

Modelling of local anodic oxidation of titanium oxide nanostructures formation process

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Abstract. A model for the oxide nanostructures formation by the local anodic oxidation method is presented. Dependences of height, depth, and diameter of titanium oxide nanostructures on the applied voltage pulse duration are obtained, as well as the oxide nanostructures profile for given technological parameters.

1. Introduction

The development of components of modern electronics, in particular memristor structures for resistive random access memory (RRAM) elements, requires application of new methods for the formation of nanostructures that possess high precision and reproducibility [1-8]. One of such methods is local anodic oxidation (LAO), which has high precision accuracy and allows forming structures with thickness less than 5 nm [9-16]. Other advantage of this method is the absence of complex photoresists and chemical etchants. Oxide nanostructures (ONS) obtained by LAO can be used to form profiled nanostructures and masks for surface selective etching [11-12]. Another promising application of titanium ONS is the memristor structures for resistive memory and synaptronic elements.

However, the LAO process has not been sufficiently studied. The analysis of the publications shows that the LAO mechanism consists of the oxygen ions generation and drift to the metal surface, where an oxidation reaction takes place with the oxide formation (Fig. 1). In this case, the application of voltage pulses plays a key role in the LAO process, since the generated electric field leads to the oxygen ions generation due to the electrical dissociation of water molecules in the air and on the substrate surface, and also stimulates the drift of the formed oxygen ions to the reaction region.

The goal of the work is to develop a mathematical model and to calculate an algorithm of titanium ONS formation obtained by LAO.

2. Model

Since the LAO process is associated with the generation and transfer of oxygen ions in the probe-air-oxide-substrate system and subsequent substrate oxidation, it is necessary to calculate the oxygen ion flux at each point of the substrate surface. For this purpose, it is necessary to solve the system of Poisson and continuity equations:



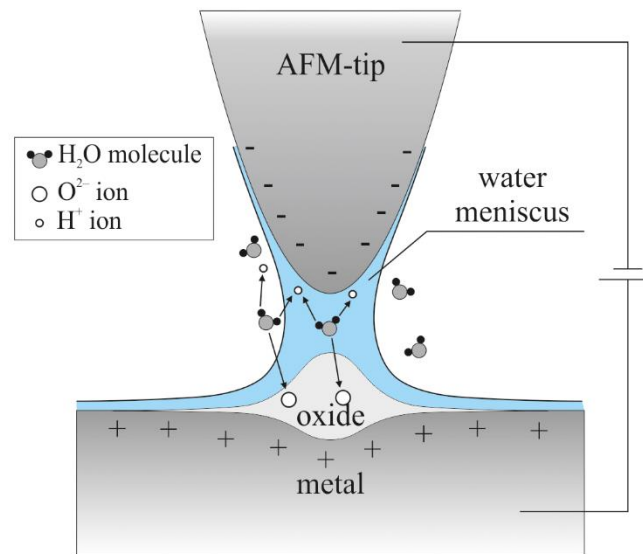


Figure 1. Schematic representation of the oxygen ions generation and drift process in the LAO.

$$\begin{cases} \nabla(\varepsilon \nabla \varphi) = -\frac{\rho(N)}{\varepsilon_0}, \\ \nabla(-\mu N \nabla \varphi + D \nabla N) = R(\varphi). \end{cases} \quad (1)$$

where ε is the relative permittivity, φ and N are the distribution of the electric potential and the concentration of oxygen ions in the system, ρ is the volume density of electrical charges, ε_0 is the electric constant, μ and D are the mobility and diffusion coefficient of oxygen ions, and R is the generation rate of oxygen ions in air.

Solution of the equations system (1) will allow calculating the flow of oxidizer ions and the oxide growth rate by formula:

$$v = -\frac{M_o}{\rho_o}(-\mu N \nabla \varphi + D \nabla N), \quad (2)$$

where v is the oxide growth rate, M_o and ρ_o are the molar mass and density of the oxide.

In addition, it was shown in Ref. [17] that the height ratio h_1 and the depth ratio h_2 of the ONS are determined by the expression:

$$h_1 : h_2 = \left(1 - \frac{M_s \rho_s}{\rho_o M_o}\right) : \frac{M_s \rho_s}{\rho_o M_o}, \quad (3)$$

where M_s and ρ_s are the molar mass and density of the substrate.

3. Results

Based on the developed model, the titanium film LAO process was numerically simulated using the MATLAB software package. For this purpose, the system geometry containing the AFM-probe, air, oxide, and metal film, for which the equations system (1) solution located was considered. Then, on the basis of equation (2) and the calculated values of the electric potential φ and the oxygen ions concentration N , the oxide growth rate was determined and, based on the relation (3), the oxide height and depth were calculated.

As a result of simulation, it is possible to obtain the titanium ONS height, depth, and diameter dependences from duration of impulses of the applied voltage (Fig. 2), the electric potential and oxygen ions concentration distribution (Fig. 3), and also the profile of the titanium ONS (Fig. 4) at the given values of the applied voltage amplitude and duration, the distance of the probe-substrate, the relative humidity level in the process chamber, and the geometric parameters of the AFM probe.

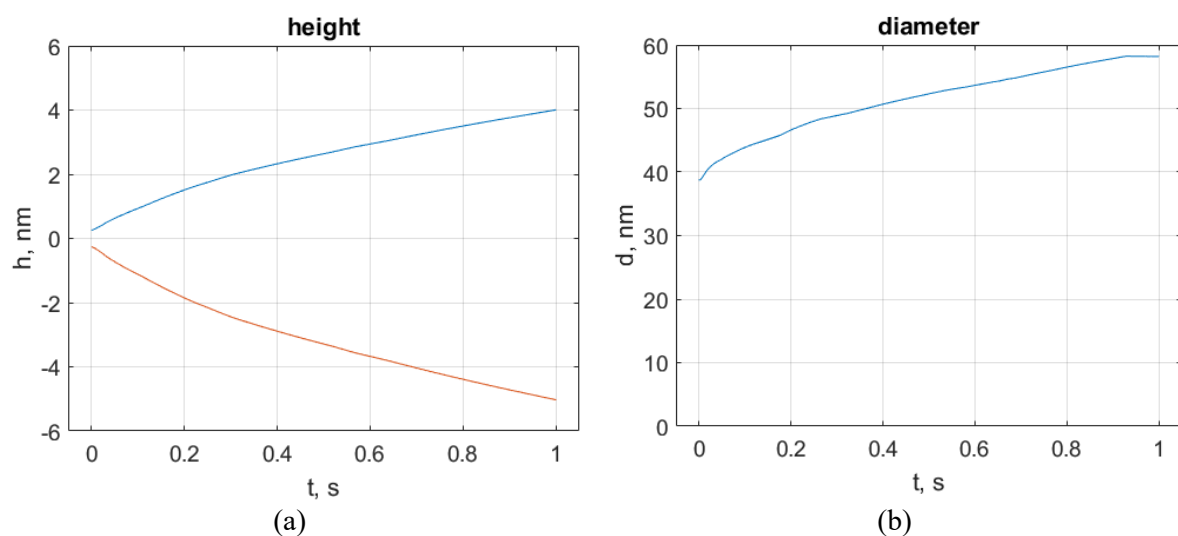


Figure 2. Dependences of (a) height and (b) diameter at half-height of titanium ONS on the duration of the applied voltage pulses.

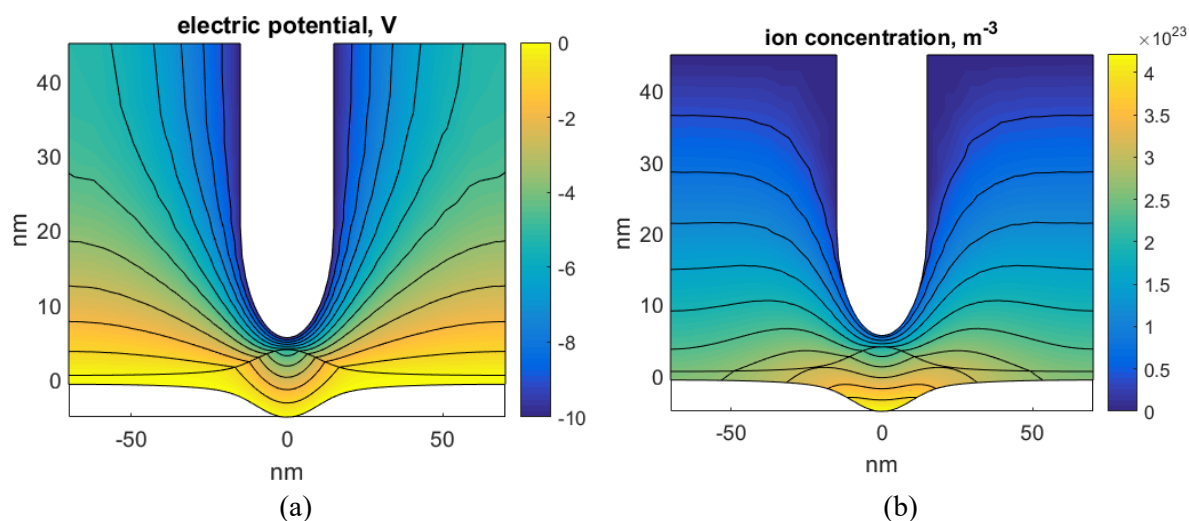


Figure 3. Spatial distributions of (a) electric potential and (b) oxygen ions concentration.

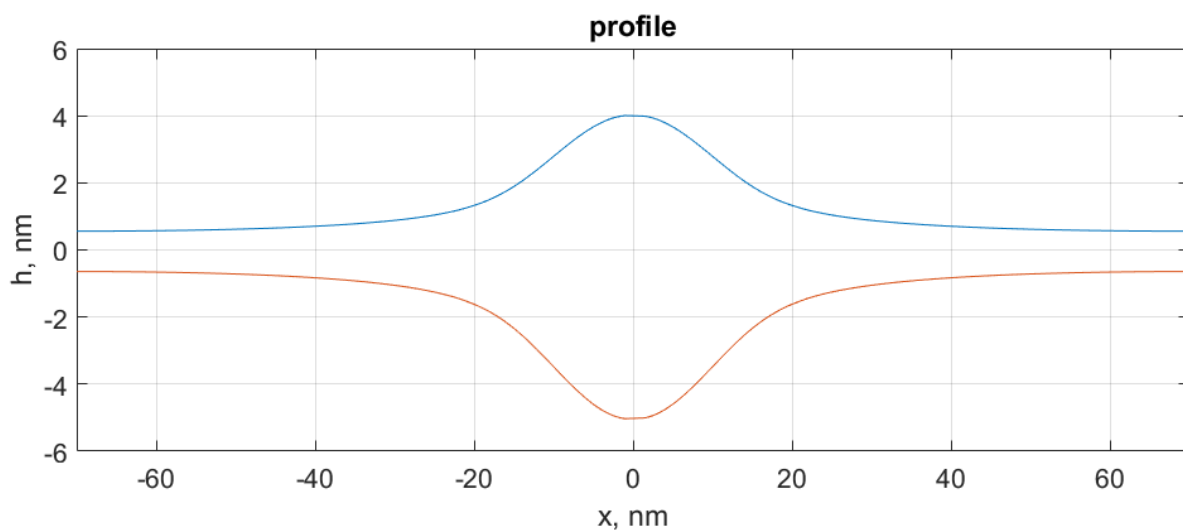


Figure 4. Titanium ONS profile.

4. Conclusion

The paper presents a model for the oxide nanostructures formation by the local anodic oxidation method, based on the electric potential distribution and the oxygen ions distribution calculation in the system. Dependences of height, depth, and diameter of titanium oxide nanostructures from duration of impulses of the applied voltage are obtained, as well as the oxide nanostructures profile for given technological parameters.

The obtained results correlate with the data obtained in Ref. [18] and can be used in the development of technological processes for the fabrication of the RRAM element based on titanium oxide nanostructures.

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