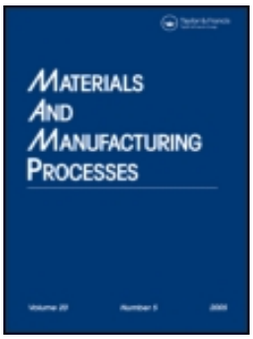

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Genetic Algorithms, a Nature-Inspired Tool: Survey of Applications in Materials Science and Related Fields

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Genetic algorithms (GAs) are a tool used to solve high-complexity computational problems. Apart from modelling the phenomena occurring in Nature, they help in optimization, simulation, modelling, design and prediction purposes in science, medicine, technology, and everyday life. They can be adapted to the given task, be joined with other ones (this leads to combined or hybrid methods), and can work in parallel on many processors. The uses of GAs reported in literature represent a wide variety of approaches and led to solving of numerous computational problems of high complexity. In materials science and related fields of science and technology the GAs open possibilities for materials design, studies of their properties, or production at industrial scale. Here, the recent use of GAs in various domains connected to materials science, solid state physics and chemistry, crystallography, biology, and engineering is reviewed. The listed examples taken from recent literature show how broad the use of these methods is. Emphasis on description of particular results is put in order to direct the reader's attention to valuable new applications as well as interesting or promising ways of solving specific tasks. Trends in method development and application-field extensions as well as some possible future implications are briefly discussed.

Keywords Application; Artificial intelligence; Evolution; Genetic algorithm (GA); Global search; Optimization; Parallel computing; Prediction.

Observez la nature, et suivez la route qu'elle vous trace. (Observe nature and follow the route she traces out for you.) – Jean-Jacques Rousseau ("Emile," 1762)

1. INTRODUCTION

Search for an optimum in a large multidimensional space, especially if the function landscape is complex and the criteria and constraints are numerous, is a difficult mathematical problem. Various numerical methods have been created; among them there is a family of so called *population-based methods*. In population-based global-search and optimization methods, the population is formed from a (usually constant) number of individuals which have some relation to solutions of the problem. Typically (but not always, cf. the discussion in [1]), an individual represents a single trial solution. Many of such methods, named as *evolutionary algorithms* or *evolutionary computations*, exploit selected principles of evolution observed among living organisms. The best known classes of such methods are genetic algorithms (GA), evolutionary strategies (ES), genetic programming (GP), evolutionary programming (EP), and artificial life (AL). Properties and efficiency of various PBMs including the evolutionary algorithms have been discussed and/or tested, e.g., by numerous authors and teams [2–26]. The present study is focused on GAs constituting a subset of PBM algorithms that are frequently used in materials science.

Materials science, a large interdisciplinary research field that joins solid-state physics, chemistry, biology, and crystallography creates many challenges for computations. More than 50 years ago, the subject of scientific and technological materials science studies was mostly metals, so the name of metallurgy was most frequently applied then. At its early incubation stage, starting from stone, bronze, and steel ages, the materials-related problems were mainly solved using trial-and-error approach combined with experience and intuition. The production experience and secrets were transferred from one technologists' generation to another, for centuries written documentation has not been created. Many important discoveries have thus been lost and only recent modern-materials-science experimental studies are helpful in breaking these secrets, as for example those of production of technologically advanced porcelain [27] in ancient China, or of metallic objects: Etruscan gold jewelry (technique of massive production of gold microspheres) [28], laminated composites (metal-containing laminated composites produced starting from 2750 BC in ancient Egypt) [29], Damascus steel (carbon nanotubes discovered in a Damascus steel sword from 17th century) [30], astrolabes (achievements of early metallurgy of brass in middle-age India) [31], and Japanese swords (elaboration of ancient swords in Japan) [32]. Deep understanding of materials properties started to be achieved in the first half of the 20th century on the basis, in particular, of discovery of the atomic structure of the matter. This gave grounds to systematization and prediction of material properties and to materials design and created the need for finding suitable computational methods.

Materials can be categorized according to various features. A simple scheme, taking into account four most important attributes: dimensionality, structure, composition, and properties, is shown in Fig. 1. The ultimate aim of many materials-science tasks is to find a material suitable for the specific application. The material must satisfy a number of criteria (technical, economic, safety, etc.). For the given case, particular attributes are involved

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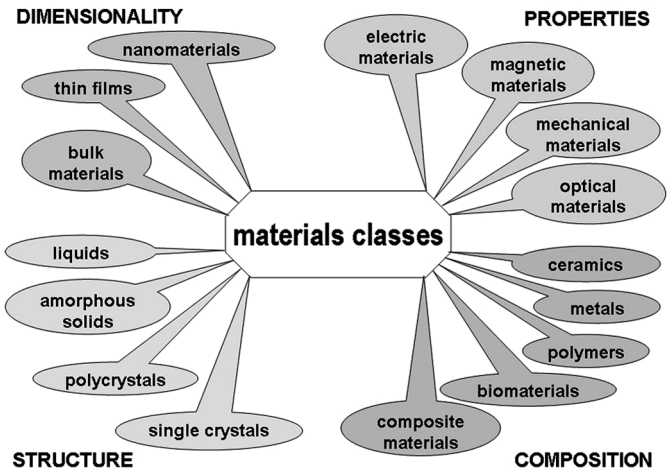

FIGURE 1.—The most important materials classes categorized according to four attributes: composition, structure, dimensionality, and properties. The presented selection of classes is not exhaustive. The expressions "electric, magnetic, mechanical, and optical materials" are abbreviations representing the materials whose respective electric (dielectric, conducting, ferroelectric, superconducting), magnetic (ferromagnetic, antiferromagnetic, diamagnetic...), mechanical, and optical properties are employed in the applications.

with one or more properties determining the target. Computational, experimental, or mixed methods are used for solving problems of this kind. Computational search and optimization problems involve modelling, design, analysis of properties, and the methodology and physical tools of analysis for the given class (subclass) of materials, as well as production of objects having the given material as a component. Modern methods of materials design, processing, characterization, and properties determination face the difficulty of search or optimization in a large space. This space is built from variables that define the given computational problem. The computations involve the ranges of variables, the constraints, and the search criteria. The size of the problem determines whether it can be solved "fully" (global minimum found with certainty) or partially (a progress in the search of global minimum, only).

The present review is devoted to applications of one of global search methods, the GAs, in materials science and in the closely related fields: materials physics and chemistry, crystallography, biology, materials-related industry, and engineering. The cited examples illustrate how broad and valuable this nature-inspired method is.

2. GENETIC ALGORITHMS: THEIR NATURE-INSPIRED CONCEPT, DEVELOPMENT, AND APPLICATIONS

GAs are a powerful tool applicable to solving high-complexity computational tasks. Their concept follows the old idea of learning from Mother Nature: the calculation strategies based on the genetic approach mimic the evolution of living organisms [33–35]. Their connection with living organisms forms a bridge between computer science and biology and social sciences. They can be used as optimization/simulation/modelling/design tools, and they also exhibit a high predictive power. The most classical implementations of the GAs involve the selection, recombination, and mutation operators. Nature has elaborated various mechanisms which are (or can be) exploited in GAs. Apart of the basic principles used in most classical algorithms, other features of the life can be exploited in the computations, leading, hopefully to an increase of level of success. For example, in calculations the selection is typically decided by fitness value or its ranking, which is a relatively simple method. In nature, the world of plants, animals, and humans, a wealth of models are adopted: the decision on selection may be influenced by one or two partners (male and/or female), parents or family, a cooperating species (it happens in the world of plants), partner appearance, the site-distance (a small one gives possibility of getting known), age, age difference, genetic difference (controlled through pheromones) etc.

Frequently, for small global-optimization problems an exhaustive method (systematic search, grid search) is typically sufficient. There is a limit for such search due to the barriers of speed and memory of the hardware. Metcalfe [36] has illustrated this by an example of white-dwarf studies. Astrophysical studies of white-dwarfs seismology lead to understanding of their properties, and permits for better modelling of physical phenomena occurring there, such as the nuclear reactions inside, and their periodicity, permitting for treating them as chronometers [36]. In a captivating story about astrophysical studies and the potential GA role, the cited author emphasizes the fact (more or less common for all experimental sciences) that modern instruments yield a rapidly increasing amount of data that have to be analyzed with theoretical models and that the given data set may require a treatment for which the capability of the available hardware is definitely insufficient. The models frequently have a large number of parameters of extended ranges—this effectively excludes using the grid search. As the models one uses are not necessarily the right ones, it is essential not only to look for the best solution in the frame of the initial model, but also to improve the existing models and to apply other ones. With five parameters of the computational problem studied in Ref. [36], the required 10^{10} objective-function evaluations are equivalent to the prohibitive 1,000 years computation using the fastest processors. GAs have been shown to be helpful in problems of such size.

The genetic computation proceeds in the space of variables. It mimics the evolution of living organisms represented by the points in this space ("trial solutions"). The method employs a number of operators. The given operator may have one or more individuals as arguments and create one or more output individual. Most frequently, the genetic operators include selection, crossover, and mutation. Various ways of defining these operators are known (see, e.g., [34, 37, 38]).

The genetic-algorithm methodology consists in:

Step 1: Creation of a starting "population" of individuals (trial solutions, chromosomes);

Steps 2, 3, . . . : Creating succeeding (improved) generations of solutions, using natural selection principles, i.e., selected simplified principles of plant or animal (Darwinian) evolution that depend on the fitness values.

The effective number of generations results from a specific stop condition applied.

An appropriate *objective function* (criterion, scoring, or cost function) is defined for the purpose of calculations. This function expresses the selection criteria applied in the given approach. It is practical to use in the calculation a non-negative *fitness function* built by suitable scaling of the primary objective function. Quite frequently, these two notions are not distinguished, and the fitness is just a synonym of objective function. As using the proper fitness function is often computationally expensive, methods of using fitness-approximation are under development by some groups [39].

Using the framework used by Hertz and Kobler [1], one can describe a "classical" GA as alternating cooperation/self-adaptation procedure. The selection and crossover operators create cooperation stages allowing for information exchange between the individuals, whereas the mutation operator is classified as a self-adaptation stage. High mutation rate ascertains a genetic diversity of the population during the search. On the contrary, low mutation rate conserves the property of the GAs of memorizing (in the bits of the whole population) the long-term information about the features of earlier populations. The mutation rate value (typically a single constant value, in simple implementations) must be a compromise.

In the classical genetic global-search methods, each individual is represented by a concatenated binary vector, describing the values of all fitted parameters. Real variables are discretized to binary vectors of a length permitting to achieve a required precision. (Also, genetic-like operators can be defined for real variables without any coding.) A large freedom in constructing the algorithms allows various calculation schemes to be applied. In general, any of schemes ascertains some progress in the task of minimizing a function of many variables. Possibility for finding a global minimum may depend on the nature and complexity of the problem studied, in particular: on the time necessary for calculation of the fitness value, on the ranges of variables studied, on the number and distribution of local minima, as well as on the function shape around the minima.

GA's are helpful in solving difficult static and dynamic mathematical problems which may be divided into two broad categories:

i finding a global or a local (depending on the nature and scale of the task) extremum of a complex-shape function of many variables (static case); and
ii on-line solving the time-dependent multivariable optimization problems (dynamic case).

It is noteworthy that GAs can accommodate constraints, even if complex and varying with time. This feature makes them particularly useful in large scale optimization and search studies. An additional advantage of the GAs is their ability to work in parallel—for the most time-consuming tasks one can use many processors—e.g., for modelling the oxygen implantation into silicon the reported calculation involved more than thousand processors [40]. Parallel computations ascertain the opportunity of solving large problems. In such case the migration process between the subpopulations existing at various computers or processors is introduced to provide exchange of genetic information.

Computing using GAs has its very beginning with three articles involving the evolution inspired calculations, by Friedman in 1956, Box in 1957, and Fraser in 1957 (cf. Refs. [41–43]), i.e., it can be dated for just three years after the discovery of double helix by Crick and Watson. The most commonly considered date of the GAs birth is the publication of the Holland's book [33] (although the term of GA was used even earlier, e.g., in Ref. [44]). The development of the GAs expressed through the number of answers to the suitable keywords in the INSPEC database is illustrated in Fig. 2. This database contains records from various disciplines covering natural sciences, material science, and technology. The incubation period of GAs was 1956–1974, childhood 1975–1986, fast nonlinear increase 1987–1995, and quasi-linear increase from 1996. Total number of applications steadily increases (visible if linear scale is used). The number of calls of GAs in article titles seems to saturate what can be attributed to the fact that the methods became routinely used. The figure shows also that the trend in the use of GAs correlates with dates of the milestone books and articles published in this field. The trends observed are related to those reported for applications of GAs in physics and chemistry [43]: the reported in Ref. [43] number of articles with GAs involved reached the level of 10 per year in 1980, 100 per year in 1988, 300 in 1995. Bonaccorsi [45] has studied the development of various disciplines through the number of articles published by the top 1,000 computer scientists. GAs were the first keyword studied: the above defined number rises linearly

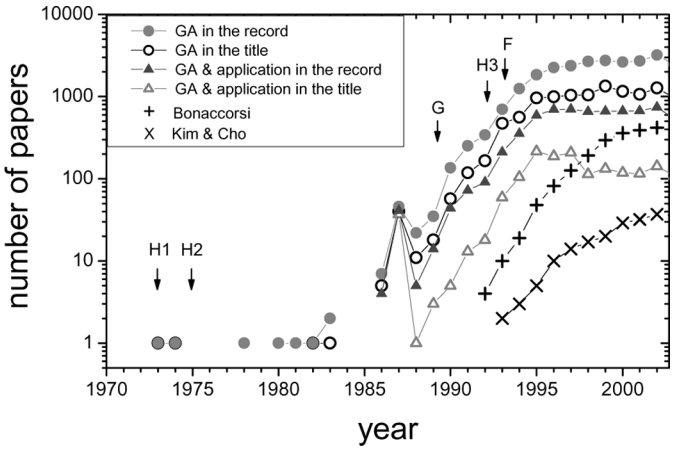

FIGURE 2.—Answers of INSPEC database (the database covered period starts in 1969) to combination of the following keywords: ♦ – *genetic algorithm(s)* in the record; ○ – *genetic algorithm(s) and application(s)* in the record; ▲ – *genetic algorithm(s)* in article title; △ – *genetic algorithm(s)* and *application(s)* in article title; + – data of Bonaccorsi [45]: use of genetic algorithm in articles of top 1000 scientists; × – data of Kim and Cho [46]: total number of GAs involving articles on robotics. The five complementary arrows represent: "H1": year of the first publication with *genetic algorithm* in its title [44] found in the INSPEC, "H2," "H3:" years of the publication of the J. H. Holland's book (first edition 1975 and second edition 1992) [33], "G" - D. E. Goldberg book [34], "F:" S. Forrest article [35].

from 4 in 1992 to over 400 in 2003. All these trends nicely correlate proving that the GAs have found their well-fixed place in applied science and are a good illustration of the rising importance of these methods. It is interesting to compare them with a broader field of artificial intelligence (AI): Kim and Cho [46] have demonstrated the increase of the number of articles on several applications of AI. Those concerning the robotics linearly rose from two in 1993 to over 40 in 2003. From among applications in engineering, these authors demonstrate that the fastest rise in this field in the same period is for AI applications in electronics and industrial design.

Many improvements or extensions of GAs have been proposed and verified in practice. Particularly useful modifications consist in above-mentioned building implementations for processors or computers working in parallel. Development of genetic code for the given problem may involve task-dependent modifications and addition of new operators, as well as joining the method with other ones (this leads to *combined* or *hybrid* methods). Alternatively, ready-to-use universal packages can be run by nonprogramming users. GAs can work in Matlab environment (opportunities are reviewed in [47]). Moreover, more or less specialized platforms exist, e.g., those reported in Refs. [48] (simulation of solids), [49] (engineering applications), [50] (catalysis), [51] (reaction mechanisms), and [52] (strain analysis for implanted semiconductor layers). Consequently, the reported uses of both own and platform GAs represent a wide variety of complexity levels and practical approaches.

As pointed out in preceding paragraphs, the expansion of GAs applications started on a large scale at the end of 1980s: at the present stage, thousands of publications on their use appear each year. Their field of action covers such crucial domains as arms race, energy production and consumption, weather forecast, bankruptcy prediction, road traffic control, as well as such exotic subjects as above-mentioned aestroseismology or modelling the spider-web structures discussed in Section 3.6. The applications are so numerous, that they cover almost all domains of life, science and technology, medicine, economy, from the fight for peace through environment monitoring and protection to weapon construction, from medical diagnosis based on image analysis through noninvasive microbe recognition based on odor detection to hospital care evaluation, from Web exploration through server control and data mining to database construction, from fashion design to aircraft design. Reviews of achievements in various fields may be found, e.g., in Refs. [46] (field: general), and for various subjects like materials design and processing [53], physics and chemistry [43], chemistry including molecular modelling [54], structure of clusters [55], molecular diversity and compound classification [56], crystal structure solving [57], productions and operation management [58], steel industry [59], oil industry [60], business [61], finances [62], control engineering [63], system engineering [64, 65], image enhancing [66], engineering design [67–70], packing [71], assembly line balancing [72], nuclear magnetic resonance spectroscopy) [73], chemometrics [26, 74, 75], computational chemistry [76], feature selection and weighting [77], electromagnetics design [78], medicine

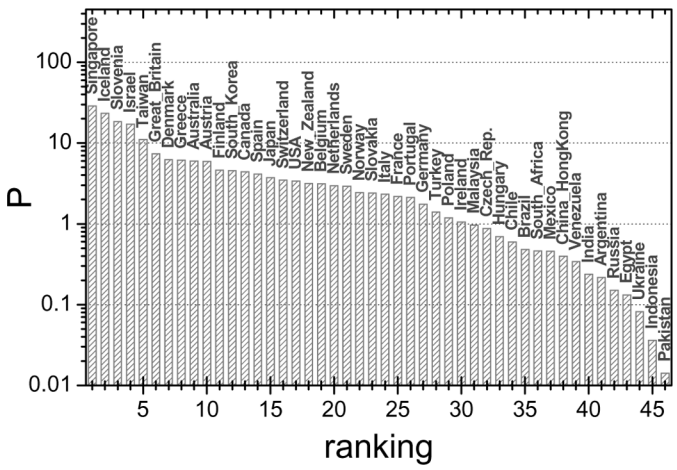

FIGURE 3.—Number of articles (P) on GAs per million of inhabitants having at least one affiliation of the given country. The data (derived from SCI-Ex database) cover the period 1996–mid-2004.

[11], chemistry, biology, and crystallography [76], and seismology [79]. Figure 3 reflects the interest in various countries during the steady growth stage (1996–2004) through the number of articles having at least one of the authors affiliated in the given country, normalized to the number of inhabitants. Data are derived from the SCI-Ex database containing the abstracts from journal articles. The interest in GAs expressed through the number of articles depends on the country, and the likely factors influencing it are the level of academic computer science as well as the local need for industrial applications. The ranking leaders are some small countries for which the total number of articles is not so high (note: geographical distribution has been studied in Ref. [43] for applications limited to physics and chemistry).

3. EXAMPLES OF APPLICATION IN MATERIALS SCIENCE AND CLOSELY RELATED FIELDS

The materials-science related applications are divided below into six thematic groups. For each group, a bibliographic table is given showing examples of problems treated by GAs in the given field. Some of the listed examples are discussed in the text. The choice of the bibliography and examples is arbitrary, aiming to document the large variety of studied problems, rather than to attempt for exhaustive or historical survey. In some cases the ascription of the subject to the group is arbitrary, as well: for example, modelling of clusters might belong to physics, chemistry, or crystallography.

3.1. Materials: Design, Processing, Damage, Basic Features

Applications of GAs in materials science cover a wide spectrum of problems (for examples see Table 1). One of most important tasks in materials processing is the so-called *reverse heat transfer problem*. It consists in finding possible input parameter combinations that lead to the given temperature field profile (static or dynamic).

TABLE 1.—Examples of applications of GAs in basic materials science.

Field	Application
General	Materials design and processing [53]
Crystal/layer growth	Optimization of chemical vapor deposition (CVD) process for carbon nanotubes fabrication [80]
	Control of thin-layers growth by molecular-beam epitaxy [81] and CVD [82]
	Industrial crystal growth [83]
	Identification of crystallization kinetics parameters at nonisothermal conditions [84]
Optimization of material preparation process	Control of unsteady solidification using a magnetic field [85, 86]
	Aging process optimization [87]
	Finding the parameters of nanoparticle milling [88]
	Design of spray reaction synthesis of mesoporous c-ZrO_2 spherical particles [89]
	Welding parameters for the joined brass [90]
	Ferrite to austenite transformation in steel welds [91]
	Optimizing the stainless steel welding process [92]
	Optimization of polyethylene terephthalate (PET) reactor [93]
Materials design	Design of alloys according to required properties [94]
	Design of composite materials [95]
	Design of self-assembling composite materials [96]
	Design of conducting polymers [97]
	Electromagnetics design [78, 98]
	Alloy/steel design [99–101]
	Designing steel of improved ductility [102]
	Optimization of modified multicomponent binders [103]
	Optimization of Li^+ content in carbon nanotubes [104, 105]
	Reconstruction of structure of a composite material [106]
Materials damage	Calculation of fatigue limit criteria [107]
	Fatigue crack mechanisms studies [108]
	Identifying the structural damage [109]
	Delamination identification [110]
	Crack-tip analysis [111]
Surface preparation and synthesis	Preparation of smooth surface by grinding [112]
	Prediction of grain surface roughness after milling [113]
	Grinding of silicon carbide with diamond wheels [114]
Phase diagrams	Phase-stability analysis [15]
Material properties	Material properties identification [115]
	Identification of factors governing mechanical properties of steel [116]
	Estimation of thermal properties of composites [117]
	Predicting materials mechanical properties [118]
	Sonic (sound attenuating) crystal optimization [119]
Temperature field	Heat transfer in a liquid layer heated by electric arc [120]

Due to complexity and nonlinearity of heat transfer equations, solving the reverse problem is very difficult. It has been shown [120] that the problem may be treated using a real-coded GA approach. The example presented consists in finding the values of input variables for a liquid layer locally heated at its surface, the heat source linearly moving. The model involves the conservation of mass, momentum and energy. The output of the method includes the temperature field and the cooling rate. The results have been experimentally confirmed. A 3D temperature profile solved using a GA at a different scale is also mentioned in Section 3.6.

Experimental optimization of the welding process is costly and time-consuming. The use of GAs for optimization of the stainless steel welding process has been investigated by Vasudevan et al. [92]. The quality of the weld seen through its shape and mechanical properties (bead width, depth of penetration, and reinforcement height) depend on the welding process parameters (current, voltage, torch speed, arc gap, shielding gas and its flow rate, kind and geometry of the electrode). The reported methodology included building up regression models correlating the process parameters with the bead shape parameters. The GA parameters have been optimized. Close agreement has been found between the calculated process parameters and the parameters of the target weld. Moreover, the study has resulted in discovery of alternative paths for achieving the required weld-bead geometry [92]. The kinetics of transformation of α-ferrite to γ-austenite in steel welds during heating of 1005 steel has been assumed to be described by a nonisothermal Johnson–Mehl–Avrami equation [91]. The model involves the fluid flow and heat transfer parameters as well as the phase fraction of γ-austenite measured at several locations across the heat-affected zone at a weld in steel. The phase fraction data have been determined using X-ray diffraction employing small-diameter beam generated at a synchrotron. The use of GA leads to improvement of the agreement between experiment and calculation results. Another welding model has been successfully used for welding of brass plates [90].

GAs are well suited to optimize processes [121], e.g., for crystal growth, growth of thin films or nanocrystals. It is well established that catalytic action of metallic nanoparticles is helpful in growth of nanotubes and nanowires. The process of growth involves many parameters and is time consuming. For example, the number of trials needed to optimize the growth of nanowires of given chemical composition, using the molecular beam epitaxy

method, is of the order of 10^2 [122] taking the laboratory time of about one year. This is a serious limitation, so employing any AI method enabling a reduction of the effective time, cost, and the manpower engaged is worth considering. Grujicic et al. [80] have described application of a GA to chemical vapor deposition (CVD) growth optimization of the carbon nanotubes. The growth method was based on catalytic hydrocarbon decomposition. The carbon nanotube grows along the normal to the substrate. The catalytic mechanism is connected with the Co nanoparticles remaining, during the process, at the top of the nanotubes growing on a substrate. The goal of the calculation is enhancing the nanotube growth whereas the simultaneous growth of amorphous-carbon component must be maintained at the lowest possible rate. The CVD reactor is built from a tube where the working gas flows through and, at a specific distance from its beginning, the substrate is located. The gas composition, pressure, temperature as well as the substrate temperature form the set of growth parameters to be optimized. The result of the computation led to a solution ($T_{\text{gas}} = 773\,\text{K}$, $T_{\text{wall}} \sim 1380\,\text{K}$, pressure 0.25 atm, CH_4 concentration $\sim$16.3%)—other solutions have been discussed as well—which is consistent with that found experimentally in an earlier work by another group [123]: the latter result gave the rate range 0.0031–0.0055 μm/min. The experimental range of deposition rate obtained in Ref. [80] for various solutions is 0.001–0.007 μm/min, and technologically important information was the rate profile along the reactor tube. The deposition rate achieved with the best solution was 0.003 μm/min, i.e., the growth of the nanotubes was about ten times faster than that of the amorphous component. A second example of CVD process is described in Ref. [82]. The process of tetraethylorthosilicate (TEOS) growth has been optimized and the growth parameters (three rate constants TEOS concentration and intermediate species concentration) calculated and successfully verified by the experimental values. The promising conclusion is that the conventional reaction modelling can be replaced by the introduced GAs-based one permitting for automation of research and development in this field. A widely applied method of thin film deposition is molecular beam epitaxy (MBE). The growth of monocrystalline films using this method can be monitored using ellipsometry exploiting the polarization of the light reflected from the surface of the growing layer. Meng et al. [81] have studied the applicability of a GA combined with simulated annealing to the control of growth of one of basic optoelectronic films, (Ga,Al)As on GaAs substrate. Getting the properties of the layer from the experiment is mathematically difficult, and the method of solution must take into account the presence of false minima. The authors have demonstrated the applicability of the computational method for the case of the experiments keeping the Al cell temperature constant and adjusting the Ga cell temperature (in feedback manner) in order to achieve the required Al content.

Another complex process that requires an intelligent optimizer is the milling of the material leading to formation of nanoparticles. Su and Hou [88] have described construction of an algorithm aiming for optimization of wet-milling of titania nanoparticles. In the mill, the collisions between the milling balls and the material particles cause fractures into smaller particles. The use of glycol solvent permitted to form a colloidal solution. The quality criteria of the nanoparticles include the mean grain size and the grain size variance that are experimentally determined before and after the process. The five process parameters studied in the paper are the milling time, flow velocity of the circulating system, agitator-shaft rotation velocity, solute-to-solvent weight ratio, and number of grinding balls. The requirements that the grain size is small while the variance remains small are conflicting; therefore, a multiobjective optimization procedure must provide a way to a compromise solution. The authors have combined several approaches to construct their algorithm that divides the population into two, each performing optimization according to a single criterion. The procedure yielded the Pareto-optimal solutions achieving the desired product qualities of the process of nanomilling.

Various materials have been studied as candidates for lithium ion batteries. Any of materials may require optimization. An example is the graphite–lithium system. In order to reduce the weight of the battery, one can consider the carbon–nanotube–lithium system. A study of this system was presented in Ref. [104] aiming for optimizing it with the particle swarm and differential evolution methods. Five kinds of metallic and semiconductor carbon nanotubes were considered. A suitable energy functional was used as a basis for energy minimization of the system where lithium ions are located inside a nanotube. In the calculations, the carbon atoms remained fixed. Using the described approach, ground state symmetries of the Li-containing nanotubes were successfully determined for each kind of nanotube.

3.2. Physics of Materials

The use of GAs in solid state physics and related branches (see Table 2) helps in design of materials with desired physical or structural properties, in working out modern devices based on specific physical principles. GAs are also widely applied as a tool in spectroscopic analysis of materials.

For determination of the density and temperature of laboratory or astrophysical plasma, iterative and neural network-based methods of analysis of X-ray spectral data have been applied before 2002. For most complex cases, the analysis with such methods becomes difficult and the GA appears to constitute a useful tool for this purpose [154]. In the cited implementation, the parameters describing the spectrum (temperature, density, and spectrum shift) are encoded in a 15-bit string. The algorithm employs elitism and n-point crossover. The results of calculation for exemplary spectra show that the applied algorithm provides a valuable method of studying the spectra of plasma. GAs are concluded to be a valuable general method of analysis of spectral data.

Another example [145] shows the usefulness of a GA for analysis of Mössbauer spectra. Analysis of Mössbauer spectroscopy data requires a large computational effort and is time consuming, especially if the phase composition of the studied material is unknown. The difficulty of analysis

TABLE 2.—Examples of applications of GAs in physics of materials.

Field	Application
General	Applications in physics [43]
Solid state physics: electronic and other properties	Bound states, nonlinear density functional calculation [124]
	Strain distribution determination for fiber Bragg grating reflection [125]
	Binding energy calculation [126]
	Band structure calculation [127]
	Thermodynamics of incommensurate $Sn_2P_2Se_6$ phase [128]
	Spin glass relaxation [129]
	Study of strain in InAs/GaAs quantum dot system [130]
	Electronic structure of a quantum dot [131]
	Numerical modelling of quartz luminescence [132]
	Optimizing electronic properties of (Ga, Al)As [133]
	Predicting the electronic properties of semiconductor nanostructure architectures [134]
	Design of holographic structures [135]
	Simulation of implanted oxygen atoms in a silicon substrate [40]
	Energy minimization of N point charges system [136]
	Classification of perovskites [137]
Optical properties	Design of reflective filters based on III–V nitride layers [138]
	Optimization of InP waveguide based photodiode [139]
	Photon assisted tunneling between quantum dots [140]
	Strain in quantum dots [141]
	Simulation of quantum effects in nanoscale magnetic systems [142]
	Thermoluminescence of quartz [143]
Spectroscopy (*)	Interpretation of high-resolution spectra [144]
	Studies of Mössbauer spectra [145–147]
	Quantitative spectroscopic analysis [148]
	Ellipsometric data analysis for a MOS structure [149]
	NMR data analysis [150–153]
	Analysis of X-ray spectra of plasma [154]
	Inverting positron lifetime spectroscopy [155]
	Infrared spectroscopy [156]
	Interpretation of complex spectroscopic (FTIR) data [157]
	Fluorescence spectroscopy [158]
	Femtosecond laser pulse shaping [159]
	Chromatography [160]
	Mass spectrometry [23]
	Structural studies by photoelectron diffraction [161]
Design	Design of a (Ga, Al)As based quantum confined Stark effect moderator [162]
	Quantum-well design [163]
	Photonic-waveguides design [164]
	Photonic bandgap structure design [165, 166]
	Optimization of X-ray waveguides [167]
	Design of optics for sample implantation/irradiation with ion beams [168]
	Design of multilayer Mo/Si mirrors applicable for attosecond laser pulses [169]
	Optimized design of semimagnetic semiconductor-based spin-filters [170]

*for EPR studies see Table 3.

of such spectra consists in building a starting model from a number of subspectra. In the cited study, the fitness was defined as inverse of χ^2 computed on the basis of the trial model and the experimental spectrum. The elaborated method is concluded to solve the spectrum in a short time even by a less experienced analyst. In Ref. [146], another application of a GA to fitting of Mössbauer data has been presented: in this case, a GA has been combined with fuzzy logic.

Modern optical devices require highly reflective filters. Their efficiency depends on the chemical composition, the number of bilayers, surface morphology, and strain at the mismatched interfaces. Optimization of the mirrors has, as a goal, approaching to 100% of reflectivity. Design of reflective filters involving the III–V nitride layers has been demonstrated in Ref. [138]. The authors have found valuable solutions in the space of thicknesses and compositions (the composition is described by Al content in the (Ga,Al)N solid solution) in each layer of the designed stack. The results of the calculation allowed for designing a system which is less sensitive to errors in thickness and to the strain caused by the unavoidable lattice mismatch. A GA has been also successfully used for the determination of the optimum thickness for Mo/Be/Mo X-ray waveguides [167]. Thickness values of the component layers have been found which should give the best performance.

Due to complex thermoluminescence physics, a large number of parameters describing the thermoluminescence of quartz requires a special method for its modelling. This has been performed with success using a GA [143] in a semiautomatic way permitting for description of the thermoluminescence phenomenon. The authors have build a simplified model of the quartz thermoluminescence and studied the calculation results for four different samples of quartz. The model includes a simulation of the measurement sequence and solving of the charge-transport equations

for the given sequence. The implementation involves a population of 300 entities. Predefined selection rules have been used in order to ascertain that the best individuals have a significant contribution to creation of the next generation. The authors have concluded that their work opens new possibilities for studies of the quartz properties.

One of valuable applications of GAs is the determination of the optimal atomic configuration leading to the required band structure properties: a study for the (Ga,Al)As case has been presented in Ref. [133]. The calculation steps for the given configuration involve the relaxing of atomic positions, calculation of the atomic potential and solving the Schrödinger equation. The authors have optimized the algorithm parameters (population size, number of generations, number of new individuals created at the given generation, the crossover probability, and the mutation rate). One of the authors' result is the discovered achievability of a wide range of bandgaps for the studied (Ga,Al)As system.

GAs have also been helpful in solving a complex task of finding the values of thermodynamical parameters for the incommensurate (IC) $Sn_2P_2Se_6$ phase [128]. The authors of the study have applied a phenomenological model to explain some experimental data for ferroelectric $Sn_2P_2Se_6$ in the IC phase. The developed model has resulted in a set of material parameters leading to good reproduction of experimental order parameter, the wave number, and the anomalous heat capacity. The results show that for $Sn_2P_2Se_6$ the role of nonlinear effects is important.

3.3. Chemistry of Materials

Applications of GAs in chemistry cover the studies of molecular design, chemical reaction, and catalysis (Table 3). They help in design of materials with desired physicochemical properties and in understanding the catalytic properties of the given material, and have been successfully used for studying of complex-reaction mechanisms and in search for new or improved catalytic materials.

TABLE 3.—Examples of application of GAs in chemistry of materials.

Field	Application
General	Applications in chemistry [43]
	Various applications in analytical chemistry [171]
	Applications in chemometrics [26, 74, 75]
	Applications in chemistry including molecular modelling [54]
	Determining molecular structures [172]
Design and modelling	Modelling of long chain molecules [173]
	Molecular design and drug design [22, 174–177]
	Small molecule geometry [178]
	Photodynamics of molecules [179]
	Design of fuel additives [180]
Chemical reactions and processes	Reaction path construction [181]
	Studies of complex reaction mechanisms [51]
	Chemical reaction kinetics [182]
	Carbonate-alcohol interaction [183]
	Polymerization [184]
Spectroscopy classification & analysis	Analysis of EPR spectra [185, 186]
	Molecular diversity & compound classification [56]
	Chemical analysis of multicomponent system [187]
	Molecular recognition [188]
Catalysis	Search for new catalytic materials [189]
	Catalysts for ethane production [190]
Theory	Molecular potential energy minimization [191]

Traditional local refinement of EPR spectra leads to finding the nearest local minimum. To find a global minimum, application of global search techniques is necessary. Implementation of GAs for automated analysis of the EPR spectra has been studied in Ref. [185]. Vanadia–zirconia catalysts exhibits catalytic properties being a function of V_2O_5 loading, thermal treatment and the chemical state of the support. The mean square error representing the difference between the experiment and model was taken as the fitness function. For an example of real EPR spectra of tetravalent vanadium in VO_x/ZrO_2 catalysts, applicable to oxidative dehydrogenation of propane, the undertaken analysis has revealed speciation of vanadium into two kinds of vanadyl entities and isolated bulk V–Zr(x) ions due to solid-solution formation near to the surface. The authors of Ref. [189] have used a hybrid genetic approach completed by an artificial neural network for search of new catalytic materials. The method is concluded to permit for reduction of the number of necessary experiments. The neural network serves for establishing relationships between the materials properties and their catalytic performance. The performance of the method is illustrated by successful search for catalytic compositions applicable to the same goal as that of Ref. [185], i.e., the oxidative dehydrogenation of propane.

Maeder et al. [51] have applied a GA, combined with a gradient search method, for investigation of complex reaction mechanisms. In the approach applied in this study, the following features of the GA have been adopted: a half-uniform crossover, crossover not allowed for strings with small Hamming distance, the limit being progressively reduced during the calculation. A similar reduction is applied for the mutation rate, replacement method has been used for creation of the new generation (the fittest individuals are selected from the list of parents and children). The method has been successfully applied to simulated kinetic measurements with the reaction mechanism described by a single equilibrium constant and two rate constants, as well as to kinetic measurements of the complexation of Cu^{2+} by 1, 4, 8, 11-tetraazacyclotetradecane involving determination of two equilibrium and two rate constants that must be determined. The applied approach can be applied to any reaction. Furthermore, the success of these calculations opens the way to extension of the approach aiming for explaining the reaction mechanisms.

Ghosh et al. [180] have presented an application of GA to design of fuel additives. These additives control the deposit formation on the intake valves of the automobile engine. They affect the fundamental properties of the car and its engine such as driveability, cold-start efficiency, knock characteristics, and emission components. The mechanisms of formation of these deposits are quite complex so developing efficient physical models for the involved phenomena is impossible. The statistical approach is inappropriate due to large noise in test data. The authors have proposed a way of designing the fuel additives by using a GA. The calculations included the parameters (such as

fuel characteristics and temperature) adopted in the ASTM tests of additives. The space size (number of points where the grid search is performed) was evaluated to be of the order of one million. Number of trials as remarkably low as 625 has led to a set of valuable solutions of the problem.

3.4. Crystallography

In crystallography, the GAs offer solving of difficult problems (Table 4) such as structure prediction, determination of complex crystal structures, modeling of clusters, understanding of the biological genetic code, or interpretation of X-ray reflectivity patterns. Interpretation of X-ray reflectivity patterns, for which (if only a local search is used) even a small inadequacy in the starting-stack model leads to a false solution, was highly facilitated by application of the genetic approach. X-ray reflectivity technique is important for modern-electronic-device technology. It exploits the fact that the reflection profile depends on thickness, density and roughness of each component (three parameters for each component layer). Additional parameters should be considered for experiment conditions and systematic errors. The profiles coming from complex multilayer systems are extremely difficult to analyze using local optimization, unless a good starting model is known. A particularly large number of GA-based programs have been written for the purpose of reflectometric analysis (see Table 4). Patented numerical solutions [259, 260] are known in this field.

Indexing powder-diffraction patterns (ascribing the Miller indices to powder diffraction peaks) is a trivial task when the unit cell size is known. It becomes difficult for low symmetry substances (monoclinic and triclinic) where four (monoclinic case) or six (triclinic case) cell parameters have to be found in a large space. Additional parameters are used for description of systematic errors that affect the peak position. The objective-function shape is

TABLE 4.—Examples of applications of GAs in crystallography.

Field	Application
General: crystallography	Evolutionary algorithms in crystallography [192]
Crystal structure modelling and prediction	Prediction of carbon crystal structures [193]
	Prediction of inorganic crystal structures [194, 195]
	Prediction of high-pressure structures [196]
	Prediction of protein crystal structures [197–200]
	Modelling crystal structures [201, 202]
	Structural optimization of tubular nanostructures [203]
	Prediction of ternary chalcopyrite formation [204]
Crystal structure solving	Powder pattern indexing [205–208]
	Solving heavy atom positions in macromolecules [209]
	Solving structures of crystals [210–216]
	Solving structures of pharmaceuticals [217]
	Solving structures of proteins [218]
	Structure refinement [219]
	Determination and refinement of disordered crystal structures [220]
General: structure of clusters	Structure of clusters [55, 221–224]
Modelling of clusters and low-dimensional system	Cluster modelling [225]
	Structure of carbon clusters [226]
	TiO_2 nanoparticle structure [227]
	Silicon clusters [228]
	Germanium clusters [229]
	Aluminum clusters [12, 230]
	Mixed clusters [231]
	Aluminum oxide clusters [232]
	Structure optimization for Na_xCl_{x+1} clusters [233]
	Structure optimization of Pd–Pt clusters [234]
	Structural transition and magnetic properties of Co_mPt_n clusters [235]
	Ab-initio determination of solid-state nanostructure [236]
	Prediction of formation of exotic dipolar monolayers [237]
	Structure and properties of Ti nanowires [238]
Characterization of surfaces and thin films	Surface structure determination [239]
	Surface reconstruction determination [240–242]
	Oxygen adsorption at the Mo crystal surface [243]
	Simulation of reflectivity data (general) [244, 245]
	Simulation of reflectivity data for Langmuir–Blodgett films [246]
	Simulation of reflectivity data for liquid crystals [247]
	Simulation of reflectivity data for thin solid layers and multilayers [248–251]
	Thin-layer structure [252]
	Rocking-curve simulation [248]
	High-resolution diffraction analysis [253]
	Strain distribution in implanted layers (software) [52]
	Multilayers aperiodic order based on X-ray diffraction from GaAs-AlAs heterostructures [254]
Other crystallographic tasks	Helix design [255]
	Indexing crystal faces [256]
	Texture analysis [257, 258]

characterized by numerous deep but narrow local minima which are difficult to locate using traditional computing methods. Shape complexity of functions applicable in global optimization-based indexing algorithms has been illustrated, e.g., in Refs. [206, 261]. Even for the case of two structural parameters one observes hundreds narrow local minima within the space. Various methods exist for solving the indexing task. Among them there is the global search/optimization in the lattice parameter space using the GA approach [205, 206, 208]. One of the reasons of failure of methods of indexing is the systematic absences and very weak intensities for a considerable fraction of peaks. The difficulties grow if statistical or systematic errors affect the reflection positions, or if spurious peaks due to secondary phases appear. If the unit-cell is large and the resolution is insufficient to separate nearby located peaks, then the most classical approach based on peak positions may fail: the approach based on full-profile-matching-based criterion function described in Refs. [206, 207] is a promising alternative.

Modelling molecules is a difficult task, because, as noted in Ref. [191], the number of local minima grows exponentially with the molecule size. Therefore, constructing tools able to avoid the problem of trapping at local minima is of fundamental importance. Deaven and Ho [226] have demonstrated the effectiveness of GA approach to energy minimization of clusters. Showing the solution for various n in carbon clusters, C_n (for $n < 60$), these authors have traced out the way for numerous further studies in this domain. Moreover, they have shown that the GA approach is much more effective than that of simulated annealing. With the cited work, a whole branch of computational studies has been initiated: the number of articles in this field systematically increases each year. One of most recent ones describes the application for modelling the structure of tubular nanostructures [203]. The promising results indicate the opportunity of finding new such structures using the applied procedure. The ground state of n-atom clusters has been studied in Ref. [228] using a hybrid GA as a tool permitting for analyzing the scalability of the algorithm. The extensions consisted in adding a local-search routine and seeding the initial population with lowest energy structures of a smaller cluster. This technique is found to provide near-optimal solutions scaling subcubically instead of exponentially as for a poorly designed evolutionary algorithm. Such achievement shows a way to calculation of larger or more complex clusters using the GA-based techniques.

Structure and properties of Ti nanowires have been studied using a GA with a tight-binding potential [238]. Ultrathin metallic nanowires can be considered as candidates for elements of molecular electronics. The starting population in the GA run has been generated at random. The child configuration obtained from a pair of parents was further locally relaxed by molecular-dynamics and replaced the parents in the population if it had lower binding energy. Up to 10,000 iterations have been found to be sufficient to detect the global minimum. Helical multiwalled cylindrical structures are the result of calculation, with pentagonal atomic packing for wires of diameter in the range of 0.747 to 1.773 nm. The thicker ones adopt hexagonal packing. Computational discovery of the pentagonal nanowires is in agreement with experimental observations.

Surface structure and properties play a significant role in the practical applications of semiconductor and metal crystals. Understanding the surface state frequently requires formulation of global optimization tasks. One example is the surface reconstruction problem, where the location and symmetries of surface atoms are determined. The surface reconstruction of Si (001) surface based on molecular dynamics is described in Ref. [240]. For modelling the surface, the authors consider a slab of three atomic layers and, for dangling bond termination, a 32 hydrogen atom layer at the bottom. To save computing time, all atoms except the first Si layer remain fixed. Appropriate boundary conditions are imposed. The Cartesian coordinates of the first layer atoms form the space of variables. Within the procedure, a step of local search consisting in a relaxation to the nearest local minimum is adopted. For comparison, the authors have performed in parallel a computation using simulated annealing method. Both methods have been found to give the same solution, the symmetric buckled-dimer structure. The GA advantage is the opportunity to find structures of complex topology. The interest connected with the (001) silicon surface is due, in particular, to its use for molecular beam epitaxy substrates. Also high index surfaces can have practical applications—they are known to serve for growth of low-dimensional objects (nanodots or nanowires). Chuang et al. [241] have studied the reconstruction of Si(105) surface. Here, a thicker slab of atoms was permitted to relax during the program run. The authors have considered models involving various periodicities, and the obtained results are verified with the independent work by other groups. Related findings have been reported by the same group for Si(114) surface [242]. Oxygen adsorption at the Mo(112) crystal surface has been modeled in Ref. [243]. Comparison of the stabilities of the predicted models obtained by a combination of a GA with density functional theory shows that different $p(1 \times 2)$ and $p(1 \times 3)$ structures may coexist over a wide range of oxygen pressures. The results of the computations are fully supported by experimental data collected by various techniques.

3.5. Biology and Genetics

Many applications in biology concern structural problems connected with proteins and with RNA and DNA (Table 5). An interesting computation has been performed in order to model the web geometry. The spider web is an unusual tool designed by nature. Despite an extremely small thread thickness (of the order of 1 μm) and low density, it can support a relatively large load (during capturing of large insects), it is also used for transportation by the wind of young spiders of some species when a wind comes. Properties of the web material make it an attractive material for applications, in particular its use as a component of nanocomposite with silica is considered [284] and its production is discussed [285]. The web strength deciding about the capture efficiency depends on the structure of the thread and on the geometrical structure of the web.

TABLE 5.—Example of applications of GAs in biology and genetics.

Field	Application
Biology	Protein-ligand docking [262]
	Protein folding [174, 176, 263–267]
	Protein-structure alignment [268]
	Nucleic acid sequence alignment [269]
	Multiple sequence alignment [270]
	Protein engineering [271]
	Protein translation [272]
	Conformational angles of biomacromolecules [273]
	Biological engineering [274]
	Spider-web modelling [275]
Genetics	Genetic mapping [276]
	Analysis of gene expression data [277]
	DNA sequencing [278]
	DNA analysis [279]
	RNA folding [280]
	DNA sequence assembly [281]
	RNA secondary structure analysis [282]
	Identification of toxicity-relevant genes and pathways [283]

Its crystal structure and even the process of crystallization during (in vivo) silking has been understood only recently, thanks to the outstanding experimental opportunities at highly collimated X-ray synchrotron beams [286–288], as well as the structural changes with rising temperature [289] or with interaction with CO_2 [290]. Krink and Vollrath [275] have compared the properties of webs built by true and cyber spiders. These properties depend on many factors such as geometry, web size, prey size/density. Factors like spider-energy consumption are thought to play a role in the web construction. The authors of Ref. [275] have performed both experiments using living spiders and calculations using GAs. The method permitted to explore local minima of the fitness function being connected with different web geometries. The simulations involved a relatively small population (size of 24), divided into 4 subpopulations. The GA-optimized results were characterized by geometrical parameters. One of results of the calculations established that one of basic spider-web parameters, the GA-optimized spiral distance, compares well to the experiment. The results of simulation are found to be improved in respect to previous geometrical and other approaches.

3.6. Engineering and Industrial Applications

The instances in engineering involve, among many others (see Table 6), the design of optical lens, planning of the river dam construction on the basis of the physical properties of the available concretes, and control of the complete steelmaking process.

Massive constructions (dams, foundation slabs, bridge decks, etc.) require a minimization of their building times and huge costs, and avoiding the cracking risks. The risks are dependent on the materials used and on the mounting schedule. An important element of the problem is the hydration reaction influencing the cracking ability of the construction. The reaction is exothermic which leads to severe limitation of the building rate. Fairbarn et al. [294] have studied the optimization of such constructions using GAs. Many parameters describing it have been taken into account, in particular the thermomechanical properties of the materials used, the placing temperature, and frequency. The success of the GA-based method has been illustrated on an example of a river dam. In the cited study, a proper dam model has been designed and tested. The model represented a relatively small dam of fixed size. The construction requires an optimized material (its properties influence the reaction with water, energy dissipation, shrinking, all of these factors being decisive for the process of construction). The computational procedure involves: the material, layer thickness, time distance between layer depositions, starting temperature, and the temperature field. No safety compromise is adopted: cracking must be avoided. Solving the problem in a different way is difficult, due to the complexity and nonlinearity of heat-transfer equations. The approach may be extended to any massive concrete constructions like bridges or viaducts. This GAs application in materials processing is of high economic importance due to the expected financial gain.

Design of optical system of lenses has been a goal of the work of Ref. [296]. Purely geometrical design is not appropriate for lenses systems because of image distortions. The authors have constructed a bi-objective fitness function based on the spot size and image flatness criteria. Minimizing both the spot size and the image curvature leads to reduced aberrations. The quantities describing the lenses shapes and materials (refraction indices) have been used as parameters of the algorithm. Chromatic aberrations can be reduced by using different materials for the system components. The problems encountered with the poor precision of the GA have been overcome by performing additional runs of the program with progressively reduced search-space size. The authors emphasize the useful results obtained, the extreme simplicity of the algorithm making possible to combine it with already existing optical designers, and the opportunity to apply it for systems being more complex than the test one described in the article.

Efforts on GAs application to a reactor-core design are described in Refs. [320, 321]. This problem has been solved using a niching GA. The calculations involved optimization of the reactor cell parameters (dimensions, enrichment, materials). The applied search method led to improved exploration of the search space as compared to classical approaches. West and Sherif [308] have optimized a model of multistage vapor-compression (MVC) system. The model involves five refrigerants, and the parameters describe the system construction as well as the pressure (total 9 parameters). The authors encountered difficulties in reaching a consensus optimum and attributed them to the termination criteria and mutation rate applied. Nevertheless, the calculation provided valuable information concerning the favorable (vapor) parameters. They are hoped to lead to improved effectiveness of the system. Thanks to the computations, one of refrigerants turned out to be clearly better than remaining ones. The authors noticed that the model of the MVC system required taking account of more parameters than those studied in the article.

Insulation from noise has an environmental aspect: so-called *noise pollution* is included in the activity program of some governments (for background of the problem see Ref. [340]). The barrier size, shape, and material decide about attenuation efficiency. In the modelling, not

TABLE 6.—Examples of applications of GAs in engineering and industry.

Field	Application
General	Engineering design [67, 70]
Design of industrial products, massive constructions, and scientific equipment	Shape and topology optimization [291]
	Aerodynamic shape design [292]
	Mechanical component design [293]
	Design of mass concrete construction [294]
	Design of vibration-free carriage arms for a hard drive [295]
	Design of optical lens/telescopes [296]
	Semiconductor device design [162]
	Multilayer X-ray mirror parameters from X-ray reflectivity patterns [297]
	Design of an adhesively bonded functionally graded lap joint [298]
	Studies of mechanical properties of an adhesive [299]
	Optimization of steel [300]
	Optimizing the low-carbon steel [301]
	Construction of anti-noise barriers [302–304]
Device optimization	Optimization of a synchrotron wiggler [305, 306]
	Optimization of an insertion device at a synchrotron source [307]
	Optimization of vapor compressions systems [308]
	Cooling the electronic devices [309]
	Stereolitography apparatus optimization [310]
Vehicles, ships, motors	Synchronous motor design [5]
	Design of ship's engine room [311]
	Engine mount design [312]
	Vehicle modeling & design [313]
Aircraft	Shape design of a missile [314]
	Aircraft design [315]
	Aircraft wing design [316]
	Wing tailoring for supersonic aircraft [317]
	Aircraft-engine diagnostics [318]
Nuclear and chemical plants	Instrumentation design for methanol plant [319]
	Nuclear reactor core design [320, 321]
Automation and instrumentation control, control systems	Cutting operation optimization [322, 323]
	Control of shape memory alloy actuators [324]
Industrial production optimizing	Optimizing the hard-disk drive production [325]
	Steel production [59, 326, 327]
	Operation of an integrated steel plant [328]
	Dynamic optimization of an industrial polymerization reactor [329]
	Continuous steel casting [330, 331]
	Prediction of silicon content in the hot metal during ironmaking process [332]
	Steel plate processing [333]
	Optimization of a scheduling system for steel reheating furnace [334]
	Modelling noisy blast furnace data [335, 336]
	Oil stabilization [337]
	Milling operation optimization [338]
	Optimization of radar-absorbing composite structure [339]

only the efficiency but also aesthetic and financial aspects are important. In particular, the barrier may not be too high. The early achievements using GAs can be found in Refs. [341, 342]. In more recent articles, technical means against noise and construction of noise barriers are described [302, 303]. The solutions found show that the classical T-shaped barriers should be replaced by more effective barriers of complex shape [303]. A study exploiting a hybrid genetic/local search technique shows the advantages of multiple edge barriers [304]. The field of studies is large here, as still a little is known about the best choice of the barrier material. The authors of the cited study have expressed their expectation that the studies will be continued and will permit to achieve a good balance between the barrier effectiveness and cost.

Applications of GAs in steel industry have been recently reviewed [59]. The article shows how fast this subfield of their use is expanding. A clear advantage of the method is its flexibility permitting to accommodate to various models and data. The method is applicable also to online processes (e.g., to casting control), although then its speed may require optimizing. As for specific tasks several features of a metallurgical process have to be fitted at the same time, multiobjective GAs are frequently elaborated for such purposes. In the cited article, six examples from recent literature are briefly discussed, touching various elements of steelmaking: gas injection during the process, transport phenomena, charging of the blast furnace, chemical composition of the molten metal, slag forming, desulphurization, continuous casting and spray cooling, as well as the requirement for flatness of hot-rolled steel strips. One of the conclusions says that the present quality requirements in the steel industry make that use of optimizers such as GAs has a great potential. Another study in the field is worth mentioning here. Fujii et al. [326] have described an automatic scheduling system for a complex large-scale task of steelmaking process from refining converter to continuous caster. A specific

difficulty here is the particular constraints and varying production requirements of the individual process. The applied computational procedure applies multiconstraints to the reduction of the search space. Introduction of the method in NKK Keihn works permitted for replacing the daily scheduling by a weekly one. This result is crucial from the economic point of view.

A chemical-process optimization problem has been solved through the use of GA involving the constraints specific for the (mathematically difficult) task of oil stabilization [337]. The oil stabilization process is used to separate a feed containing 12 hydrocarbon components (methane to decane and heavier), into a specified multicomponent gas and liquid products. Due to the nature of the separation technologies, design of the process is difficult. The design involves capital cost models of the units (flash vessels and compressors) and the aim is to maximize the annual profit. The design includes specific constraints such as the oil-vapor pressure range. The authors have proposed an improved methodology involving a combination of visualization, data analysis, learning procedures, penalty functions, and a GA, what helps in identifying the feasible ranges of each variable and consequently in finding the solution of the problem. The implementation has been found to provide a valuable tool for this kind of computational problems.

A group in Japan has been working for at least a decade on design of aircraft wings (see, e.g., Ref. [316]), using GAs as one of basic tools. In the most recent study, these authors have used GAs for design of a wing of a small supersonic aircraft. The study involves as many as 35 variables describing the wing shape (nine parameters describe the sections) accompanied by three geometrical constraints, one constraint involving the target Mach number, and one constraint limiting the wing volume. The population size equal eight has been used. The computation led to the optimal aircraft wing shape. The authors conclude that their approach will become a standard one in a short time.

The design of both photonic and electronic devices requires a systematic approach to identify optimal devices of earlier designed structure as well as quite new ones. Modern computational methods create such opportunity. To reach this goal, one solves the inverse problem, namely, finding the optimal configuration for the user defined problem described by the target function, i.e., determines the spatial configuration of the semiconductor (hetero)structure. In case of (Ga,Al)As semiconductor heterostructure studied in Ref. [162], the authors demonstrate this approach for the design of a quantum-confined Stark-effect (QCSE) optical modulator. Intelligent searches are performed for various target functions. The approach has provided interesting and unexpected solutions representing the previously unknown layer-stacking variants. This result leads to expectation that further investigations of this kind will lead to valuable discoveries of structures exhibiting new properties. The authors' conclusion is that such methods will be of great use both for the design of devices and for the discovery of new device functionalities.

4. Discussion

GAs have numerous advantages, but it is well known that for some purposes the computation speed and convergence may be better for other types of algorithms. For example, in ab initio determination of solid-state nanostructures [236], the sport-inspired LIGA algorithm has been concluded to be considerably better than the genetic one used in the cited article. However, in many cases, GAs have been demonstrated to work more efficiently than other global search/optimization methods. Because of their flexibility, opportunity to work on many processors, and easiness of combining with other methods, they remain a very popular class of AI methods. Some improvements and tests are included in a number of articles cited in the present survey, e.g., the hybrid approach in Refs. [146, 191, 213, 228, 252, 278, 318, 337], penalty functions [337], progressive reduction of the search space [296], other strategies (seeding, predation, mutation operator variation) [234].

Global optimization methods based on genetic approach find practical applications in solving static as well as dynamic problems. GAs create possibilities for materials design, and for studies of their properties. The present survey starts from reminding that explaining the secrets of ancient materials science is due to modern materials science studies methods. The GAs can largely contribute to solving the secrets of present materials (as noted in Ref. [343]), of ancient materials technologies, but also to discover *all yet undiscovered* in this domain, i.e., to contribute in present and future materials-science challenges: uncover, modelling, design, understanding, as well as elaboration of improved methods of materials characterization.

Because of the broad applications in various domains, GAs may start to interact or interfere at various levels—either mutually or with the natural evolution. A striking example of GAs application can be given for the evolution of humans: the proposal of the authors of Ref. [344], (the idea has been rediscovered in Ref. [345]) that the marriage partners are selected using a GA caused the natural gene-based evolution of humans to be completed by a second (computational) genetic mechanism. It is easy to conclude that if this is realized on a larger scale, a question would arise about the consequences—would it lead to acceleration of the human evolution process? As for materials science, a good interaction example is the feedback application of GAs in synchrotron sources design (here mentioned: wigglers and insertion devices that are essential in forming of intense beams of extremely low divergence). These sources are widely exploited in advanced studies of materials (here mentioned: the web structure studies [275], investigation of the welding process [91]). Synchrotrons can contribute to a fast development in materials science in particular due to the idea of "compound libraries" (two-dimensional thin layers of composition varying as the function of coordinates). Such libraries, as proposed by DiSalvo [346], scanned by narrow synchrotron beam would provide information now missing on multicomponent phase diagrams and structural and physical properties of these systems: this idea is now being realized [347–350] what augurs well for future acceleration of knowledge on phase diagrams. The materials

science studies at synchrotrons contribute to permanent improvement of electronic circuits hardware used in GA-based computations. *The circuit is thus closed.*

As it is mentioned in the introduction, the evolution-inspired studies were published starting from 1956, i.e., they are only one year older than the Space exploration. So in parallel to the Space Mission, the computer scientists have contributed to the Explore-the-Parameter-Space Mission for already half a century. In materials science, they have a lot to do.

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