coatings

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Supporting Information

Plasma Enhanced Atomic Layer Deposition of Tantalum (V) Oxide

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Ellipsometric study of dielectric functions

Since ellipsometry [1] is not a direct method for measuring dielectric functions, refractive indices n, absorption k and layer thickness, a suitable model must be used to determine them. For transparent layers, the Cauchy model is most commonly used [2]:

$$n(\lambda) = A + B/\lambda^2 + C/\lambda^4 \quad (1)$$

$$k(\lambda) = D + E/\lambda^2 + F/\lambda^4 \quad (2)$$

where A, B, C, D, E, F are the Cauchy coefficients.

Figure S1 shows the measured angles ψ and Δ for a sample with 1000 cycles (Table 1). As a result of calculations using models (1) and (2) and fitting the parameters, the Cauchy coefficients and the corresponding dependences n (λ) and k (λ) were determined, as well as the thickness of the Ta-O film d = 46.3 nm.

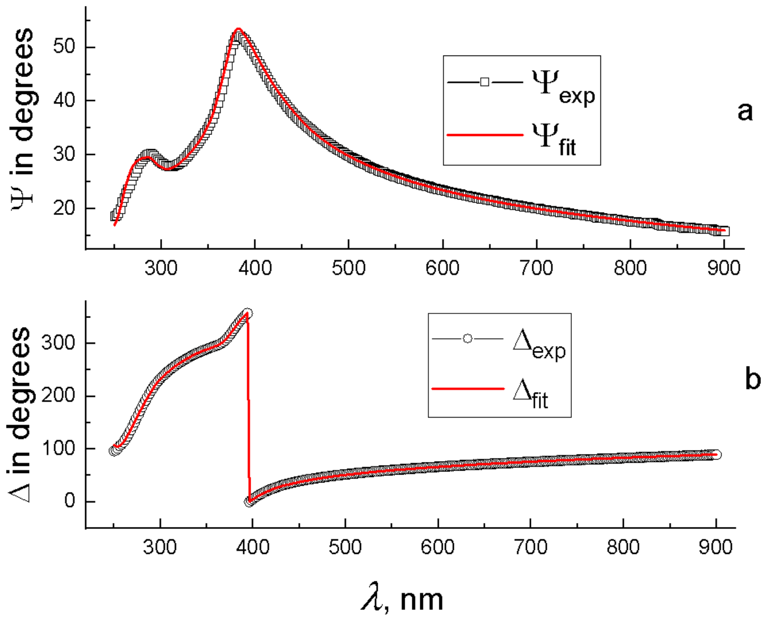

Figure S1. The measured and calculated spectra of ellipsometric angles ψ (a) and Δ (b) at an angle of incidence φ = 70 ° for a Ta-O layer with a thickness of d = 46.3 nm.

The dependences of the dielectric functions ε1 and ε2 were obtained from the functions n (λ) and k (λ) using the formulas: ε1 = n2 - k2 and ε2 = 2nk and are shown in Figure S2. The same Figure S2 shows the data from the graph in [3] for the Ta_2O_5 layer, which was obtained by evaporation of tantalum in an atomic oxygen plasma on a Si substrate dielectric functions ε1 and ε2 were also determined using spectral ellipsometry. This data is selected for only a few points for comparison with the ALD layer.

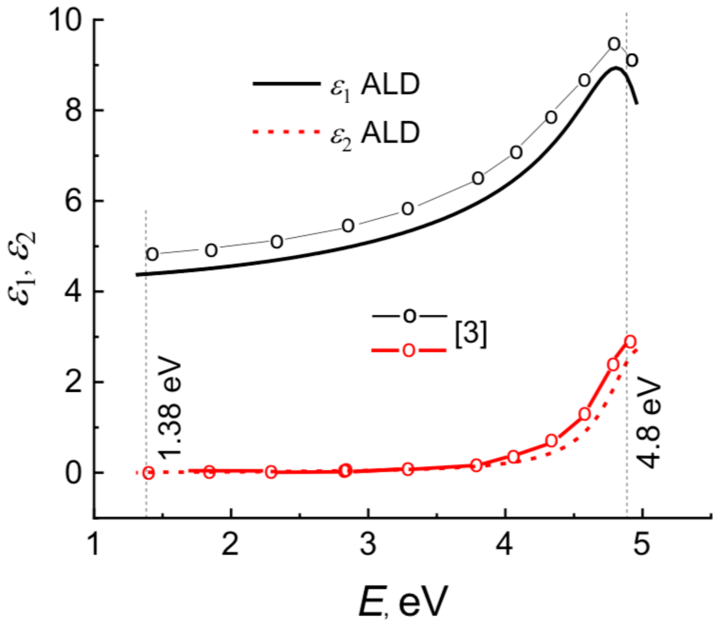

Figure S2. According to the ellipsometric angles, the real ε1 and imaginary ε2 parts of the complex dielectric function for the ALD Ta-O sample with the layer thickness d = 46 nm were calculated by Cauchy model [2]. Comparison with the data from [3] for Ta-O deposited layer (d = 48 nm) by evaporation of tantalum in atomic oxygen plasma. In both cases, there was a Si substrate.

In the energy range E from 1.3 to 4.8 eV, the values of the real part of the dielectric function ALD of the Ta oxide were in the range ε1 = 4.3 - 9.0, while for the plasma oxide Ta [3] this range was ε1 = 4.8 - 9.5. On the other hand, the values of the imaginary part of the dielectric function ALD of Ta oxide in the energy range E from less than 3.5 to 4.9 eV turned out to be in the range ε2 = 0 - 2.7, while for plasma oxide Ta - in the range ε2 = 0 - 2.8 eV, that is, in this case, they differ little by this parameter.

The structure of the ALD layer of tantalum oxide was formed under less "harsh" conditions and, apparently, was not "burdened" by the action of the electron plasma. The nature of the ε1 and ε2 dependences and the convergence of the ellipsometric data and the values calculated within the Cauchy model indicate the formation of a transparent structure in the visible spectral range for the ALD layer of Ta oxide.

Study of the effect of annealing on the dielectric function ε1

A Ta-O sample with an ellipsometrically determined dependence of the real part of the dielectric constant ε1 and thickness dTaO = 25.0 ± 1 nm was heated to 800 ° C. As a result, dTaO (dTaO = 25.5) remained practically the same. Still, the ellipsometric parameters (ψ and Δ) changed, as can be seen in Figure S3 (a and b).

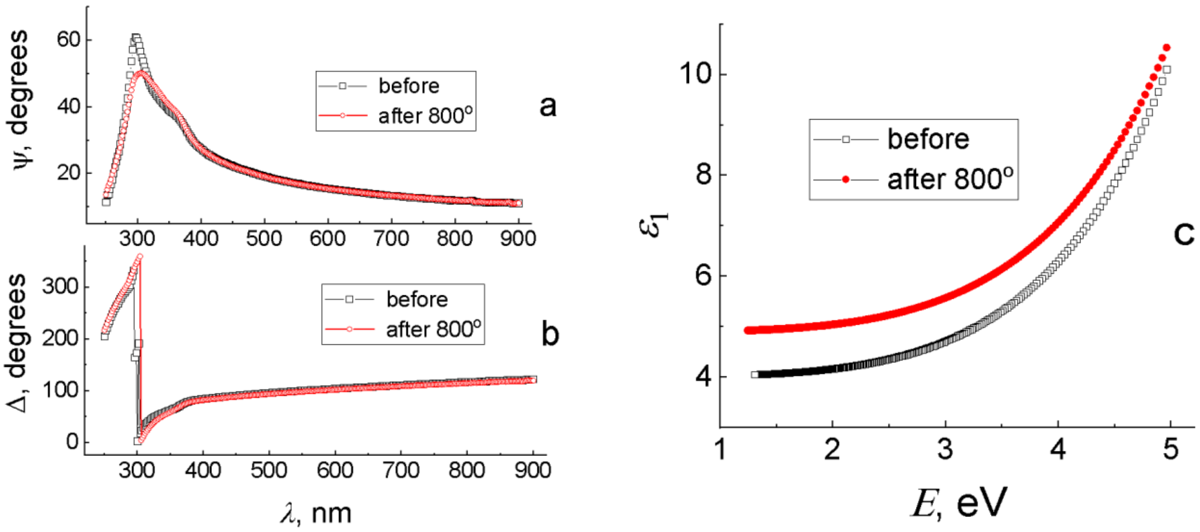

Figure S3. Ellipsometric angles ψ (a) and Δ (b) for the TaO sample before and after annealing (800 °) and the corresponding dependences of the real part of the dielectric function ε1 (c).

The dependences n (λ) and k (λ) calculated using the Cauchy equation were transformed into the real part of the dielectric function ε1 and compared before and after annealing in Fig. S3 (c).

Study of the effect of annealing at T = 800 °C on the characteristics of the Ta-O layer (thickness and dielectric function ε1).

True, this was done for one sample Ta-O_11 (25 nm): ε after annealing (800 °C) increased, which agrees with the conclusion about the appearance of a crystalline phase of Ta_2O_5 oxide from the results of XRD studies for other samples in Fig. 5.

References

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2. Fujiwara H. Spectroscopic Ellipsometry: Principles and Applications // Spectrosc. Ellipsom. Princ. Appl. 2007. P. 1–369.
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