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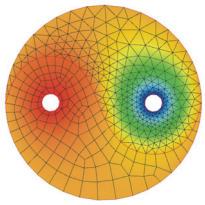

APPLICATIONS OF GENETIC ALGORITHMS IN NANOMATERIALS SCIENCE: A SHORT SURVEY OF RECENT RESULTS

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Abstract

Global-search procedures are an important element of materials design, processing, and properties determination. Genetic algorithms, a subset of algorithms based on evolutionary computation methods, are an example of global optimization methods inspired by biological principles of evolution. In materials science and related fields of science and technology, these algorithms are successfully used, e.g., for optimization of material elaboration and for design of materials with desired physical or structural properties, in working out modern devices based on specific physical principles, as well as in elaboration of improved methods of materials characterization. Nanomaterials science is a rapidly growing subfield of materials science covering various objects characterized by nanometric size. In this review, examples of recent applications of genetic algorithms in nanomaterials science are presented. Representative examples illustrate how useful are such computational methods for solving the scientific tasks, e.g., for thin-film growth modeling and characterization, for optimization of quantum-dot systems and of nanoparticle based medical therapies, for design of hard nanocomposite materials and for optimization of nanomaterial-based optical nanodevices and sensors of various gases.

Key words: genetic algorithm, application, evolution, optimization, artificial intelligence, prediction, parallel computing, global search, modeling, materials, science, engineering

1. INTRODUCTION

Many tasks in computational materials science are of complex nature and cannot be described in an analytical way. Therefore, they require a support by numerical global-search or optimization procedures. Such computations frequently face the difficulty of search in a large parameter space. Genetic algorithms (GAs), a subset of a family of algorithms inspired by biological principles of evolution (Holland, 1975; Goldberg, 1989; Baeck et al, 1997; Arabas, 2004; Affenzeller & Wagner, 2009) can be used for such purpose. Their advantages include (i) the easiness of hybridization with other methods, (ii) the ability for adaptation to the given computational problem, and (iii) an opportunity for parallel work on multiple processors [*e.g.* for modeling the oxygen implantation into silicon the reported calculation involved more than thousand processors, cf. (Takemiya et al., 2006)],

In science, medicine and technology, genetic algorithms have been found to be useful for optimization, modeling, design and prediction or analysis purposes. The use of GAs in materials science and related branches helps in optimization and design of materials of desired physical or structural properties, working out modern devices based on specific physical principles, as well as in elaboration of improved methods of materials characterization. Reviews have been presented on GAs applications in materials optimization, design and processing (Chakraborti, 2004; Kim & Cho, 2006; Maier, et al. 2007; Aland-

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er, 2008; Paszkowicz, 2009; Paszkowicz, 2013), applications in chemistry and chemometrics (Alander, 2000; Leardi, 2001; Luke, 2003; Hageman, 2004; Luo, 2006), applications in physics (Alander, 2000), materials design (Jóhannesson et al., 2002), structure of clusters (Johnston, 2003; Sastry, 2007), in machining parameters optimization (Yusup et al., 2012), reliability related applications (Ye, et al., 2010), spectroscopy and chemometrics (Koljonen et al, 2008), polymer production (Mitra, 2008), and in crystal structure prediction (Woodley & Catlow, 2008; Oganov & Glass, 2008; Oganov et al., 2011a), Day *et al.,* 2009, Oganov et al., 2011b).

2. GaS IN NANOMATERIALS SCIENCE

Nanoscience and nanotechnology exploit new physical phenomena that occur in crystals characterized by nanoscale dimensions. If the length scale of such objects is of the order of tens, hundreds or several thousands of atoms, new physics occurs because, unlike in larger solids, this scale is comparable to such physical quantities as Fermi wavelength of electrons and spin-coherence length for electron spins in transport. The physics of such small objects typically has quantum mechanical grounds and may lead to new functionalities. The physical properties of zero-, one- and two-dimensional nanostructures may thus be a basis for new devices applicable in nano-optoelectronics, nano-bioelectronics, nano-mechanics, nano-robotics, etc. Some nanosystems can be designed as productive, i.e. they can fabricate precise parts of other nanosystems. An industrial evolution may be expected at a time when nanotechnology finds massive applications.

Nanomaterials science covers various materials characterized by nanometric size in one or more direction (e.g. thin films, heterostructures, nanofibers, nanowires, quantum dots, and nanopores). An example of unconscious use quite a long time ago is noticed: carbon nanotubes have been discovered in a Damascus steel sword from 17th century (Reibold *et al*., 2006). Conscious use of nanomaterials is developing for the last decades, only. In this review, the applications of genetic algorithms in nanomaterials science are briefly reviewed. Representative examples taken from recent literature show how such computational methods are useful for solving the scientific tasks for thin-film growth modeling and characterization, for optimization of quantum dots systems and of nanoparticle based medical therapies, for design of hard nanocomposite materials, as well as for optimization of nanomaterial-based optical nanodevices and gas sensors.

2.1. Studies of nanocrystal growth, characterization and properties

Thin film growth processes by any of methods (molecular beam epitaxy, MBE, atomic layer deposition, ALD, pulsed laser deposition, PLD, chemical vapor deposition, CVD, sputter deposition, SD, etc.) involve multiple physical and technological parameters causing a complexity of process design, modeling and optimization tasks. Many studies have already demonstrated the usefulness of genetic algorithms in this area. For example, Meng *et al.* (1998a, 1998b) have implemented a genetic algorithm, in combination with simulated annealing process and optical and neural net models, for the control of MBE growth of one of basic optoelectronic films, (Ga,Al)As, on GaAs substrate. The calculations led to estimation of values for both, the complex refractive index and the deposition rate of this material. 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 a feedback manner) in order to achieve the required Al concentration in the grown film.

Due to the physicochemical properties (large bandgap, easiness of incorporation of *3d* metals into the lattice), zinc oxide is one of most extensively studied II-VI-type semiconductors. In CVD growth method, understanding the chemical reactions leading to the final product is a main stem leading to the successful film growth. Takahashi et al. (2005) have constructed reaction models for a CVD growth process of silica. These models involve various deposition species and gas-phase and surface reactions. A genetic algorithm has been found to be helpful in analysis of reaction mechanisms of the studied processes and to be able to replace earlier applied, more conventional procedures. Ko et al. (2009) have studied the growth rate for ZnO thin films grown by PLD method. In the calculations, a neural networks algorithm has been applied, whereas the growth process has been optimized via a genetic algorithm, showing that this calculation method can be successfully used to design the semiconductor manufacturing process.

X-ray reflectivity is one of basic methods of thin film characterization. Due to complexity of reflectivity profiles, which grows with the number of param-

eters (at least three parameters for each component layer), their interpretation requires application of global search methods. X-ray reflectivity technique is important for modern-electronic-device technology because the physical properties of the given multilayer are determined by its structural features (thickness, composition, density, roughness of individual layers). Many GA-based programs are available for the purpose of reflectometric analysis, e.g. that described by Björck & Andersson (2007).

In the studies of implanted layers, one of goals is understanding of the distribution of implanted ions and of the distribution of strain. Such tasks may require a particularly large computational effort. For example (as mentioned in the Introduction) for modelling the oxygen ions implantation into silicon, the reported calculation involved more than thousand processors (Takemiya et al., 2006). For analysis of strain in implanted semiconductor layers, the genetic-algorithm-based software analysing the rocking-curve profiles is highly helpful (Bleicher et al., 2004).

Improvement of multilayer systems requires a large experimental effort. Modeling using the genetic algorithms is frequently time consuming, due to the need of looking for the global solution in a large space. The difficulties connected with relatively slow operation of genetic software can be strongly reduced through the use of GP GPU cards (cf. Baumes et al., 2011). Recently, a neural network combined with a genetic algorithm have been used for optimization of transparent conductive indium tin oxide/aluminum multilayers deposited on glass (Cho et al., 2012) ("ITO" stays for indium tin oxide, a material being a rare example of transparent and conductive material). The genetic algorithm is shown to be useful for tailoring the transmittance and resistance, according to the technological needs. The calculated parameters have been employed in an experiment, confirming the obtained calculation results.

Spider webs are built from silk, which is a protein fiber of micron or submicron thickness. They exhibit valuable mechanical properties (strength, extensibility and toughness). In an interesting study of spider web structure and properties, Krink & Vollrath (1997) have compared the properties of webs built by true and cyber spiders. Spider energy consumption is one of key factors in such considerations. In the theoretical part, GAs have been used as a tool. One of results of the calculations, the GA-optimised spiral distance, compares well with that determined experimentally.

The process of nanowire growth involves many technological parameters and is time consuming. Structure and properties of ultrathin titanium nanowires have been studied by Wang et al. (2001), using a genetic algorithm. Such nanowires can be considered as a candidate for components of future molecular electronics. The calculations have led to helical multi-walled cylindrical structures, with pentagonal atomic packing for wires of diameter as low as about 1 nm. This computational discovery of the pentagonal nanowires has been demonstrated to be in agreement with experimental observations.

Double quantum dots exhibit interesting electron-transport properties (van der Wiel et al., 2002). Grigorenko, Speer & Garcia (2002) have studied photon assisted tunnelling between quantum dots. In the studied case, the electron tunneling between two metallic reservoirs coupled through a double quantum dot has been induced by an ultrashort pulse of electric field. A genetic algorithm has been employed in optimization of the shape of the electric field, in order to maximize the transferred charge. It has been found that when using a sequence of pulses of different shapes, a considerable enhancement of the current takes place. Genetic algorithms have been successfully used also for such tasks as calculation of bandgap in Si quantum dot arrays (Gómez-Campos et al., 2009) and for optimization of multi-quantum well structures (Passaro et al., 2010). In quantum dot systems, both hydrostatic and biaxial strain occur. A genetic algorithm has been developed for the purpose of analysis of the strain state (Korkusinski et al,, 2009). The usefulness of quantum dots in white-light emission has been documented by Zhong et al. (2012). In the cited study, the color proportion and the FWHMs of the color components have to be modeled in order to provide the optimal white spectrum of the emitted light. This analysis, performed through the use of multiobjective genetic approach, has shown that the use of quantum-dot nanophosphors causes an increase of the emission by 13% to 32% as compared to white LEDs based on traditional phosphors.

Çamkerten et al. (2012) have studied the properties of a nanocomposite material built from nanosilica and styrene particles. The polystyrene has been prepared in a reactor with temperature control performed by a self-tuning PID controller. The controller parameters were determined using a genetic algorithm. The final material obtained shows an improved hardness and thermal stability; an increase of

performance with rising silica-to-styrene proportion has been observed.

Heat transfer is a means used in medical therapies. In particular, it can be applied to destroy tumors. Mital and Tafreshi (2012) have optimized a GA-assisted therapy based on introduction of magnetic nanoparticles (such as iron oxide) into the tumor area. The known method of therapy consists in heating the particles using an alternating magnetic field, leading to damage of the tumor. In the cited paper, a simple model of the heat transfer is constructed and its parameters are optimized using a genetic algorithm. The genetic approach is a proper one, as the fitting function, which has been built for the given task, is of relatively flat shape in the vicinity of the optimum, causing substantial difficulties in localizing the global minimum. Optimizing the power dissipation consists in maximizing the heat delivered to tumor cells, whereas that delivered to other cells must be as low as possible.

Dudiy & Zunger (2006) have studied the properties of rare-earth doped gallium phosphide. The study, performed with the use of a genetic algorithm, has shown that the dopants are present in the matrix in the form of clusters and that their presence modifies the bandgap. For quaternary systems such as (Ga,In)(As,Sb), an opportunity exists for designing structures fulfilling the conditions of lattice matching to a given substrate and a specific value of bandgap at more than one chemical composition. Piquini et al. (2008) have used a genetic-algorithm in order to study the above-mentioned system. The results of the calculation have open the way to still more advanced bandgap engineering studies. Calculations performed by D'Avezac *et al.* (2012), employing the genetic algorithm approach, have demonstrated a possibility for construction of a direct gap superstructure from indirect gap components, Si and Ge. The proposed solution of the problem is founded on a configurational motif of $SiGe_2Si_2Ge_2SiGe_n$ on $Si_xGe_{1-x}(001)$ substrate. It shows a direct and dipole-allowed bandgap. The mentioned finding, if experimentally confirmed, would be of high importance for the science and technology of optoelectronic materials.

Nanoporous metal-organic frameworks (metal-based clusters interconnected by organic linkers, abbreviated by MOF) attract interest because of their properties such as high surface area, tunable functionality and pore size, hosting the guest molecules. Due to these properties caused by hybrid structure, the MOFs exhibit ability for sensing, drug delivery, gas storage, gas separation and catalysis. Combinations of the building units with organic linkers create one-, two- and three-dimensional periodic structures. Modeling such structures is a multi-parameter global optimization problem. A computational genetic-algorithm based approach suitable for design of MOFs has been proposed by Tafipolsky and Schmid (2009). This approach has been subsequently used, e.g., for prediction of structure and properties of boron-based organic frameworks (Amirjalayer et al., 2012).

2.2. Studies of nanocrystal-based devices

(Ga,Al)As semiconductor heterostructure has been studied with the help of a genetic algorithm by Thalken et al. (2005) with the aim of design of a quantum-confined Stark-effect (QCSE) optical modulator. The searches have been performed for various target functions. The approach has provided interesting and unexpected solutions representing previously unknown layer stacking. Using the proposed or a similar approach for other semiconductor systems may lead to finding new structures exhibiting valuable characteristics.

Future European Community regulations will probably include a continuous monitoring of ammonia level in atmosphere of big towns. The level of the order of 30 ppb is considered as normal whereas higher levels may serve as an indication of an environmental problem. Installation of a low-cost monitoring systems is thus highly desirable. Chiesa et al. (2012) have reported a study on implementation of an ammonia monitoring grid based on nanostructured chemresistor gas sensors permitting for such monitoring. This is an alternative to systems, such as that employing quantum cascade lasers sensing the ammonia remotely, as described by Corrigan et al. (2009).

Optimization of MOS memory devices has been performed by Dash et al. (2012) for devices built with silicon nanocrystals and single-walled carbon nanotubes confined in a layer in the gate dielectric oxides, separately. The authors have demonstrated that the MOS characteristics can be improved by optimization of both high-field and low field tunneling currents, employing a genetic algorithm.

One of goals of nano-biotechnology is building synthetic molecular machinery from DNA (Bath & Turberfield, 2007). The molecular motors could carry cargoes within living cells. Kovacic et al. (2012) have used a genetic algorithm for developing

one-dimensional DNA-based track for an artificial molecular motor. Another device has been recently worked out by Forestiere et al. (2012). These authors have presented a genetic algorithm approach to the design of metallic nanoparticle arrays providing a large enhancement of electric field. The applied method has been experimentally validated by surface-enhanced Raman scattering measurements, and it has been concluded to be valuable for construction of various nanoscale optical devices.

3. DISCUSSION

The examples presented in the previous section concern only a small fraction of possible directions of studies of nanomaterials using the genetic algorithms. These examples concern various scientific and technological tasks, such as:

- growth of thin films and the reflectometric method of analysis of films and multilayers,
- modeling of metallic Ti nanowires applicable in electronics,
- various studies on quantum dots of several types, in particular those used in optoelectronics for generation of white light,
- preparation of a nanocomposite material offering interesting mechanical properties,
- improving the nanoparticle based therapy aiming for destroying tumors,
- construction of a direct gap superstructure from indirect-gap components,
- design of a functional nanoporous metal-organic framework,
- design of a nanodevice for a continuous monitoring of ammonia level in atmosphere of big towns,
- optimization of MOS memory devices,
- construction of synthetic molecular machinery from DNA.

The subjects of these studies, and of other ones cited in sec. 2, illustrate the diversity of tasks solvable using the GAs. Up to now, results of multiple GA-assisted nanomaterial-related investigations have been obtained in such fields as modeling thin films, multilayers and clusters, and in solving metallurgical tasks. In a number of other domains, one can find promising examples of application, just opening the ways for future research.

It is interesting to note that in specific studies two different GAs can be involved, or a genetic algorithm can interact with a natural genetic code. For example, a GA-assisted thin film growth process can produce a film which is subsequently analyzed using a genetic-algorithm-based reflectometric analysis method. Another example of such combination is mentioned in sec. 2: the construction of molecular machinery has been designed combining the use of a genetic algorithm and a (genetic) DNA molecule (Bath & Turberfield, 2007). With the expected development of GA applications, such combinations will become more frequent.

All nanomaterials can be classified using a suitable scheme. An example of a possible single classification is shown in figure 1 which combines the nano-objects (eleven basic nanomaterial types are grouped according to their dimensionality inside the central ellipse) with the broad opportunities of genetic-algorithm support (ten key GA-based categories of studies are distinguished outside the ellipse). The data in the figure 1 are not exhaustive. In particular, for simplicity, the listed eleven 0D, 1D and 2D nanomaterial types do not include more complex and more exotic ones such as compound libraries, core-shell structures, waveguides, nanocrystal (nanowire) arrays and assemblies, webs, nanoplasmonic materials, nanocomposites, nanobelts, nanorings, nanocables, nanorobots, nanodevices, etc. The figure schematically demonstrates that all these (listed and not listed) nanomaterials can be potentially studied with the assistance of genetic algorithms. The GAs can serve for prediction, preparation, design, modeling, improvement engineering and production of such objects. Moreover, nanomaterials can be investigated with the aim of better understanding the crystal or electronic structure and of recognition of their physicochemical properties, what is necessary for improvement of their functionalities.

In summary, the nanomaterials science, a rapidly developing field, requires a support from global optimization methods. One of such methods are genetic algorithms. as show the cited examples from recent literature, Genetic algorithms are useful in nanomaterials science for tasks of global optimization, modeling, prediction and design. They are commonly used in some subfields of nanomaterials science, in many others they have been proven to be useful. A simple graphical cllassification scheme may be helpful in indication of future, yet unexplored, application directions. The contribution of genetic algorithms is likely to increase with time, owing to the flexibility of the method, to the possibility of its hybridization with other search methods. The future applications will progresively become more accessible to non-specialists, due to growing availability of user-friendly software.

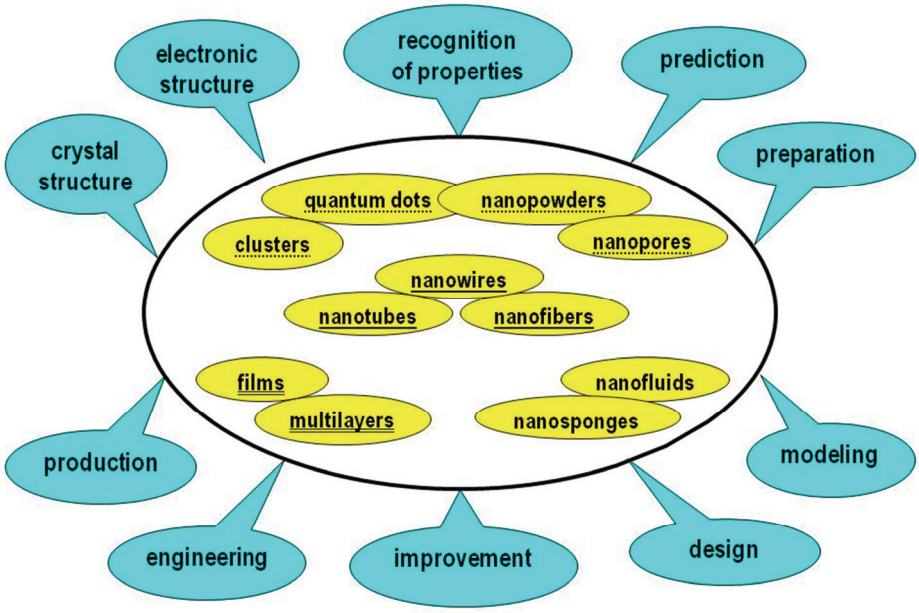

Fig. 1. *Fields of action of genetic-algorithms in nanoscience. They serve for prediction, preparation, modeling, design, improvement, engineering and production, as well as in studies of crystal and electronic structure, and in recognition of physicochemical properties. Eleven basic nanoscale material types are distinguished within the large central ellipse: zero-dimensional (underlined by dotted line), one dimensional ones (solid line), two-dimensional (double solid line) and others (not underlined).*

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ZASTOSOWANIA ALGORYTMÓW GENETYCZNYCH W DZIEDZINIE NANOMATERIAŁÓW: KRÓTKI PRZEGLĄD OSTATNICH WYNIKÓW

Streszczenie

Procedury przeszukiwania globalnego są ważnym elementem projektowania materiałów, ich wytwarzania i określania właściwości. Algorytmy genetyczne, stanowiące podzbiór algorytmów opartych o obliczenia ewolucyjne, stanowią przykład metody optymalizacji globalnej inspirowanej przez biologiczne prawa ewolucji. W nauce o materiałach i w pokrewnych dziedzinach nauki i techniki, algorytmy genetyczne są z powodzeniem stosowane, na przykład, w celu optymalizacji wytwarzania, przy projektowaniu materiałów o pożądanych właściwościach fizycznych lub strukturalnych, w opracowaniu nowoczesnych urządzeń działających na podstawie określonych zasad fizycznych, jak również w udoskonalaniu metod charakteryzacji materiałów. Nauka o nanomateriałach jest szybko rozwijającą się dziedziną materiałoznawstwa obejmującą różnorodne obiekty charakteryzujące się rozmiarami w skali nano. W niniejszym przeglądzie zaprezentowano przykłady ostatnio opisanych zastosowań algorytmów genetycznych w nauce o nanomateriałach. Reprezentatywne przykłady ilustrują, jak przydatne są takie metody obliczeniowe w rozwiązywaniu zadań naukowych, np. dla celów modelowania wzrostu cienkich warstw i dla ich charakteryzacji, dla optymalizacji układów kropek kwantowych i terapii medycznych bazujących na nanocząstkach, dla projektowania materiałów nanokompozytowych o wysokiej twardości i dla optymalizacji nanourządzeń optycznych i czujników różnego rodzaju gazów.

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