Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 594-595

P8-4

Genetic Algorithm Approach to Functional Molecules for Nanoscale Devices

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1. Introduction

Molecular devices are potential candidates for the next step towards nanoelectronic technology, and they would make it possible to realize the most advantageous applications [1]. Since Aviram and Ratner suggested that a unimolecule with a donor-spacer-acceptor structure would behave like a diode [2], a great deal of experimental work has been carried out to demonstrate an element of such an electronic device using either a single- or a finite-number of small organic molecules [3-6]. In addition, this trend has been further supported by a number of theoretical studies that have been published [7-10].

Recent investigations into unimolecular devices using experimental methods have raised important questions about the characteristics that are required for such a unimolecule to achieve functionality, such as the stability of its structure, the role of any functional groups, the localization of the frontier orbitals and the availability of an adsorption site on a metal electrode. Important problems that are pertinent to the development of unimolecular devices are the choice of suitable molecules for future nanoelectronic circuits and the requirement to establish a suitably smart method of surveying for them.

A genetic or evolutional algorithm applies the principles of evolution found in nature to some kind of optimization problem. A Genetic Algorithm (GA) [11, 12] is classified as an algorithm that mimics the natural process of Evolution and Darwin's principle of "Survival of the Fittest". In this case, it refers to the acceptance of the best solution, generated from previous solutions by the use of genetic operators such as crossover and mutation. Genetic Algorithms, as in the case of the Darwinian model of evolution, rely heavily on random experiments of reproduction. The next section describes outlines of the basic concepts and a procedure for implementing GA in a computer model.

2. Procedure of Genetic Algorithm

Figure 1 shows a general flowchart for the genetic algorithm used in the present study. The procedure used in the present study is as follows. (1) Firstly, an initial population of candidate molecules for the molecular devices is identified. We prepare a set of typical oligomers as the input data, for example, acetylene, phenylene, thiophene oligomer, etc. (2) The structures of the individual molecules are evaluated by using the Gaussian03 program [13]. In order to save computational time, we use molecular mechanics and a semi-empirical method to obtain a stable structure and the HF/STO-3G level to examine the electronic properties. (3) The selection procedure is based on these evaluation results. The selection procedure is inspired by the role of natural selection in evolution. In the present study, we assume that advanced members of the population may survive. The criterion for this is the number of points obtained in the evaluation procedure. The aim of the present study is the discovery of a suitable molecule for a molecular wire application, and therefore the evaluation allocates high points in the case of a small number of atoms in a molecule and a small HOMO-LUMO gap. (4) Some good candidates are selected as "permanent" parents. In a conventional GA approach, two parents are chosen from the same generation. However, in the present method, "father" parents are chosen from the "permanent" parents, while the "mother" parents are selected from each generation. The reason why we adapt this crossover strategy is that "descendant" generations have no fundamental molecule. "Mother" parents of "descendant" generations are not fundamental molecules, so crossover between "mother" parents cannot evolve step-by-step. Therefore, we need the "father" parents to be small molecules. (5) and (6) The "Crossover" and "Mutation" strategies are chosen with probabilities of *P*c and *P*m, respectively. The mutation process is inspired by the role of mutation of an organism's DNA in natural evolution. Namely, these mutations are adding or deleting a bond and an atom, changing an atomic element, or changing the coordination of partial atoms in the molecule. The crossover process is inspired by the role of sexual production in the evolution of living things. In the present study, an evolutionary algorithm attempts to combine elements of existing solutions in order to create a new solution, with some of the features of each parent. By analogy to the natural model, each candidate would be called a chromosome in a conventional GA. Each chromosome consists of genes, which represent a parameter or feature of the solution. In the present "crossover" strategy however, the "father" and "mother" parents are simply merged. In other words, each chromosome is merged, i.e. each molecule is connected by a small substituent such as a single hydrogen atom. In the present mutation process, the atomic elements and the coordination of the candidate molecules are replaced by others to change the molecular structure. (7) Finally, we can obtain a next-generation population. The generation process continues by returning back to step (2) until the convergence criteria are met.

The drawback of any GA approach is that a solution obtained using a GA is only "better" by comparison with another specified solution, i.e., we cannot say "This

molecule is the best" in finite terms. However, the Genetic Algorithm approach is still a powerful optimization tool, and we used it to survey for the appropriate molecule.

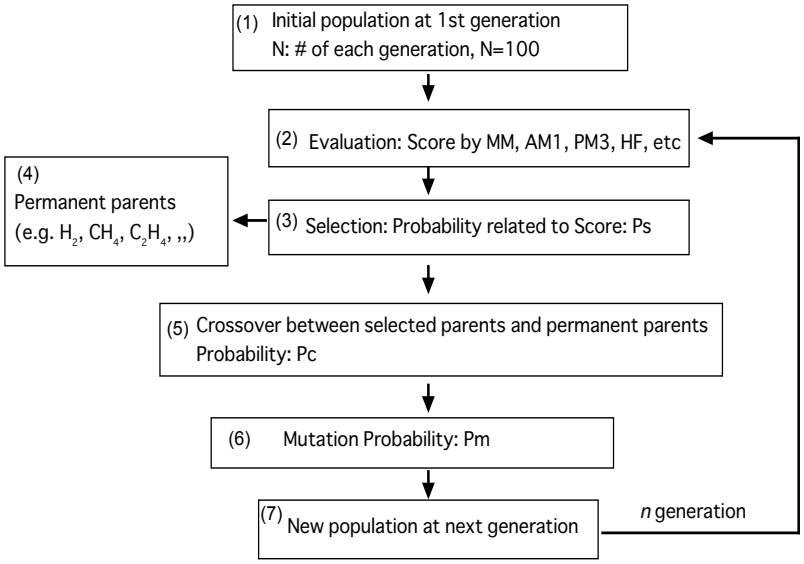

Fig. 1 General flowchart for the present genetic algorithm. Steps (1) to (7) are described in text.

3. Results and Discussion

In the present work, we adapt a GA technique to survey for an appropriate molecule to use as a molecular wire, i.e. we try to identify a molecule that possesses a specific length (20 Angstroms), a small number of atoms and a small HOMO-LUMO gap. In the present study, molecules that possess these features receive positive marks in the evaluation procedure, which start with small oligomers such as acetylene, phenylene, thiophene oligomer and so on as the first generation molecules. Therefore, we can identify relatively long molecules that have a specific length in the early generations. We examine the average length, the number of atoms in a molecule and the HOMO-LUMO gap for such "elite" molecules at various generations. With each successive generation, the number of atoms and the HOMO-LUMO gap gently decrease, while the length is almost constant, and is comparable to the specified length. Finally, we can obtain several molecules that have an elongated shape and a small HOMO-LUMO gap.

4. Conclusions

For many years, progress in microelectronics has been associated with the reduction of the minimum feature size of integrated circuits. However, this trend, described by Moore's law, seems to be ending due to process and physical limitations[14], therefore, a new paradigm shift has been expected. Molecular device is a potential candidate and would make it possible to realize the most advantage devices[1]. In this paper, we proposed a novel GA technique to survey a molecule in order to a good candidate for molecular electronic application.

Acknowledgments

The authors would like to express their sincere thanks to the Center for Computational Materials Science of the Institute for Materials Research, Tohoku University, for their continuous support of the HITAC SR8000-G1/64 supercomputing facilities. This study was performed through Special Coordination Funds for Promoting Science and Technology from the Ministry of Education, Culture, Sports, Science and Technology of the Japanese Government and a Grant for Basic Science Research Projects from the Sumitomo Foundation.

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