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Effect of Coulomb blockade on the switching time of Ag–Ag_2S–Pt atomic switches

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ABSTRACT

A theoretical model based on the single electron tunneling phenomenon is employed to calculate the time-dependent electrical resistance of an Ag–Ag_2S–Pt atomic switch at different applied voltages. While a negative voltage is applied to Pt electrode, Ag atoms precipitate on the surface of Ag_2S electrode where they form Ag clusters. The resistance of switch decreases as Ag clusters grow larger between two electrodes. Our model calculations imply the time required to decrease the resistance of switch below the resistance quantum (switching time) is mainly determined by the Coulomb blockade effect of Ag clusters. The switching time is found to decrease exponentially with increasing the applied voltage, which agrees very well with the experimental observations.

1. Introduction

Atomic switches are solid electrochemical nanodevices, which operate based on the diffusion/reduction of metal ions between two electrodes. Their resistance changes reversibly by changing the polarity of applied voltage. This fascinating electronic property makes them suitable to perform as memory devices and artificial neurons [1–7]. Although there have been significant experimental investigations on the electrical property of these switches, the theoretical understanding of how these switches work requires further investigations.

An atomic switch can be fabricated by using Ag and Pt as its electrodes where silver sulfide (Ag_2S) is grown on the surface of Ag electrode leaving a tunnel junction (TJ) gap between Pt electrode and Ag_2S. In the absence of applied voltage, the resistance of these switches (R_{OFF}) can be as low as few kΩ or as high as few TΩ depending on the size of TJ gap and the width of electrodes. The TJ can be controlled by applying a voltage to the switch [8]. If a negative voltage is applied to Pt electrode, electrons tunnel from Pt electrode to Ag_2S and neutralize Ag ions that diffuse within Ag_2S from Ag electrode resulting in formation of Ag nanowires within Ag_2S and precipitation of Ag atoms on the surface of Ag_2S [9,10]. This process continually decreases TJ gap between two electrodes while the voltage is applied, because Ag atoms keep growing between two electrodes. As a result, the resistance of switch decreases. This is a reversible process where by applying a positive voltage to Pt electrode metal reduction/oxidation occurs and Ag atoms diffuse back to the Ag electrode and TJ gap begin to increase [8]. The time that it takes to decrease the resistance of a switch below the resistance quantum [11] ($R_Q \approx 6.5$ kΩ, for the single spin electron transport phenomenon) is called switching time (t_{SW}). The growth/reduction rates are functions of tunnel current, amplitude and polarity of the applied voltage. The experimental investigations have shown t_{SW} is exponentially decreases with increasing the applied voltage [12]. Currently, there is no theoretical model based on first principle calculations to describe this process.

Here, by using first principle calculations based on the single electron tunneling phenomenon we show Coulomb blockade (CB) effect of precipitated Ag clusters on the surface of Ag_2S plays a major role to determine t_{SW} of an atomic switch. To model the time-dependent electrical property of the atomic switch, Matlab software was used to write a home-made code to calculate t_{SW}. The model calculations indicate t_{SW} decreases exponentially with increasing the applied voltage. This occurs, because at higher voltages electrons have higher electrostatic energy to overcome the CB effect of Ag clusters, hence, the growth rate of Ag clusters increases and t_{SW} decreases exponentially. Our findings agree very well with the experimental observations.

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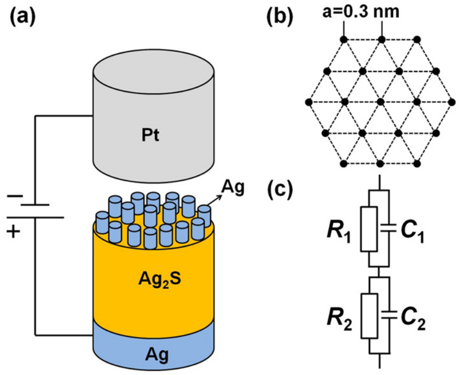

Fig. 1. (a) Schematic of an Ag–Ag_2S–Pt atomic switch where Pt electrode is connected to the negative pole of a DC power supply. (b) Double-concentric hexagonal base of an Ag nanowire with Ag–Ag bound length of $a = 0.3$ nm. (c) Equivalent circuit diagram of the atomic switch.

2. Theoretical model

Fig. 1(a) shows a hypothetical experimental setup where a power supply provides a negative DC voltage to a circular cylindrical Pt electrode with radius $r_{Pt} = 5.5$ nm. The second electrode made of Ag with a similar geometry is connected to the positive pole. Here, we assume a very thin Ag_2S layer is grown on Ag electrode so the diffusion time of Ag atoms becomes negligible compared to the time that it takes to form Ag clusters on the surface of Ag_2S. Therefore, t_{SW} is mainly determined by the time required to form Ag clusters between two electrodes.

While a voltage (V) is applied to the switch, Ag ions diffuse to the surface of Ag_2S and they are neutralized to form Ag clusters. Due to the surface defects, Ag clusters will grow at different locations on the surface of Ag_2S and they can grow in parallel between two electrodes. We assume the average distance between clusters is 2 nm. To simplify our calculations, Ag clusters are treated as cylindrical nanowires with a double-concentric hexagonal base as shown in Fig. 1(b). This assumption allows us to use an appropriate Ag–Ag bond length ($a = 0.3$ nm) in nanowires [9] and to arrange hexagonal bases on the surface of Ag_2S conveniently. Although the CB energy of total Ag clusters plays a major role to determine t_{SW}, the CB energy of an individual cluster confined between two electrodes is mainly determined by its volume and it weakly depends on its geometry.

Fig. 1(c) shows the equivalent circuit diagram of the atomic switch, $R_1(t)$ is the TJ resistance between Pt electrode and Ag_2S, $C_1(t)$ is the capacitance of that TJ, R_2 is the TJ resistance between Ag nanowires and Ag_2S (because the Ag–Ag bond length in nanowires within Ag_2S is also $a = 0.3$ nm) [9], and C_2 is the capacitance of that TJ. As the TJ between Pt electrode and Ag_2S is larger than the other TJ, the tunnel current passing through the switch can be calculated as [13]

$$I(t) = I^{+}(t) - I^{-}(t),$$
$$I^{\pm}(t) = C\exp\left[-\beta^{\pm}(V_1,t)l(t)\right]\frac{E_c(t) \pm eV_1(t)}{1-\exp[(E_c(t) \pm eV_1(t))/k_BT]}, \quad (1)$$

where $C = 1.25 \times 10^{21}$ $(\mathrm{C.\Omega})^{-1}$ is a constant related to the tunneling cross-sectional area and the density of electronic states at the Fermi level of Ag clusters, e is the electron charge ($e > 0$ to ensure the sign of tunnel current agrees with the direction of conventional current), $V_1(t)$ is the potential difference between Ag nanowires and Pt electrode, k_B is the Boltzmann constant, T is the absolute temperature, $l(t)$ is the TJ gap between Pt electrode and the top of Ag nanowire, $E_c(t)$ is the CB energy of Ag nanowires (the electrostatic energy required to add one electron to Ag nanowires), and $\beta^{\pm}(V_1,t)$ is the tunneling decay constant

$$\beta^{\pm}(V_1,t) = 4\pi h^{-1}\sqrt{2m\left[U + E_c(t) \pm eV_1(t)\right]}, \quad (2)$$

where h is the Planck constant, $m \approx 9.11 \times 10^{-31}$ kg is the effective mass of the electron, and $U = 3$ eV is the height of the tunnel barrier, which is lower than the work functions of Pt and Ag due to the image charge effect [14]. The CB energy is a function of time as Ag nanowires grow larger and it is calculated as [15]

$$E_c(t) = \frac{e^2}{2C_T(t)}, \quad C_T(t) = N\left[C_1(t) + C_2 + C_3(t)\right], \quad (3)$$

where $C_T(t)$ is the total capacitance of Ag nanowires and $N = 16$ is the number of Ag nanowires, $C_1(t)$ and C_2 are the coupling capacitances of Ag nanowires to Ag_2S and Pt electrodes respectively. To calculate the CB energy it is assumed there is no initial excess charges [13,15] on Ag nanowires before the electron tunneling occurs. Furthermore, the radius of Ag nanowire is $\approx 2a$ where $a = 0.3$ nm is the Ag–Ag bond length in nanowires (Fig. 1(b)). The coupling capacitances are calculated by considering Ag nanowires as parallel plate capacitors where

$$C_1(t) = \frac{4\pi\varepsilon_0 a^2}{l_0 - n(t)a}, \quad C_2 = 4\pi\varepsilon_0 a, \quad (4)$$

where ε_0 is the permittivity of free space, l_0 is the initial TJ gap between Pt electrode and Ag_2S, $n(t)$ is the number of double-concentric hexagonal layers in each Ag nanowire. The self-capacitance of an Ag nanowire is calculated as [16]

$$C_3(t) = 2\varepsilon_0 a\left\{8 + 6.95\left[\frac{n(t)-1}{2}\right]^{0.76}\right\}. \quad (5)$$

It is important to note that $C_1(t)$ and C_2 are connected in series and $V_1(t) = VC_2/[C_1(t) + C_2]$ (Fig. 1(c)), but to calculate $E_c(t)$ the power supply is turned off and its internal resistance is assumed to be zero, so $C_1(t)$, C_2 and $C_3(t)$ are treated as if they are connected in parallel.

In order to calculate the t_{SW}, first, the tunnel current, $I(t)$, is calculated by using Eqs. (1) and (2) where initially $E_c(t) = 0$. Then, the resistance of switch $R(t) = V/I(t)$ is calculated and it is compared against the resistance quantum $R_Q = h/4e^2 \approx 6.5$ kΩ [11].

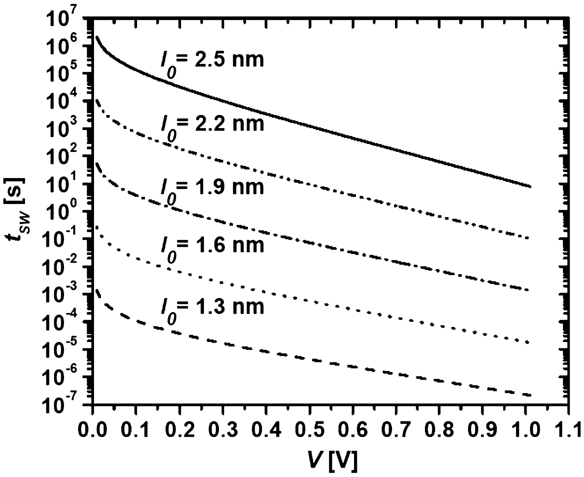

Fig. 2. The switching time (t_{SW}) of the atomic switch at $T = 300$ K as a function of applied voltage for five different initial TJ gaps (l_0). The negative pole of the power supply is connected to Pt electrode.