Fault Tolerance Analysis of a Bis-Ferrocene QCA Wire

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***Abstract*—Molecular Quantum Dot Cellular Automata (mQCA) are among the most promising emerging technologies for the expected theoretical operating frequencies (THz), the high device densities and the non-cryogenic working temperature. In this paper, we performed an analysis of the possible fabrication defects of a molecular QCA wire built with ad-hoc synthesized bis-ferrocene molecules. We then evaluated the fault tolerance of a real QCA device and assessed its performance in non-ideal conditions, by defining a new methodology for the fault analysis in the mQCA technology.**

I. Introduction

The reason at the root of the expectations on Quantum Dot Cellular Automata devices as successful CMOS substitutes [1] is that no charge transport is involved, but only local field interaction determines the information transfer. Power consumption is then expected to be dramatically reduced. According to the Lent theory [2], the smallest and most performing QCA cell could be implemented with a molecular system. The simplest demonstration of logic propagation that could be performed according to this paradigm is a molecular wire (see Fig. 1(B)). In [3], [4] some possible candidate molecules were presented: all these molecules are ideal systems and are studied in vacuum, so they are not suitable for a real circuit. In this work we addressed our fault tolerance analysis to a real molecule, the bis-ferrocene (see Fig. 1(A)), synthesized ad hoc for QCA purpose [5], [6]. Both the QCA properties and the fault tolerance of this molecule have been already proved in [6], [7], [8].

II. Defect models

In order to experimentally demonstrate the QCA functionalities, we are preparing a bis-ferrocene molecular wire like the one in Fig. 1(B), based on a gold nanowire upon which the molecules can be binded through the thiol element. During the gold substrate preparation and the molecule deposition, some defects may occur and they are schematically sketched in Fig. 2: i) misalignment of deposited molecules, due to the defects of the grain or the irregularity of the hexane-dithiol monolayer (Fig. 2(A)); ii) huge vertical distance between two dots, caused by the roughness of the gold substrate (Fig. 2(B)); iii) variations of the distance of two nearby molecules, in case of many hexane-dithiol elements between consecutive molecules (Fig. 2(B)). These defects might cause faults and mis-behaviors of the cells in the molecular QCA wire.

In order to evaluate the fault tolerance of a molecular QCA wire, we defined a methodology focused on a system composed of an ideal emulated driver, a bis-ferrocene molecule under test (MUT) and an ideal receiver, as part of the molecular wire. The state of the driver should localize the MUT charge on one of the active dots. Referring to the above mentioned

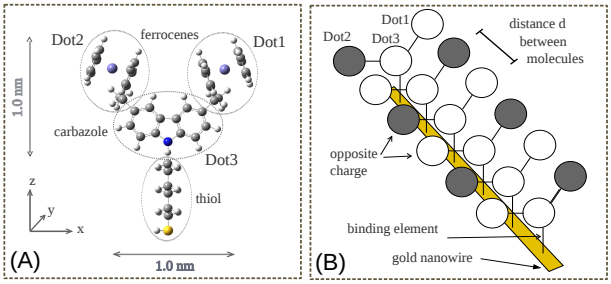

Fig. 1. (A) Bis-ferrocene molecule: two ferrocenes (active dots) are linked together by means of a carbazole central group (central third dot). An alkyl-chain and an ending thiol (-SH) group provide the binding to a gold substrate. (B) Molecular QCA wire: bis-ferrocene molecules aligned over a gold nanowire.

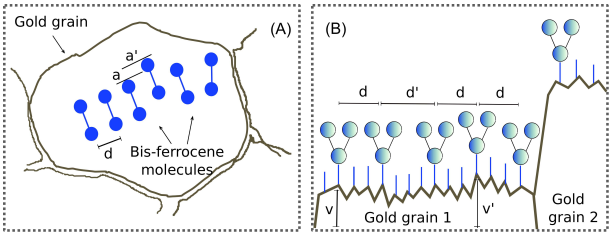

Fig. 2. Fabrication defects in the case of a QCA wire made of bis-ferrocene molecules. (a) Top view of a gold grain after molecule deposition: misalignment and tilt defect are sketched. (b) Section of a bis-ferrocene SAM on gold: vertical shifts may occur due to the roughness inside a gold grain or at the interface of two grains; higher molecule-molecule distance is caused by the number of hexane-dithiol elements.

defects classification, we modeled the three types of defects varying the position of the driver, as sketched in Fig. 3: firstly we considered the misalignment of the driver with respect to the two dots (delta X, Fig. 3(A)), due to the defects in the orientation of the gold grain (see Fig. 4(A)). Then, we varied the distance between the driver and the MUT (delta Y) to model a non ideal squared cell (Fig. 3(B)) in case of different number of spacers between two molecules as depicted in Fig. 2(B). Finally, the roughness of gold grain is modeled as the shift of the driver along the vertical axes of the MUT as shown in Fig. 3(C) (delta Z).

Since the charge localization inside the molecule is the main requirement for QCA bistability validation, we need to evaluate the charge distribution of the MUT under different bias conditions (different positions of the driver).

III. Results and conclusions

Fig. 9 displays the results for the driver shifting along the vertical axes, defines as delta Z. The graph includes the results for three different distances from the MUT (equivalent to three

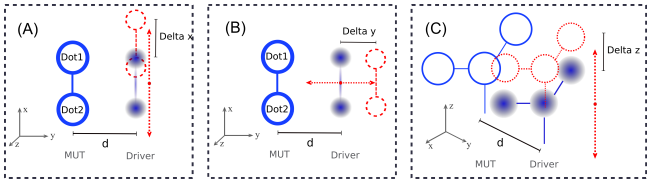

Fig. 3. Three possible fabrication defects are modeled moving the driver with the respect to its ideal position: (A) the driver is not perfectly aligned with the two dots, (B) it is placed at a distance different from the ideal *d*, (C) the displacement is along the vertical axes of the molecule.

values of delta Y), considering the driver logic state at 1. The charge difference between the two dots of the MUT decreases when the value of delta Z is incremented, which is enhanced for longer distances from the molecule (higher delta Y). In particular, in the range related to the roughness of the gold substrate inside a grain ($\pm 0.2 \div 0.4nm$) the molecule still works properly, that means that the free positive charge is mainly localized on one of the two dots, encoding a valid logic state. On the contrary, when the driver-MUT interaction is at the interface between two gold grains (equivalent to $deltaZ = \pm 2.0nm$) the molecule is in an undefined state, because the charge of the two dots is almost the same.

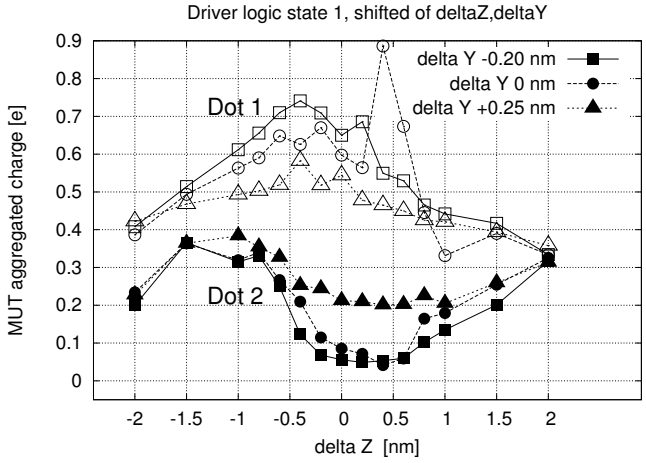

Fig. 4. Dot charges as function of the driver shifting along the vertical axes (*delta Z*) for three different distances from the molecule (*delta Y*).

Regarding the driver misalignment with the respect to the two dots of the MUT (delta X), the trend of the dot charges is reported in Fig. 5 for the ideal distance between the MUT and the driver (delta Y = 0). In this case, we reported simultaneously both the driver logic state at 1 and at 0, in order to check immediately the MUT bistability for a specific driver position. In particular, for a given delta X value it is possible to check if the positive charge inside the MUT moves between the two dots when the driver changes its state from 1 to 0 and the difference between them is great enough to be considered a valid state. Figure 5 reveals that in some cases of driver misalignment the interaction with the MUT is still preserved.

The results we obtained in this work are fundamental to address the fabrication of a molecular QCA wire on gold. In particular, the fault tolerance analysis discussed here highlights the feasibility and functionality of the MQCA wire also in presence of several defects we faced during our experimental

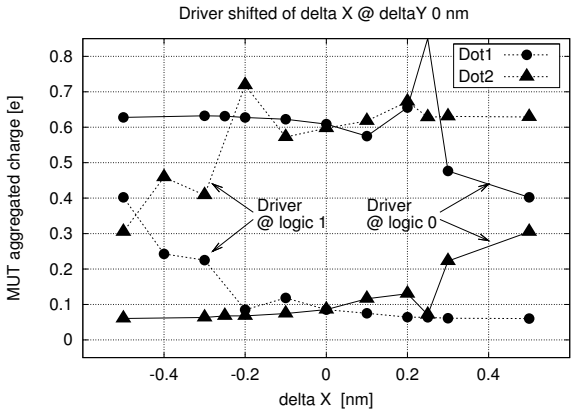

Fig. 5. Dot charges as function of the driver misalignment with the respect of the two dots (delta X) for a fixed molecule-molecule distance (delta Y=0)

processes. These results are promising for the development of molecular QCA circuits and, at the same time, give an important feedback to improve the technological process.

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