From wave-functions to current-voltage characteristics in silicon single-nanocrystal Coulomb blockade devices

Johann Sée, Philippe Dollfus, Sylvie Galdin and Patrice Hesto
Institut d'Électronique Fondamentale (CNRS UMR8622),
Université Paris-Sud, 91405 Orsay, FRANCE
email: johann.see@ief.u-psud.fr

In the search for innovating solutions likely to ensure the perenniality of silicon microelectronics which will have to face up to technological as well as theoretical limits within a few years, the concept of semiconductor single-electron devices has revealed promising assets [1,2]. By exploiting the electric charge granularity through Coulomb blockade phenomenon, these type of devices may offer new functionalities or even an alternative to CMOS circuits while remaining compatible with current technologies.

From this point of view, a theoretical examination by various approaches of physical simulation appears to be of first interest in order to predict the behavior of these future generation devices and to give information on the appropriate design [3]. This work aims at studying elementary Metal–Insulator–Silicon quantum dot–Insulator–Metal (MI*Si*IM) structures (cf Fig. 1) thanks to a physical description using only fundamental parameters of the system (oxide thicknesses, metal work function, quantum dot size and shape, temperature,...). The model consists in calculating *(i)* the electronic structure of Si nanocrystal using the Hartree method [4], *(ii)* the tunneling transfer rates in Bardeen's approach [5] and *(iii)* the current using a Monte-Carlo technique. The main advantage of this approach lies in the accurate calculation of tunneling rates including the effect of bias voltage on the wave-functions in the quantum dot and tunnel barriers [6].

To achieve such simulations, the description of the quantum electronic states of the silicon island is obtained from a three-dimensional self-consistent Schrödinger-Poisson solver within the frame of Hartree approximation. This method allows us to have all necessary informations on the electronic wave-function to calculate tunnel transfer rates in the Bardeen's approach of weak coupling, as shown in figure 2 for the tunneling rate from the right electrode to the dot containing no electron and the tunneling rate from the dot containing one electron to the left electrode. These tunneling rates turn then into the main parameters of a Monte-Carlo algorithm to determine the current flowing in the structure as a function of the bias voltage. Typical current/voltage characteristics are shown in figure 3 at different temperatures for a MI*Si*IM structure with a 30 Å radius silicon spherical quantum dot.

For larger quantum dots, the influence of bias voltage on wave-functions and tunnelling rates may induce negative differential resistance effects. The details of the model will be presented and the influence of geometrical parameters of the structure on *I(V)* characteristics will be discussed at the conference.

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[5] J. Bardeen , *Phys. Rev. Lett.* **6**(2), 1961, pp. 57–59.
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A full journal publication of this work will be published in the Journal of Computational Electronics.

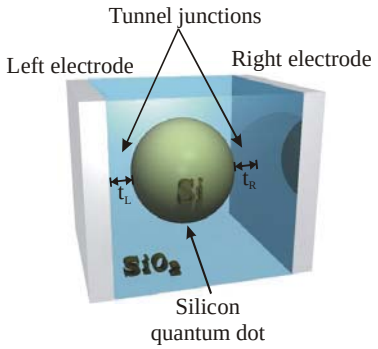

Figure 1: Schematic of the MI*Si*IM structure under study: a spherical silicon quantum dot embedded in a silicon dioxide layer and connected to electrodes by two tunnel junctions. The left and right tunnel junction thicknesses are t_L and t_R, respectively.

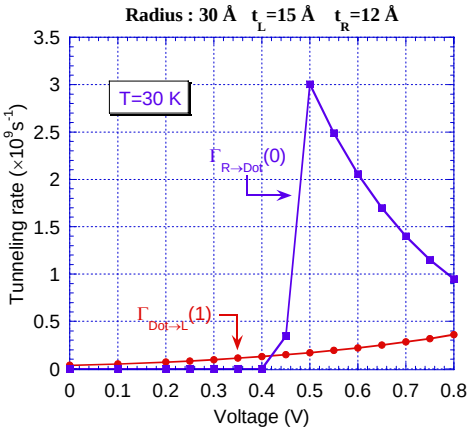

Figure 2: Evolution of tunneling rates as a function of bias voltage for a MI*Si*IM structure with a 30 Å radius silicon spherical quantum dot (t_L =15 Å and t_r =12 Å). $\Gamma_{R\rightarrow Dot}(0)$ represents the tunneling rate from the right electrode to the dot containing no electron and $\Gamma_{R\rightarrow Dot}(1)$ is the tunneling rate from the dot containing one electron to the left electrode.

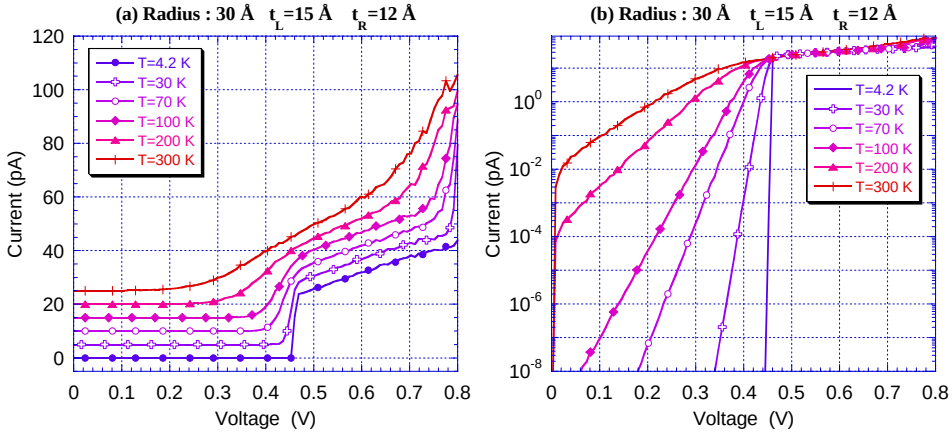

Figure 3: Temperature dependence of *I(V)* characteristics in (a) linear and (b) logarithmic scale for a MI*Si*IM structure with a 30 Å radius silicon spherical quantum dot. The left and right tunnel junctions are 15 Å and 12 Å thick respectively and the electrodes are made of aluminium. In case (a), the curves have been shifted vertically for clarity.

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