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BREAKDOWN AND CONDUCTIVITY SWITCHING IN NANOSIZED HAFNIUM DIOXIDE

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I. INTRODUCTION

At the present time nanostructures based on hafnium dioxide are promising for use as gate insulators in MOSFETs (metal-oxide-semiconductor) and non-volatile resistive memory with random sampling (RRAM). Hafnium oxide has a high dielectric constant, a relatively high energy of the forbidden band, and forms a thermodynamically stable interface with silicon. It is worthwhile for resistive memory, since its dielectric breakdown leads to switching to a low-resistance state, and formation of high density of traps, that makes possible the long-term storage of charge (up to 106-107 s). Therefore, the methods for fabrication of nanosized hafnium dioxide on a silicon substrate and nanostructures based on it are being developing, and its electrical, structural and spectroscopic characteristics and parameters, as well as peculiarities of hafnium dioxide properties appearing as a result of electroforming, are being studied [1, 2]. In this area practical results have been already achieved, the main of which is the production of a stable nanosized layer of hafnium dioxide, switchable by a low potential. However, there are still many unsolved problems, the most important of which are the identification of a mechanism for switching of hafnium dioxide from a high-resistance to a low-resistance state, identification of mechanisms of current transfer in the presence of a high concentration of traps, and the determination of the contribution of thermal processes.

II. MODEL

In this paper, we propose a model of breakdown and a fast switching of the conductivity of nanosized hafnium dioxide containing bistable electronic states. Such states in hafnium dioxide are obtained by electroforming in an electric field with the formation of conductive current filaments. At electrical breakdown of nanosized hafnium dioxide, filaments with a diameter of about 50 nm are formed. A strong heating of the material up to its boiling point takes place. In fact, there is an electrical explosion of matter in the channel, which is limited by solid walls. Plasma is formed, a fast growth of pressure on the walls of the channel and its expansion occurs, as well as a certain release of matter from the channels due to local heating of the electrodes, which leads not only to a deficiency of oxygen atoms in the channels, but also to the release of the compound itself [3]. Due to the strong heating and the subsequent increase of pressure on the walls and electrodes, the substance in the channels is pressed against the walls, like spreading along them, some of it is pushed to the electrodes closer to the anode, and part of the electrode material, mainly the cathode, is pressed into the channels. After removing the electrical impulse and cooling down of the substance in the channel, i.e. after the finishing of the electroforming, the evaporated material sedimentate on the channel walls, is amorphized under pressure in the anode region and after cooling turns into a glassy nonequilibrium disordered system. Between the cathode and the glassy region, apparently, an area is formed in which the substance is absent, i. e. a vacuum cavity.

Upon further application of the electric field, the current transfer mechanism changes. Now we must take into account the thermal emission of electrons from the cathode, which have energy higher than the Fermi energy of the cathode and can be accelerated in the vacuum gap. These electrons, interacting with the glassy region near the anode, activate metastable trap states in it, facilitating the transition of this region to a high-conductivity state, but without heating the substance up its to melting and evaporation. The removal of the field leads to the return of the system to a low-conductivity state.

Such glassy region near the anode can capture electrons, forming a space charge after removing the field, or may not form it at all. In the first case, for the subsequent switching it is necessary to apply an external bias with the opposite sign, and this will be a bipolar switching. In the second case, the potential of the opposite sign is not required, and we obtain a monopolar switching.

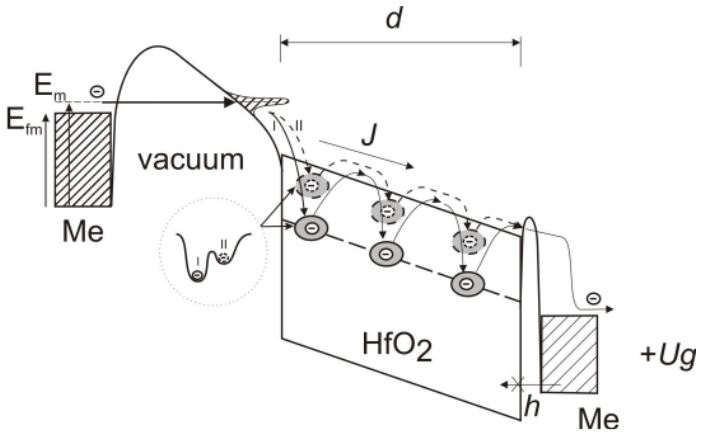

Figure 1 – Energy diagram of breakdown channel in hafnium dioxide with vacuum gap.

The current flow through the glassy region near the anode happens by means of the activation mechanism of metastable trap states (Figure 1). Several mechanisms are possible here. One of them is the excitation of trap states by electron impact with an energy of the order of several eV. Here it will be nonequilibrium hot electrons for the glassy region. The excitation of trap states leads both to a change in the ionization energy and to the cathodoluminescence of this region with the emission of photons. For bistable states, the interaction with hot electrons leads not only to transition to the excited state, but also contributes to a decrease of their ionization energy up to their delocalization. Also, in this case, bistable trap states can pass into upper energy state not by direct interaction with hot electrons, but due to the influence of noise and periodic force. In this case the appearance of noise is facilitated by charge fluctuations under the influence of hot electrons, which are associated with their defect scattering. The vibrational modes of trap centers act as a periodic force in that case. The transition of the whole system of traps to a highly conducting state occurs due to the stochastic synchronization effect, which requires a specific interaction between the traps [4]. In this case, it can be either a Coulomb interaction or a dipole interaction.

To model the traps switching, a bistable switching model is used in the presence of a periodic force associated with the electron-phonon interaction and the noise impact. The general form of the time-dependent generalized configuration coordinate of the trap x(t) is [4]:

$$\frac{dx}{dt} = \frac{dV(x)}{dx} + A\cos(\omega t + \varphi) + \sqrt{2D}Noise(t), \quad (1)$$

where φ is the phase shift, A is the periodic impact amplitude, D is the noise level. The bistable potential of the trap state is:

$$V(x) = V_0(x^4 + \xi x^3 - \eta x^2), \quad (2)$$

where $V_0 = \frac{1}{2}k_0 a_0^2$, k_0 – characteristic atomic quasi-elastic constant, a_0 ~0.1 nm – characteristic atomic length, ξ и η – structure parameters, x – configuration coordinate.

The simulation of the switching of bistable trap states in hafnium dioxide is carried out using the bistable oscillator model under the assumption that its switching is induced by noise and is described by the equation:

$$\frac{d(y)}{dt} = ay + by^2 + cy^3 + Acos(\Omega t + \varphi) + \sqrt{2D}\xi(t), \quad (3)$$

where y – the generalized coordinate of the trap state, characterizing the form of its potential energy, a, b, c – parameters that determine the shape of the potential well of the trap, A, Ω, φ – the amplitude, the frequency and the phase of the oscillations of the center , D – the noise intensity, ξ(t) – the white noise generating function.

Using the system of equations (3), the main regularities of fast switching of the conductivity of oxide dielectrics containing bistable electronic states in strong electric fields are revealed.

III. RESULTS AND DISCUSSIONS

The simulation of electronic switching of bistable trap states was carried out on the example of hafnium dioxide: the thermal ionization energy of the traps was 0.48 eV, the oscillation frequency was 10-12 GHz, the trap concentration was 10^{19} cm^{-3}, and the noise intensity was 0.08-0.15.

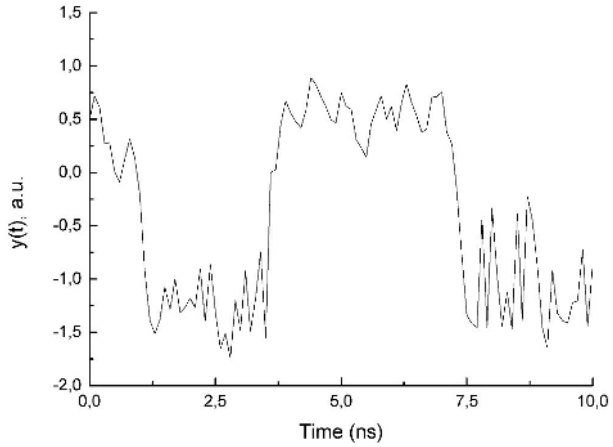

Figure 2 – Transitions between metastable states of the bistable center under the action of driving force and noise: A=0.25, φ=0, Ω=1, D =0.02, a=1, b=-1, c=-1

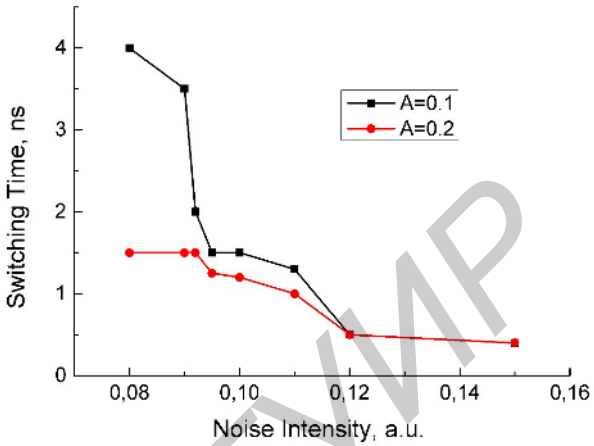

Figure 3 – Switching time vs noise intensity at different amplitudes noise amplitudes A

The calculations of the influence of the configuration parameters on the electronic properties of bistable centers have shown that in the presence of periodic impact and noise the transitions from one metastable state to another state are possible. These transitions substantially depend on potential wells depth ratio and are determined by the noise level.

IV. CONCLUSIONS

The bistable potential of the trap center under the action of weak periodic modulation undergoes the transition from one state to another only under the noise impact. It is shown that the noise exposure leads to a switching of the trap state in hafnium dioxide from one metastable state to another during a few nanoseconds. Upon the noise intensity growth the scatter of the output signal values y(t) increases and the switching occurs. With the growth of periodic impact amplitude the switching frequency from one state to another increases. The periodic action frequency growth leads to increase of switching frequency and with the phase growth the time of finding of the trap center in the metastable state increases. The characteristic switching time is of unities of ns.

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