Mechanism of charge transport in Si/Al_2O_3/Al structures

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Abstract. The investigation of current – voltage characteristics of structures Si/Al_2O_3/Al on the basis of aluminium oxide layers obtained by a method atomic layer deposition is carried out. It is established, that the possible mechanism of charge transport in structure is the space charge limited currents. The charge carrier concentration (N_t), concentration of traps (n_0) and electron mobility (μ) in Al_2O_3 layer are calculated.

1. Introduction

Aluminium oxide possesses a number of interesting physical and chemical properties - high melting point, heat conductivity and the dielectric parameters, increased radiation stability, high electrical specifications, opacity to alkali ions and stability, wide-gap region, minor external impact resistance, shows no chemical reaction at contacted materials, thus causes its wide application as an active element in modern microtronics and electrooptics. During the recent years films of aluminium oxide have been analyzed as a dielectric layer in condenser structures. Thanks to high dielectric capacitance amorphous films of Al_2O_3 are considered as one of alternatives of replacement of silicon oxide in the process of formation of superfine gate dielectric layers in technology of metal-oxide-semiconductor structure [1].

Nature of films' conductivity depends on film thickness, film coating conditions, electrode system, substratum material, and applied voltage direction. Authors [2] investigated properties of cold cathodes on the basis of nanoflake of Al_2O_3 applied on Indium Tin Oxide. It is revealed that addition of a dielectric layer in thickness up to 11 nm essentially increases emission current. At a field, smaller than $2\cdot10^7$ V/m, prominent mechanisms of emission current formation are trap tunneling and Frenkel-Poole thermoactivation. In the field of $E \leq 6\cdot10^7$ V/m carrier tunneling in vacuo according to Fowler-Nordheim mechanism involving traps is carried out, and at $E \geq 6\cdot10^7$ V/m the emission mechanism changes from resonance to direct Fowler- Nordheim mechanism. Hickmott examined Al–Al_2O_3–Au structures with thickness of a dielectric layer ≈ 30 nm [3], [4] and found out that at voltage up to ≈ 15 V the Fowler- Nordheim mechanism of tunneling is carried out, and the height of a potential barrier makes up 1.5 eV. At the thickness of the insulation layer of 100 nm and at the voltage of 1 V density of injection current was equal to $8\cdot10^6$ A/cm^2 . Many researchers interpret the conductivity of Al_2O_3 within Frenkel-Poole model [5], [6], [7], [8].

It is known that when using TMA (trimethylaluminum, $Al(CH_3)_3$) and water as reagent in the process of synthesis of amorphous aluminum oxide, crystalline grains of the structure represent modification α-Al_2O_3 (hexagonal, distance between the closest atoms of aluminum and Oxygen is $R_{Al\text{-}O}$ = 0,176Å) [9]. A unit cell of α-Al_2O_3 belongs to a rhombohedral crystallographic system (R3cR) and contains 10 basic elements. Lattice constant: a_1 = 5.160 Å and θ_1=55.286^0. Atoms of oxygen are fourfold coordinated by atoms of aluminum. Atoms of aluminum are coordinated by six atoms of oxygen, and three next atoms at distance of 1.866 Å and three following the next atoms at distance of 1.983 Å are available [10], [11]. The valance band of α-Al_2O_3 consists of two subbands divided by an ionic gep, the lower band is formed generally by 2*s* – oxygen states, the top band is created by 2p – oxygen states with a contribution of 3*s*-, 3*p*-states aluminum. Values of forbidden-band width (E_g) is 6.0 – 8.2 eV for α-Al_2O_3 [12].

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Excess of aluminum in a crystal latitude of amorphous aluminum oxide that has not been subjected to annealing is caused by existence of its own (structural) defects such as vacancies of oxygen (anionic vacancy) which are the donors capable to double ionizing event, and their concentration defines the volume of conductivity of aluminum oxide. In connection with what the size of a potential barrier for electron injection out of metal into the isolator conducting band goes down and makes up according to source [13] $\varphi_B = 1.23$ eV . If the concentration of traps is great, the distance between traps isn't enough, so electrons from a metal electrode have possibility to tunnel directly onto traps and to pass isolator – hopping conductivity that we observed within the limits of frequencies from 10^3 up to 10^5 Hz at constant voltage of 1 V.

Electron density n in conduction band is connected with electron density on the n_t -traps in the following relation :

$$n = \theta n_t , \tag{1}$$

where θ is the constant specifying the extent of trap filling, it depends on depth of trap occurrence traps E_t.

Existence of traps (vacancies) leads to considerable reduction of current since being originally empty, they entrap injected electrons not allowing them to move in electric field. Consequently, the entrapped electrons make up a volume characteristic, and don't participate in current transfer through isolator. Electron density on the traps [14]

$$n_t \approx \frac{\varepsilon\varepsilon_0 U}{ed^2} = \frac{\varepsilon\varepsilon_0 E}{ed} . \tag{2}$$

The purpose of work is research of current-voltage characteristic (*I-V* characteristic) of films of amorphous aluminum oxide, for identification of the mechanism of charge transportation within $Si/Al_2O_3/Al$.

2. Methods and Materials

Films used in work are received through method atomic layer deposition (ALD) on *p*-type silicon Si (100) surface-supported substrate with its resistivity of ρ = 10 Ohm • cm from a mixed gas of trimethylaluminum of $Al(CH_3)_3$ (TMA) and water vapour at substrate temperature of 300 K. Directly before the loading of the fin into the ALD reactor cell Si-fin were processed by one-percent solution of fluorohydrogen acid HF for the purpose of removal of natural SiO_2 oxide. Aluminum contact points in area of 0.24 mm^2 were applied on isolator with thermal evaporation in vacuo. The thickness of oxide layer measured with the help of ellipsometer LEF – 3 was 78 nm. Measurements of current-voltage characteristic are executed at room temperature on the spectrometer "Concept 41" (Novocontrol Technologies), measuring voltage on a sample was in limits from 0.01 till 1 V.

3. Results and Discussion

The most probable mechanisms of charge transportation are the following: overbarrier Schottky emission, Frenkel-Poole mechanism and the currents limited by a space charge.

I-V characteristic of the structure is measured at the room temperature and at an alternating current. By the shape of *I-V* characteristic it can be concluded that in these films the conductivity mechanism is monopolar (electronic) [15].

When analyzing the experimental data and assessing the received results we used the following measurements: dielectric capacitance of aluminum oxide at frequency of 10^{-1} Hz ε=94, high-frequency dielectric capacitance $\varepsilon_\infty = 9.2$.

I – V characteristic at logarithmic scale of lg*I* - lg*U* (Figure 1) shows existence of three marked sites corresponding to power characteristics of a current (*I*) from applied voltage (*U*).

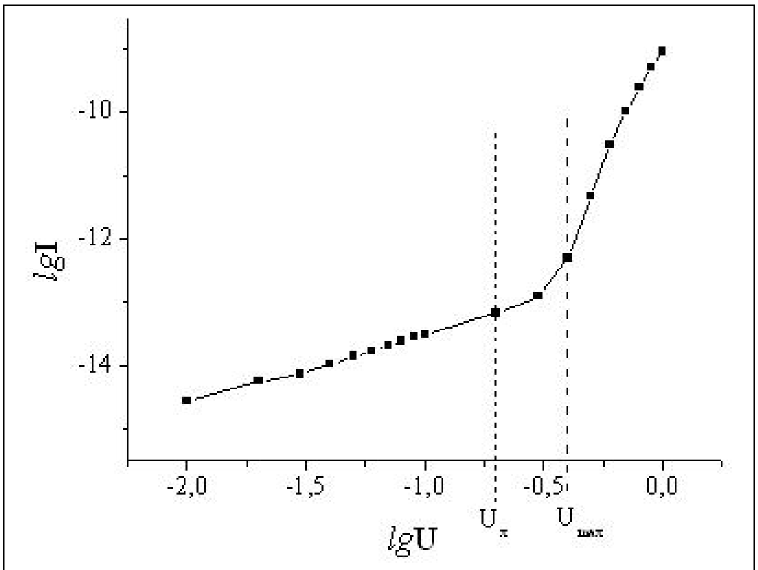

Figure 1. Sample *I-V* characteristic at the room temperature at the frequency of 10^{-1} Hz in coordinates of currents limited by a space charge

On the interval of voltage ranging from 0.01 V up to 0.2 V lgI ~ lgU, i.e. out the Ohm law is fulfilled

$$J = en_0\mu\frac{U}{d}, \quad (3)$$

where J – is electric current density in isolator, n_0 – is concentration of balanced thermally generated free carriers, μ- is current carrier mobility, U – the voltage applied to a sample, d – thickness of isolator.

The Ohm law is fulfilled at low voltages while the average concentration of n_i injected non-balanced free carriers doesn't become comparable with n_0 concentration of those carriers which are released thermally and are therefore neutralized. Existence of an ohmic site in loow fields allows to speak about existence of free electrons in isolator with n_0 concentration .

At higher voltages on the interval ranging from 0.2 V up to 0.4 V when n_i starts to prevail over n_0, current trapping quadratic dependence of voltage lg$I$ ~ 2lg$U$ is observed, *I-V* characteristic submits to dependence:

$$J = \frac{9}{8}\theta\varepsilon\mu\frac{U^2}{d^3}. \quad (4)$$

Voltage of transfer from an ohmic site of *I-V* characteristic to quadratic U_X = 0.2 V, is given by the following:

$$U_x = \frac{4en_0d^2}{3\theta\varepsilon}, \quad (5)$$

where n_0 – is concentration of free carriers at thermal balance.

The equation (4) be fair until Fermi level F is lower than level of trap occurrence E_t, at some voltage Fermi's level crosses trapping level, this voltage is called voltage of maximum trap infill

$$U_{\max} = \frac{eN_t d^2}{2\varepsilon}, \quad (6)$$

where N_t - is concentration of total number of traps in a unit of isolator volume, d - is isolator thickness, ε - is dielectric capacitance of isolator, ε_0 - is dielectric constant.

At U=$U_{\max}$= 0.4 V current starts to increase sharply, the number of injected electrons will be equal to number of traps. The received result corresponds to a case when all defects are identical and their levels lie superficially (above Fermi's level, as $U_x < U_{\max}$) (t.i. they are small). As the currents limited by a space charge are described with power like current-voltage characteristic of $I=C\cdot U^k$ type [16], growth of a current observed on chart at voltage higher than 0.4 V lg$I$ ~ 8.25 lg$U$, it allows us to assume that the main mechanism of current transportation is currents limited by a space charge. Dependence of a current on voltage is described by a formula

$$I = e\mu N_c \left(\frac{\varepsilon\varepsilon_0}{N_t}\right)^l \frac{U^{l+1}}{d^{2l+1}} = e\mu N_c \left(\frac{\varepsilon\varepsilon_0}{N_t}\right)^l \left(\frac{E}{d}\right)^l, \quad (7)$$

where N_c – is effective density of states in conduction band.

I-V characteristic in fields higher than 0.4 V proves existence of traps with exponential (continuous) distribution of density on energy in amorphous aluminum oxide.

In isolator with traps a current is in $1/\theta$ time less, than in isolator without traps. According to the schedule (Figure 1) we get $\theta = 0.85$.

According to (5) taking into account that U_x = 0.2 V, we get concentration of free balance current carriers of n_0=1,23 $\cdot 10^9$ cm^{-3}. According to (6) taking into account that U_{max}=0.4 V, we get concentration of levels of sticking (of traps) N_t=1.24$\cdot 10^{17}$ cm^{-3}. With the help of an ohmic site (3) we determine current carrier mobility in aluminum oxide: μ=2.473 $\cdot 10^{-4}$ m^2/V$\cdot$s = 247.3 cm^2/V$\cdot$s

At further increase of voltage new additional carriers of a charge are injected into isolator. These electrons already have no place to disappear, but remain in a conduct band. Therefore at voltages, higher than voltage of complete filling of traps, *I-V* characteristic will be the same, as well as for isolator without traps. That is the filled traps don't influence any more on *I-V* characteristic and they can be not taken into consideration.

Concentration of electrons in a conduct band, i.e. is higher than mobility edge

$$n = N_c \left(\frac{\varepsilon\varepsilon_0 U}{N_t d^2}\right)^l. \quad (8)$$

Characteristic energy of distribution of traps (depth of levels of sticking) E_t, is determined by a formula:

$$E_t = lkT. \quad (9)$$

The measurement l is determined by the schedule of lg I – by lg$U$ where *I-V* characteristic gives a straight line with l+1 tilt angle, and l= 7.25, E_0 = 0.19 eV.

Fermi level position is determined by a formula (will be changed accordingly to increase in voltage):

$$F = E_t \ln\frac{N_t d^2}{\varepsilon\varepsilon_0 U}, \quad (10)$$

we get F=(5.63÷6.50) eV.

4. Conclusions

Thus, the possible mechanism of charge transport in $Si/Al_2O_3/Al$ structure is the currents limited by a space charge. Concentration of free balanced current carriers in Al_2O_3 makes up (1.23±0.01)$\cdot 10^9$ cm^{-3}, concentration of traps (1.24±0.01) $\cdot 10^{12}$ cm^{-3}, depth of their occurrence, counted from a bottom of conduct band, is 0.19 eV.

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