Bridged Quantum Cellular Automata based on Si/SiO_2 Superlattices

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***Abstract*—**The new architecture for quantum cellular automata is offered. A QCA cell includes two layers nc-Si, divided by a dielectric. Among themselves cells are connected by the bridge from a conductive material. The comparison is made between this and QCA, offered earlier by C. Lent's group.

***Keywords*—**quantum cellular automata (QCA), nc-Si, Si/SiO_2 superlattices, parallel computing

I. Introduction

HEAT dissipation problem is one of the most critical one for modern high-efficiency microprocessors. Thereupon a search of new element base of nanoelectronics [1] is being actively conducted, and one of candidates on replacement CMOS-logics is quantum cellular automata. The big contribution to the development of QCA problematics was made by the research group of University of Notre Dame (Indiana, USA) – C. Lent et al [2].

Some variants of QCA (metal, magnetic and molecular) were realized, with the help of which the elementary logic functions and schemes, in particular, OR/AND/XOR, «majority votings», adders, triggers and multiplexers [3] were executed.

Metal QCA works at cryogenic temperatures. Magnetic QCA do not possess the necessary speed operation. Molecular QCA are known only in theory, and laboratory workings are in embryo; absolute obstacles are created by the present level of development of technology.

In the given work we will consider shortly in the beginning the specificity of our theoretical approach to QCA, then we will describe key features of cells and architecture of ours QCA, named «bridged», we will make some remarks on its technological realization and we will carry out the comparative analysis bridged QCA with C. Lent's QCA.

II. Our Approach to QCA

In our opinion, it is necessary to define QCA as the physical structure realizing in the strict sense classical functional model of CA (cellular automation) and containing accurately distinguished cells of micro- or nano scale for the behavioral description of which laws of quantum mechanics are essential. At the present time none of realized QCA satisfies strictness of such definition. In C. Lent's works the truncated model of pseudo-one-dimensional CA WireWorld [4] is actually considered. Watrous - Dam's model [5], trying to consider quantum character of QCA cells, complicates CA model, and it is expedient to apply it only in case when the size of cells is less about 2-3 nanometers.

At the future researches of QCA their quantum character and continuous race on reduction of the device sizes and package density increasing should not cover, as, apparently, has occurred, the aspect of parallelism of calculations inherent in them that is more important, in our opinion. It is necessary to focus on semi-conductive QCA which are technologically realizable at least in laboratory conditions and not exacting to design scale. Thus semi-conductive QCA are still represented by makeshift on a way to molecular QCA, but it is possible to investigate various parallel architectures of calculations on their element base.

Therefore, for example, the charge amount, stored by a semi-conductive QCA cell, should be big enough (in comparison with an elementary charge), so to speak about QDCA (D – dot) is to assume in advance that there are a few, probably, tens of quantum points in the cell. Detection procedures conditions of QCA cells and information output to the periphery framed with the standard CMOS-schemes are simultaneously facilitated.

While setting QCA cell in the surface of a silicon wafer, i.e. reserving two dimensions for information transfer between cells, it is expedient to take out all endocellular interactions in the third. Timing signals also should interact vertically. Anyway at designing of QCA the principle of dimensions division should be conducted more accurately.

Previously C. Lent and W. Porod have offered the concept of edge-driven computing [6]. Delevoping it and doing it more abstract, we consider three kinds of QCA cells (Fig. 1):

• approximately 5-10 % of cells keep their condition invariable, being as though a "window" of the information input in QCA;

• approximately 5-10 % of QCA cells give their charging condition, for example, for reading/detection, being as though a "window" of the information output;

• other 80-90 % of cells are managed only by timing (clocking) scheme and their array serves for low-level processing of the information.

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As a matter of fact we will not know basically what occurs inside QCA in the calculation process. The complex physical processes occurring on the set of QCA cells, undoubtedly, mean transformation of global informational QCA state, but the question is whether we can guide this transformation to the necessary direction?

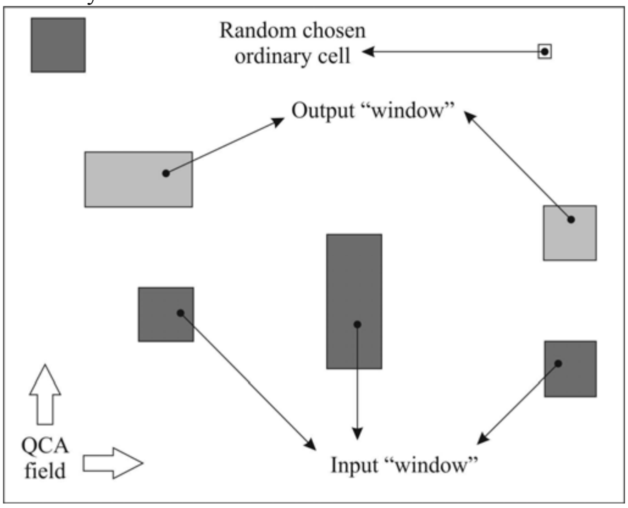

Fig. 1 Window conception of QCA computing

Process of intercellular interaction also demands controllability so that the realization of different local transition functions was possible. Therefore it is necessary to enter «binding areas» into QCA matrix that can play a role of a bridge between two adjoining cells. The timing principle in Lent's QCA is based on the blockade of electron's movements between quantum dots (QD), i.e. the purpose of timing is the cell itself. There is other timing principle that is possible – influence on binding area; it appears to be as more accurate, proceeding from QCA definition.

Though it is not realized for bridged QCA, but for the best approach to definition, the QCA cell should store not only its present, but also its last condition, and also provide information interchange between these conditions. It is the simplest way to provide synchronism and accordingly predictability of calculations.

III. BRIDGED QCA

On Fig. 2 the scheme of cells and binding area of bridged QCA is shown (the scale marker in 10 nanometers has only conditional value). All geometrical and electrophysical parameters of bridged QCA (bQCA) are described only qualitatively in this paper; as for their quantitative description quite a complicated mathematical modeling is required. The question of a choice of materials is postponed by us for the future though we will implicitly assume use of silicon and a silicon dioxide as the most widespread materials in microelectronics.

The bQCA cell contains two layers of Si nanocrystals divided by tunnel-transparent layer SiO_2. Thicker layers of SiO_2 serve as an isolating layer both from the top electrode, and from a substrate. Thus, we have an array of quantum points which can keep a charge on themselves. Charge transfer to a horizontal direction, from nanocrystal to nanocrystal, is apparently difficult enough to be described; at the preliminary analysis it is possible to abstract from details of structure of these layers and to accept model of capacitor plates. The interlaminar dielectric should be thick enough to blockade the tunneling of the electrons (at least for characteristic duration of timing), however in the presence of an external field should become tunnel-transparent. If the top layer is charged negatively we will consider a cell being in condition of logic «0»; if the bottom layer is charged negatively, this condition is logic «1». Other layer can be or electro neutral if there is surplus of electrons in the system, or is charged positively. It is difficult to estimate, what case is more preferable from the point of view of a bQCA work optimality.

The top record electrode is necessary to establish a certain logic condition of a cell depending on electric potential sign. We would like to notice that possibility of all variables zeroing is rather desirable from the point of view of the organization of calculations. The application to all cells (or in view of the "window" idea of QCA-computing to groups of cells) an average of voltage value will dump an automata state. If a dielectric layer between a substrate and the bottom layer of nanocrystals is not too thick then supplying of higher voltage on the write electrode can make possible the emission of electrons from a substrate. This effect can be used for injection of the charges in a system (or emission from a system). At carrying out of calculations the write electrode is at zero potential (except cells of input windows and the initial phase of the calculations). Low voltage on a write electrode can prevent parasitic tunneling between layers of nanocrystals, i.e. to increase a storage time of a logic condition (however only at coincidence of polarities).

Now we will describe binding (bridged) area the realizable details of which appear unclear to us. Interaction of cells is carried out by means of a jumper from a conductive material. Probably, polysilicon can serve as such material for a bQCA prototype, however, it is necessary to expect a considerable ohmic heat dissipation at the high timing frequencies, therefore at transition to small scales it is expedient to use a macromolecule as such jumper. The use of graphene appears to be attractive here as it possesses unique high conductivity.

The jumper can partially block the bQCA cell area from below to raise sensitivity to a charge, stored on the bottom layer of nanocrystals. So, on one end of the jumper the charge is induced, and owing to electroneutrality and conductivity of the jumper on its other end there is an opposite charge. This charge induces a field on other cell; normal field component changes a potential barrier to tunneling between nanocrystals layers which leads to the change of a cell logic state. Structural execution of a jumper reminds rather a floating gate in memory elements, however unlike a floating gate our purpose consists in maintenance of the jumper electroneutrality.

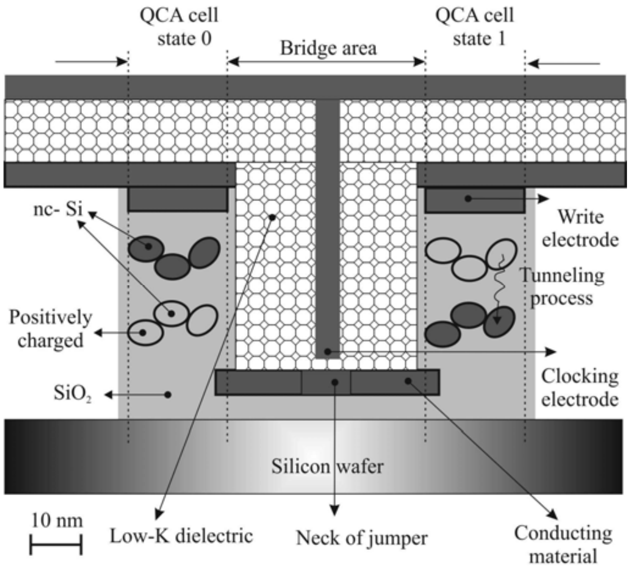

Fig. 2 Scheme of cells and binding area of bridged QCA

Timing (clocking) electrode is brought to its center for managing of the jumper. If the small and negative potential is delivered on it, then without essential change of charges on the crosspiece ends the blocking positive charge accumulates in the jumper center. Any change of logic condition of a bQCA cell is accompanied by current flow on the jumper. Blocking role of timing electrode can be understood if to remember work function on moving of charge between semispaces over the charged plane. The general charge of the jumper can be operated, delivering higher voltage on timing electrode that will cause issuing of electrons from a substrate. The field of the timing electrode should not be too extensive so that the blocking area in the crosspiece center does not deform excessively available charges at the jumper edges.

The question about a dielectric material in bridged area is not clear. On the one hand, the dielectric should not be tunnel-transparent, but on the other hand, electric field should pass rather easily through it. Apparently, it should be wide-ranged material with low dielectric permeability (low-K); probably even SiO_2 will not be too bad in such a role.

Fig. 3 presents the top view on a rectangular matrix of bQCA. The concrete layout of the cellular automata can receive features of heterogeneity due to absence/presence of jumpers in bridged areas. Besides, the variation of the jumper material (for example, a polysilicon doping) will allow realizing CA transition local functions more flexibly. Thus, we receive a constructive way of calculation management (besides timing management if to accept continuous voltage model of in-feed of timing electrodes).

Fig. 3 also specifies the possible problem connected with an arrangement of jumpers – they can electrostatically start to cooperate with each other if they are placed excessively close to the cell center. Also a tangential component of electric field takes significance in a layer of nanocrystals. Creation of mathematical models on this theme appears to be tempting. However it is possible to write out a parity of a general view for transition function:

$$X(t+1) = X(t) - \sum w_i\big(t, E(t)\big)\, X_i(t)$$

Here $X(t)$ is a cell condition (expressed by a charge of the bottom layer of nanocrystals), i – an index of the neighbour cell, w_i – weight coefficient equal to zero in the absence of a crosspiece and depending in a complicated way on many parameters, in particular, on field $E(t)$ of timing electrode. Such kind of local function, generally speaking, is peculiar to totalistic CA or even to neural networks, supposing continuous set of CA cell conditions.

As a solution of a detection problem for conditions in cells «output windows» (Fig. 1, Fig. 3) can be assumed either made the top electrode floating, i.e. not to feed it, or to expand and deduce a jumper on a wafer surface. In both cases the first end of an electrode is under the influence of a layer of nanocrystals, and on the second end the opposite charge accumulates. The second end serves as MOSFET gate, and, thus, by source-drain current we can consider a bQCA cell condition. It is important only that the induced charge on a gate has sufficient value.

Fig. 4 shows richness of bQCA perspectives, thanks to a principle of dimensions division. bQCA is shown here with cells in a kind of hexagons, and each cell has a vicinity of six neighbors which are connected in pairs by three crosspieces. The bridged area coincides with a cell in size. The lacunas presence leading to loss of ¼ of the crystal area can be considered as a lack of this bQCA modification; on the other hand, empty cells areas can be used for the best routing of timing signals on cells.

Importance of the timing organization has been perceived already for Lent's QCA; its value is even higher for bQCA, aspiring to use parallel computing potential more fully. The ideal decision, apparently, consists in diphasic scheme of one-zonal timing, i.e. the signal of all timing electrodes is identical and equal either to 0, or 1. Application of such decision for bQCA would lead to chaos; therefore bQCA is only approximation to ideal QCA, to answering its definition and to which the ideal timing scheme is applicable. The usage of the quadriphase classical scheme "switch-hold-release-relax", developed for Lent's QCA is expedient for bQCA as well. At that in a phase «hold» course of the transients connected with tunneling of electrons between and in layers of nanocrystals is still possible. Much more interesting is a question of a choice of timing zones; the presence of such zones testifies: first, an orientation of an information stream (streams), and secondly, partial asynchronism of QCA work. We will formulate two postulates regarding timing in bQCA:

- Results of calculations on identical bQCA structures, but with different organization of timing zones, generally do not coincide;
- Nonideality (partial asynchronism) of bQCA leads to occurrence of the allocated information streams (vortex) in it.

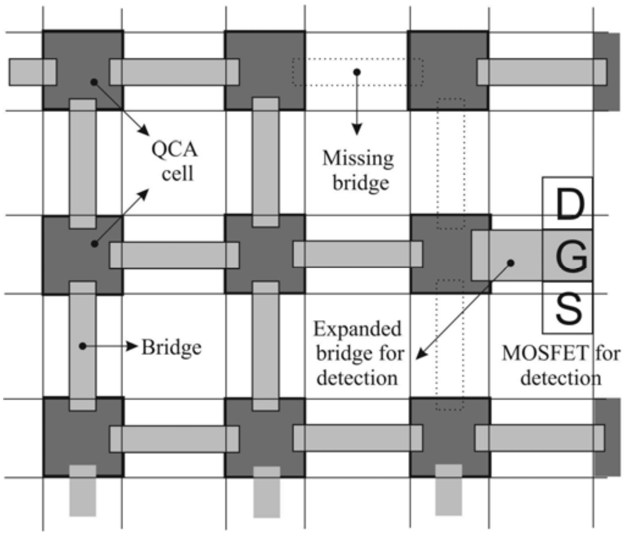

Fig. 3 A matrix of bridged QCA: the top view. Bridges are below picture plain

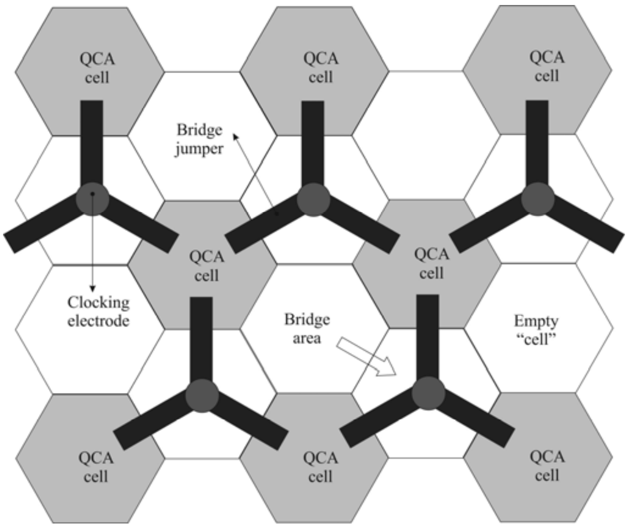

Fig. 4 Hexagonal type of bQCA

IV. REMARKS ON TECHNOLOGY

Now we can make only preliminary remarks on a process flow of bQCA creation, but it is already obvious that bQCA can be implemented on CMOS-compatible technology. Many ambiguities are connected with a jumper material and interlayer dielectrics. Further we will focus on Si/SiO2-superlattices though, obviously, general idea of bQCA supposes other concrete solutions. Our choice is justified by that technological ways of silicon dioxide thin layer formation are well studied, and the material possesses widebandness in comparison with others.

Fig. 5 represents the rough preliminary scheme of workflow initial stages. It consists of three basic stages:

• Formation of jumpers on a substrate surface according to topological layout and architecture of bQCA;

• Formation of a Si/SiO_2-superlattice which serves as preparation for the future bQCA cells;

• Removal of a superfluous material from bridged areas.

The basic problem is connected with the fact that operations of thermal oxidation and annealing are high-temperature and the way they will influence a jumper is not clear (at least it will fuse if made of aluminum, for example). In addition some difficulties exist to provide the oxygen flow under bridges; one can make jumper with holes. If we refuse the idea of bQCA cell area partial overlapping by a jumper then it is possible to put high-temperature operations in the workflow beginning. We would like to notice that only thermal oxidation of silicon provides the best SiO_2 electrophysical characteristics (for example, uniformity on a thickness, absence of pinholes). Quality of a dielectric between a jumper and the bottom layer of nanocrystals determines value of possible leaks of a charge and has key value for correct bQCA functioning.

At formation of electrode system it is necessary to also provide quality of a dielectric between timing electrode and a jumper. For decrease in static power consumption of bQCA it is necessary to reduce voltage on timing electrode, it means it is necessary to approach it to a jumper that makes possible dielectric breakdown and uncontrollable tunneling of electrons from a substrate.

Apparently, and deposition of two electrode layers can meet difficulties, especially at reduction of bQCA sizes. Also problematic is the choice of a material and manufacturing techniques of the dielectric which is placed in binding area. All these questions demand more detailed discussion.

V. COMPARISON WITH LENT’S QCA

As well as Lent’s QCA, suggested bQCA is based on an electrostatic principle. Therefore such advantages of QCA as little energy dissipation and a small number of metallization layers are fair for bQCA. However introduction of bridged areas and jumpers on which there is a charge motion reduces slightly an advantage of heat dissipation, especially in the case of signal high frequencies.

While Lent’s QCA cell contains from 4 to 6 quantum dots, we do not limit number of QD. Moreover, as a modifications of bQCA it is possible to consider a 2D-uniform layer of a material (that is inherent in heterostructures) instead of a nanocrystals layer. However the basic mechanism of cell condition change is still tunneling.

For molecular QCA the qubit third condition (ground state) is introduced; that has substantiation in Watrous - Dam’s model and is connected with peculiarities of timing. It is possible to introduce such condition (electroneutrality of each layer of nanocrystals) for bQCA as well; however it will not play any functional role and appears to be superfluous. Numerosity of nanocrystals generates a physical continuity of a bQCA cell charging conditions. Apparently, it will complicate work on bQCA logic designing.

All primitive logic elements described in Lent’s works, including QCA-wires, can be realized on bQCA base. In our opinion, for cellular automation such concepts as "trigger", "gate" etc., taken from experience of sequential calculations, appear inapplicable. In this sense Lent's QCA are much more conservative (that it is historically justified) than bQCA. In spite of the fact that a bQCA cell is larger than Lent's QCA cell, due to more active use of the second dimension, packing density is higher in bQCA.

Unlike Lent's QCA, binding area does act as a timing target rather than a bQCA cell.

VI. Conclusion

In the given paper more questions are being raised, than decided. Essentially bQCA can find a physical embodiment by means of already available modern technology of microelectronics, however numerous details of such realization demand specification. The questions of the organization of parallel computing with the help bQCA looks vaguer. There is a wish to believe that the this paper will give a new impulse to complex researches in the field of quantum cellular automata and will open extensive prospects for replacement CMOS schemes in nanodevices.

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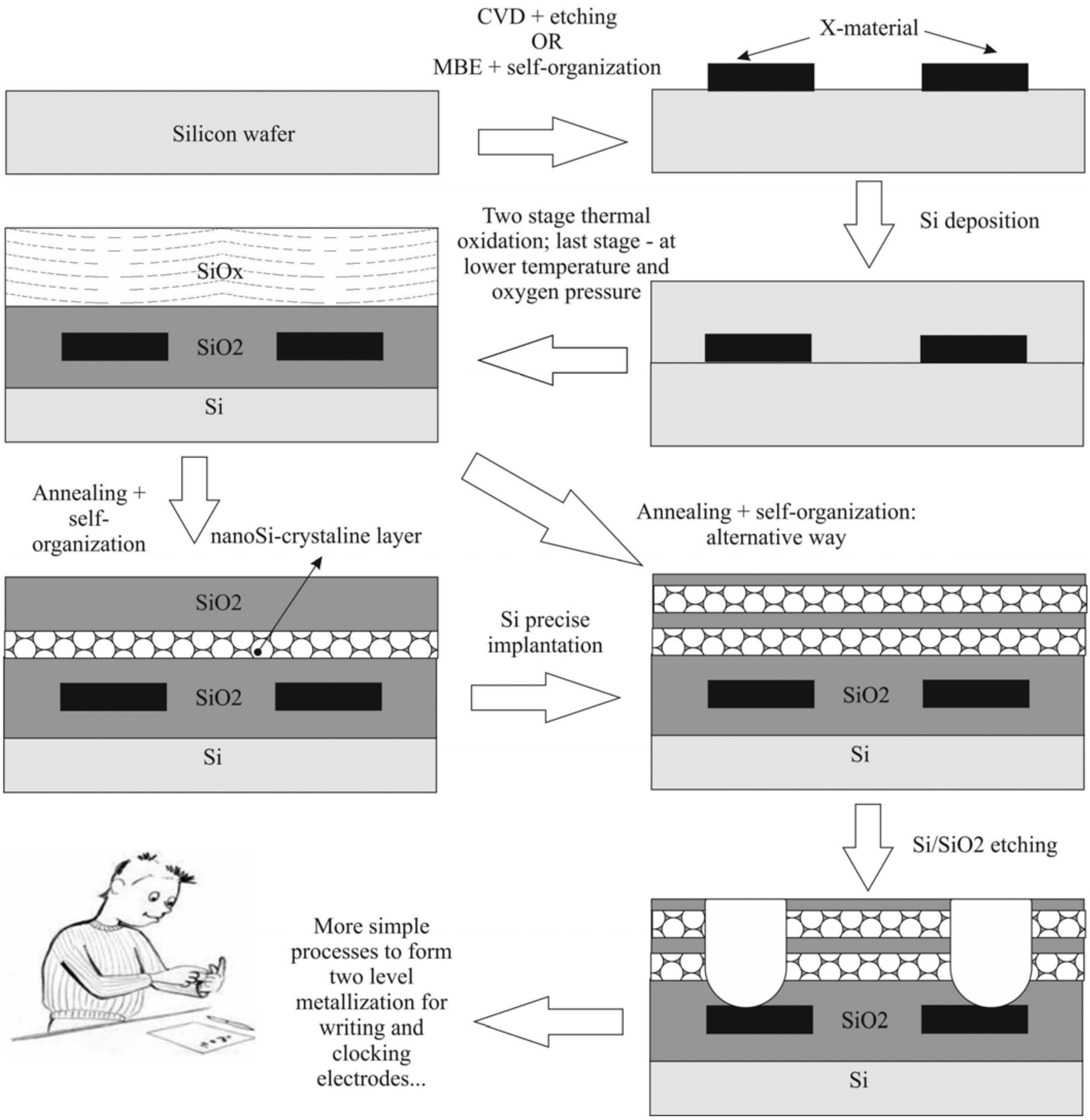

Fig. 5 The initial stages of bQCA workflow (rough scheme)