COMPUTATIONAL NANOTECHNOLOGY OF SILICON STRUCTURES: A CHALLENGE FOR BEYOND 2000

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Abstract: Devices enormously smaller than before will remodel engineering, chemistry, medicine, and computer technology. How can we understand machines that are so small? In general it is expected that computational nanotechnology should give the link between today nanometer scale science and technology and future molecular nanotechnology. I feel that the accurate modelling of nanosystems is one of the big challenges for our times. I discuss briefly some of the subject under investigation in the Technical University of Gdańsk and proposals for future research.

1. Introduction

Nanometer scale science and technology has become a complex and demanding field for physicists, chemists and engineers. Advances in physics, molecular biology and computer science are converging on the capacity to control, with molecular precision, the structure and function of mater as it was predicted by Feynman four decades ago [1].

Since the invention of the scanning tunnelling microscope (STM) just a two decades ago [2], the world has seen a revolution in the imaging and manipulation of individual atoms and molecules. With the visualising and discriminating atoms on surfaces, visualising and performing chemical operations on individual molecules, etc., a challenge is set for their basic understanding and imaginative applications. Nowadays it is possible to estimate in a conservative way that the following devices and capabilities appear to be both physically possible and practically realisable [3]:

* Programmable positioning of reactive molecules with ~0.1 nm precision
* Mechanosynthesis at > 10^6 operations/device x second
* Mechanosynthetic assembly of 1 kg objects in <10^4 s
* Nanomechanical systems operating at ~10^9 Hz
* Logic gates that occupy ~10^{-26} m (~ 10^{-8} μm^3)

* Logic gates that switch in ~0.1 ns and dissipate $< 10^{-21}$ J
* Computers that perform 10^{16} instructions per second per watt
* Cooling of cubic-centimeter $\sim 10^{5}$ W systems at 300 K
* Compact 10^{15} MIPS parallel computing systems
* Mechanochemical power conversion at $> 10^{9}$ W/m^3
* Electromechanical power conversion at $> 10^{15}$ W/m^3
* Macroscopic components with tensile strength $> 5 \times 10^{10}$ GPa
* Production systems that can double capital stocks in $< 10^{4}$s

Of these capabilities, several are qualitatively novel and others improve on present engineering practice by one or more orders of magnitude. Each is an aspect or a consequence of molecular manufacturing [4]. Molecular manufacturing is the construction of objects to complex, atomic specifications using sequences of chemical reactions directed by nonbiological molecular machinery [5]. Mechanosynthesis - mechanically guided chemical synthesis - is fundamental to molecular manufacturing. It guides chemical reactions on an atomic scale by means other than the local steric and electronic properties of reagents. It is thus distinct from enzymatic processes and present techniques for organic synthesis. Nowadays, positional chemical synthesis is at the threshold of realisation [6]. Precise placement of atoms and molecules has been demonstrated, but flexible, extensible techniques remain in the domain of design and theoretical study. The accurate modelling of these processes would allow them to be better understand and lead to important potential applications. This lead to theoretical applied science, the concept introduced by Drexler [3]. Theoretical applied science draws on the enormous body of knowledge amassed by science and engineering, but exploits that knowledge for different purposes using different methodologies. Its aim is neither to describe nature nor to build devices, but to describe lower bounds to the performance achievable with physically possible classes of devices.

Theoretical applied science can achieve its goals only by sacrificing many of goals of experimental science and of engineering. It produces analyses, not devices, and thus avoids the stringent requirement that its designs be fully specified, manufacturable, and competitive. This latitude can be exploited to mitigate the problems posed by inaccurate models and the unfeasibility of direct experimentation. Research in theoretical applied science typically makes no pretence of designing systems that can be built today, or that will be built tomorrow. Today we lack the tools, tomorrow we will have better designs.

The concept of computational nanotechnology was introduced by Merkle [7]. He recognised that, the major research objectives in molecular nanotechnology are the design, modelling, and fabrication of molecular machines and molecular devices. While the ultimate objective must clearly be economical fabrication, present capabilities preclude the manufacture of any but the most rudimentary molecular structures. The design and modelling of molecular machines is, however, quite feasible with

present technology. More to the point, such modelling is a cheap and easy way to explore the truly wide range of molecular machines that are possible, allowing the rapid evaluation and elimination of obvious dead ends and the retention and more intensive analysis of more promising designs. While it can be debated exactly how long it will take to develop a broadly based molecular manufacturing capability, it is clear that the right computational support will substantially reduce the development time. With appropriate molecular CAD software, molecular modelling software (including available computational chemistry packages, e.g., molecular mechanics, semi-empirical and *ab initio* programs) and related tools, we can plan the development of molecular manufacturing systems on a computer just as Boeing might 'build' and 'fly' a new plane on a computer before actually manufacturing it.

2. Why computational nanotechnology of silicon?

In the past few years, mechanosynthesis of diamondoid structures of carbon have become the subject of intensive theoretical investigations [3, 8, 9]. Diamondoid systems made from carbon are natural long-term goal for molecular mechanical engineering, but their fabrication will require future advanced mechanosynthetic capabilities. Considering silicon, completely different situation exist. The scanning tunnelling microscope (STM) , can be used to manipulate strongly bound silicon atoms or clusters at room temperature[10]. Specifically, by using a combination of electrostatic and chemical forces, surface atoms can be removed and deposited on the STM tip. The tip can then move to a predetermined surface site, and the atom or cluster can be redeposited. The magnitude of such forces and the amount of material removed can be controlled by applying voltage pulses at different tip-surface separations. The controlled manipulation of silicon at the nanometer scale will facilitate the fabrication of new types of devices. On the general grounds, it is expected that diamondoid structures of carbon exhibit ideal properties, whereas solid silicon and germanium present the same topological challenges as diamond, but atoms lower in the periodic table are more readily subject to mechanochemical manipulation owing to their larger sizes and lower bond strengths and stiffnesses [11]. It is known however, that middle sized silicon atoms possess properties which are far from linear interpolations between the two extremes, carbon and germanium.

The particular silicon properties are determined mainly by the difference between valence s and p orbital contraction [12]. An analysis of bonding in alkanes vs. that in silanes relates more s character to Si-Si bonds than, to C-C bonds. An important requirement for hybridization of valence s and p orbitals is similar extension in space. The resulting hybrid orbitals are more suitable for overlap. Consequently, the energy gain due to overlap of hybrid orbitals is larger than the promotion energy required to it[13]. This principle does not apply to the higher homologues in the periodic table of elements. There the valence s orbitals are more strongly contracted than the valence p orbitals[14]. On this basis the s orbitals become more "inert", a rule that has been known for a long time in inorganic chemistry as the "inert electron pair effect"[15]. An important difference may be summarised here. In

silicon, the valence 3s orbital is more strongly contracted than its 3p valence orbital. In carbon the valence s and p orbitals possess similar extensions in space and thus match perfectly for the formation of hybrid orbitals of different kinds. This is witnessed in the average distance from nucleus $< r >$ of valence s, and p electrons in carbon and silicon atoms calculated by the HFS theory[16].

	s	p
C	1.5010	1.6628
Si	2.0469	2.6082

This trend increases from Si to Sn and is known as "orbital nonhybridization" (ONH) effect [12]. The valence s-orbital contraction is common for bonding for higher main-group elements. It is witnessed in some other important chemical phenomena as well, e.g. the occupancy of an oxidation state two below the group valence. In fact, a singlet ground state of AH_2 systems comes to the fore in the order: CH_2 ($E(S_o) - E(T_o) = 10.5$ kcal/mol (73.0 maJ) < SiH_2 -18.6 (-129) < GeH_2 -19.0 (-132) < SnH_2 -19.0 (-132). As a consequence of s valence orbital contraction the bonding situation in AH_3 systems is related to that in the AH_2 cases. A non bonding orbital at the central atom is present that increases its s character with increasing contraction of ns valence orbital. Concomitantly, the inversion barrier in these systems increases in the same order. Similarly, silyl radicals adopt a non planar conformation as do the higher homologues, the germyl and stannyl radicals [13]. As a consequence of less "perfect" hybridization the bonds and deformation potentials in silanes are weaker than in alkanes; e.g., the force constant for the stretching vibration in ethane is almost three times higher than in disilane (k_{C-C} = 4.57 mdyn/A (457 N/m), k_{Si-Si} 1.73 ÷ 2.3 (173 ÷ 230)) [11]. Considering the effect of orbital nonhybridization (ONH) on bonding in the bulk element systems one can see that allotropy of carbon is rich: diamond, graphite and fullerenes [17]. The two best-known forms of carbon, diamond and graphite, differ in their physical and chemical properties because of differences in the arrangement and bonding of atoms. Diamond is denser than graphite, but graphite is more stable, by 0.69 kcal/mol (4.8 maJ) at 300 ° K and 1 atm (10^5 N/m^2) pressure. Silicon and germanium are normally isostructural with diamond. The graphite structure is peculiar to carbon, which is understandable because such structure requires the similar extension in space of valence s and p orbitals.

Silicon is readily available commercially in a very pure form and has the following characteristics[18,19]

* High modulus of elasticity: 213 GPa (same as steel)
* Low density: 2300 kg/m^3 (same as aluminium)
* Reasonable hardness: 850 kg/mm^2 (same as quartz)

* High melting point: 1720 K
* High tensile yeld strength: 7 GPa (stronger than steel)
* Essentially perfect elasticity
* High sensitivity to physical variables

Silicon structures can be very strong. A small silicon structure can easily have a yeld strength of 1.3 GPa.

With careful sample preparation, a yeld strength of 2 GPa can be achieved. Furthermore, silicon has a low volumetric thermal expansion coefficient $7.5 \times 10^{-6} K^{-1}$ at 300 K [3], which makes it very useful for making high-temperature and dimensionally stable structures.

3. Mechanosynthesis of silicon diamondoid structures

At the Technical University of Gdańsk, I have been devoted some efforts in the study of silicon diamondoid structures and its mechanosynthesis. Here I give a brief description of two topics under current investigation.

3.1 An electron transfer device based on polysilylenes

Because of the ease of writing, shifting, and detect electrons, particularly with the assistance of light, I have focused attention on a molecular device based on electron transfer [20]. Electron transport between two localised electronic states can be controlled by modifying the electronic state of polysilylene chain.

3.1.1 The polysilylenes as molecular wires

The analysis is based on a physical hybrid, consisting of a silicon VLSI-style circuit on which the molecular devices are installed. The silicon circuit will provide the means of making electronic and logical contact with the molecular structures as proposed by Hopfield at al [21]. The base silicon chip would have various metal and oxide parts exposed and be made with 0.1-μm-scale lithography. Appropriate surface treatments with cleverly designed chemicals and/or electrochemistry will then generate a surface with bonded hydrogen atoms (Si-H or O-H) on which the added polysilylene based devices are build by mechanosynthetic silylene insertion into Si-H or O-H bonds as indicated in Figure 1.

Short-range selfwiring with polysilylenes might replace certain metalization or polysilicon layers. The terminal (Si-H) bond might be simply used for specific polysilylene-to-silicon or polysilylene-to-metal end binding through dehydrocupling bond formation. To deal with inevitable errors, assuming a small fraction of the chains have the wrong length or other defects, a few tenths of chains are assembled to discharge a small VLSI floating gate in a few milliseconds.

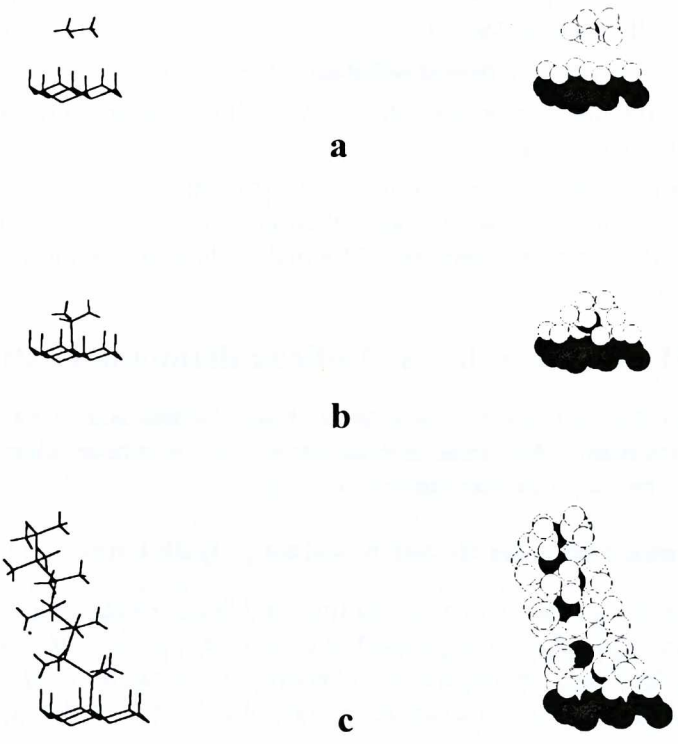

Figure 1. Communication between the VLSI circuit and the molecular world might be achieved via polysilylene wires of $(RR'Si)_n$ mechanosynthesized on chemically prepared silicon or metal surface. (a) Dimethylsilylene molecule over hydrogenated Si (1 1 1) surface. (b) Dimethylsilylene after insertion into surface Si-H bond. (c) Polydimethylsilylene wire after insertion of seven dimethylsilylene fragments.

3.1.2 Substituted polysilylene fragments as potential electric signals switches

Workers at Sandia National Laboratories and Nippon Telegraph and Telephone have studied a variety of polysilylene derivatives and found them to be excellent photoconductors[20]. In each study only positive carriers were found mobile, and nondispersive transport was observed with measured mobility's of order 10^{-4} cm^2 /(Vs) at room temperature were reported. The insensitivity of the carrier mobility's measured at room temperature to the nature of the polysilylene substituents lead to the conclusion that transport occurs via the σ electronic states of the silicon backbone rather than by hopping between sidechain substituents. The measured positive carrier mobility's depend on the applied electric field and are sensitive to temperature. The

drift mobility is thermally activated and activation energies of 0.25 to 0.28 eV have been measured. The measured activation energies are among the lowest values reported for amorphous solids and drift mobility's are quite high. Studying photoconductivity of poly-(methylphenylsilylene) have been estimated that the photocarrier generation quantum efficiency approaches 1% at high electric fields and that the carrier lifetimes are in excess of several milliseconds. Carrier lifetimes are affected by impurities and decrease mostly in the presence of certain electrondonor dopants [20].

Figure 2 shows schematically the potential application of photoinduced electron transfer in polysilylene chain to the switching of electronic signals. Application of potential difference to the polysilylene chain ends does not allow electronic migration when the chain is kept in the dark because its lowest unoccupied and highest occupied orbitals lie at too high energy with respect to the Fermi levels of the bulk silicon or metal electrodes. On light excitation, however, an electron is transferred from the highest occupied to the lowest unoccupied orbital of polysilylene, making possible the transfer of electrons between the two electrodes. Because of the possibility of modifying its electrical resistance with light, this photochemical molecular device PMD can be considered as phototransistor.

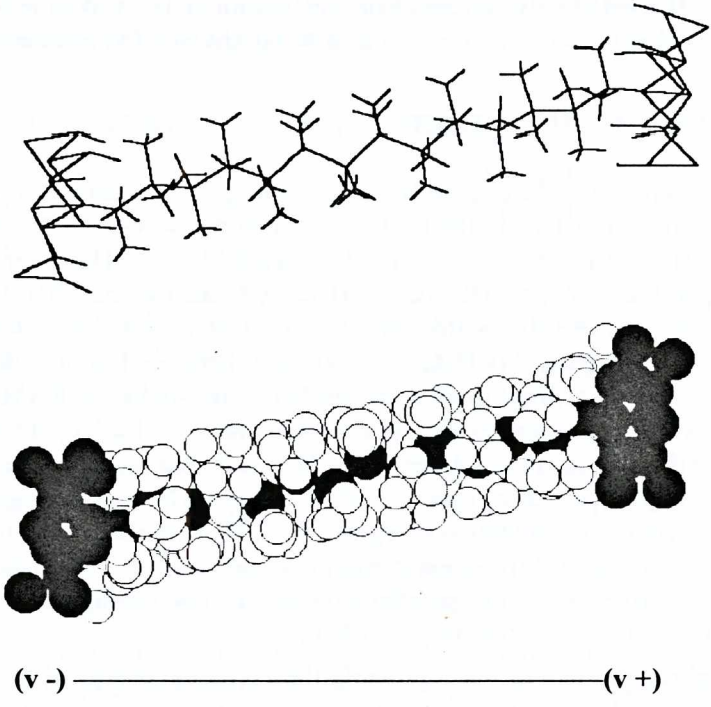

Figure 2. Schematic representation of a polysilylene based photochemical molecular device (PMD) for switching electric signals.

The molecular shift register can essentially be based on this light switching function. The idea of using single polysilylene molecules for switching and rectification purposes was first advanced by Pitt [22] and constitutes one of the basic concepts of molecular electronic devices based on polysilylenes [20].

3.1.3 Concept of information storage

The key feature of polysilylenes that makes them favourable for information storage is the strongest localisation of electrons on the polysilylene backbone in comparison to bulk silicon. This allows (at least in principle) the use of a cluster of e.g., 10 polysilylene chains each bonded with a bit storage molecule at the end, as an information carrier. It is obvious that a storage capacity of, e.g., 10^{11} b/mm^2 is attainable. Few basic aspects of this problem have been discussed in [20] together with conventional VLSI 1 μm technology.

An approach relies on the attachment of light switchable acceptor end groups (AT) to the polysilylene chain through an appropriate spacer using the terminal Si-H bond (-$(R_2Si)_n$-$(H_2C)_m$-AT). The strategy for achieving this depends on our ability to construct the spacer-AT end group and then bond it to the polysilylene chain. The most promising method for mechanosynthetic treatment is addition reaction between terminal Si-H bond of polysilylene chain and unsaturated C=C double bond of spacer [20]. This probably can be carried out as a W tip driven STM mechanosynthesis:

$$-(R_2Si)_n- H + H_2C{=}CH-(CH_2)_{m-2}-AT \longrightarrow -(R_2Si)_n-(CH_2)_m-AT$$

The acceptor may be excited by light resulting in an acceptor excited state that permits electron transfer via the bridge-spacer to the acceptor. The resulting state -$(R_2Si)_n$-$(CH_2)_m$ -AT$^{(-)}$ may be visualised as logical "1" state. However, this state can have comparable energy to -$(R_2Si)_n^{(-)}$-$(CH_2)_m$ -AT state (logical "0"). Due to tunnelling processes it is very likely that the -(R_2Si)" -$(CH_2)_m$ -AT$^{(-)}$ state will decay very rapidly into the -$(R_2Si)_n^{(-)}$-$(CH_2)_m$ -AT state and therefore lose its information[20]. Of course, one may argue that even modern semiconductor RAMs have to be refreshed every few nanoseconds and a corresponding "refresh cycle" also could be provided in this case. One should be aware, however, that power consumption is also a factor of importance. For instance, while molecularly based computation might reasonably promise computation energies of ~50 kT/b, the acceptor ended polysilylene approach makes little progress in energy per bit handled. The fundamental origin of this ineffectiveness is the parallel processing. For example, the need for 50 electrons necessitates 50 strands everywhere.

It is also important to select properly the excitation energy of the end acceptor substituent wavelength. A system designed so that -$(R_2Si)_n$-$(CH_2)_m$ -AT $\Rightarrow$ -$(R_2Si)_n^{(*)}$-$(CH_2)_m$ -AT transfer is driven by a wavelength λ_1, while -$(R_2Si)_n$- $(CH_2)_m$ -AT $\Rightarrow$ -$(R_2Si)_n$ -$(CH_2)_m$ -AT$^{(*)}$ transfer is driven by λ_2, would have the desired property. The advantage of this scheme is that the light pulses are answers to the

clock, power supply and switching problems. With light, the fabrication problems of real devices appear to lie within understood STM driven mechanosynthesis of silicon nanostructures, VLSI technology and physics of polysilylenes.

The general questions of light-driven polysilylene-based devices can be investigated with short oligomers tethered at only one end and without the need for microfabrication.

3.2 Mechanosynthesis of diamondoid structures with the STM

The theory and modelling of new mechanosynthetic strategies concerning silicon nanostructures is of main importance. Some of these problems have been addressed in recent publications [23-25].

3.2.1 Quantum-chemical molecular dynamics simulations of sila-adamantane mechanosynthesis on hydrogenated Si(111) surface using STM

On the basis of quantum-chemical molecular dynamics simulations a sequence of reactions can be constructed, with none of them requiring a higher activation energy than the silylene insertion, which give the $Si_{10}H_{15}$ silicon cluster as final product on hydrogenated Si (111) surface:

Si(111)-H	+	SiH_2	=	Si(111)-SiH_3
Si(111)-SiH_3	+	SiH_2	=	Si(111)-Si_2H_5
Si(111)-Si_2H_5	+	SiH_2	=	Si(111)-Si_3H_7
Si(111)-Si_3H_7	+	SiH_2	=	Si(111)-Si_4H_9
Si(111)-Si_4H_9	+	Si	=	Si(111)-Si_5H_9
Si(111)-Si_5H_9	+	Si	=	Si(111)-Si_6H_9
Si(111)-Si_6H_9	+	Si	=	Si(111)-Si_7H_9
Si(111)-Si_7H_9	+	SiH_2	=	Si(111)-Si_8H_{11}
Si(111)-Si_8H_{11}	+	SiH_2	=	Si(111)-Si_9H_{13}
Si(111)-Si_9H_{13}	+	SiH_2	=	Si(111)-$Si_{10}H_{15}$

where - $Si_{10}H_{15}$ means the simplest diamondoid structure - sila-adamantane. The nomenclature and optimised geometry's of the complexes investigated are shown in recent papers [23,24].

3.2.2 Quantum-chemical molecular dynamics simulations of silicon diamondoid structures mechanosynthesis on hydrogenated Si(111) surface using STM

The manipulation of silicon atoms and silylene molecules at the subnanometer scale via STM W tip provides a potentially powerful way of building silicon diamondoid structures. In recent work [25], I have been used quantum-chemical atomistic simulations to explore the feasibility of mechanosynthesis on hydrogenated Si(111) surface using STM tip. The sequence of energetically favourable insertion reactions was established leading to stable surface intermediates. Using the silaadamantane molecule as surface model the sequence is as follows:

$Si_{10}H_{16}$	+	SiH2	=	$Si_{11}H_{18}$
$Si_{11}H_{18}$	+	SiH2	=	$Si_{12}H_{20}$
$Si_{12}H_{20}$	+	Si	=	$Si_{13}H_{20}$
$Si_{13}H_{20}$	+	Si	=	$Si_{14}H_{20}$

This sequence of operations suffices to build an indefinitely large volume of diamondoid lattice. The sequence is based solely on two reactants (Si and SiH_2) with the overall charge neutrality of the structure maintained. I characterise reaction rates and energy flows, and conclude that they are sufficiently fast and simple to make this mechanosynthesis feasible.

4. The future for beyond 2000

What might one expect for the next ten years? There appear to be a number of clearly established lines of research for the computational nanotechnology. Several groups are working on computational methods which would scale linearly with the number of atoms. The goal here is to preserve the accuracy of current methods based on *ab initio* pseudopotentials, but allow much larger systems to be examined. The theory and modelling of nanostructures, as well as nanometer scale science and technology theory in general, is a young discipline. Some of these efforts will probably be successful. Today, one must admit that designing new nanosystems on the computer is still a dream. However, as computers become faster, and as the new algorithms allow more accurate descriptions of complex systems, this situation should change.

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