bibliometric) it was established that the sol–gel method is appropriate and economically substantiated for industrial applications, which should later be replaced by green synthesis, which has the advantage of using environmental organic reagents for the production of magnesium nanooxide.

The next iteration of the study, namely, its empirical part, is presented by the results of testing the hypothesis about the possibility of optimising and modernising technical and technological solutions of nanometallurgy by means of appropriate digital software. In the current scientometric landscape, a similar hypothesis regarding magnesium oxide nanometallurgy has not been investigated at the time of the creation of the current paper. It was found that BIOVIA Materials Studio is the most appropriate for the established goal of testing the above hypothesis, which correlates with the results of research on modelling other nanomaterials, which are presented in papers by S. Merezhko *et al.* [42], K. Kunene *et al.* [43], B. R. Abhiram and D. Ghosh [44].

The use of BIOVIA materials Studio significantly expands the range of obtained characteristics for the target nanoproduct—nanoscale magnesium oxide. In particular, it was possible to obtain data on the physical and mechanical structure of the nanomaterial under study (correlated with the results of empirical observations), data on the energy structure of magnesium nanooxide (discrete energy structure, density of energy bonds of nanoscale, parameters of energy-molecular dynamics), data on the elastic and mechanical characteristics of the simulated nano-MgO with correlation by the methods of Voigt, Royce, and Hill (universal anisotropy index, median speed of sound in the nanostructure, Debye elastic temperature, generalised volume modulus, shear modulus (*Lame Mu*), *Lame lambda*, Young's modulus, Poisson's ratio, hardness (relative to titanium 2012)). Based on the results of modelling in BIOVIA Materials Studio, it was possible to obtain a model of the magnesium oxide nanostructure in a comparable scale form [12].

Moreover, based on the results of modelling nanoscale magnesium oxide in the PC BIOVIA Materials Studio software environment, data were obtained on the radial distribution function, concentration distribution, x-ray intensity distribution, velocity distribution, temperature fluctuations distribution, density field distribution in the form of model visualisation, optical characteristics, and phonon dispersion characteristics. Most of all, the fact of correlation of the model representation of the distribution of magnesium oxide nanoparticle powder with empirical observations of XRD studies proves the correspondence of the formed hypothesis to the real state of affairs [9, 24, 25].

Thus, the grounds for confirming the hypothesis about the possibility of using digital software tools as an optimisation solution in nanometallurgy technology are obtained.

5. CONCLUSIONS

As a result of the current study, the results are obtained, consisting of a part of the systematised data of relevant scientific studies integrated into the profile scientometric landscape and an empirical part, with the help of which the hypothesis of the potential possibility of optimising nanometallurgy technologies by digital software means is tested.

Based on the results of a multilocal information search, which is the first iteration of the current study, the concept of recognising sol–gel synthesis as an optimal and economically viable method of synthesis and production has been preliminarily established. It is established that this method is the most adaptive for industrial production of the target nanoproduct. However, according to the results of the second iteration of the study (bibliometric analysis), not only the previous concept was confirmed, but also the next one was developed, namely, the most likely method for producing magnesium oxide nanoparticles (and other metal nanooxides) is green synthesis, which forms the eco-friendly nanometallurgy paradigm. At the same time, using the first iteration of the study, a factual array of data was obtained, which allowed approaching the third iteration of the study.

As the next step of the study, the concept of modelling is defined, which follows from the hypothesis about the probability of optimising nanometallurgy technology using digital programmes. It is established that the use of specialised software provided not only more specific characteristics of the nanomaterial but also the results that have a significant level of correlation with empirical observations recorded in the relevant profile studies. Moreover, this software product allows full use of the concept of molecular and atomic engineering, namely, to generate, modernise, adapt various physicochemical nanostructures in mono- and polysyllables and carry out their rapid (software) calculation to identify the most appropriate and adapted to implementation. That is, the hypothesis about the possibility of optimising nanometallurgy technology by integrating the design and model link into production chains is clearly confirmed, which has far-reaching results with direct economic consequences, in particular, it will significantly reduce the load on specialised laboratory equipment.

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