Optical Properties of Textured V_2O_5/Si Thin Films Deposited by Reactive Magnetron Sputtering

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Abstract – Thin films of V_2O_5 are formed on Si substrates by reactive DC magnetron sputtering of vanadium metal target in Ar/O_2 low pressure gas mixture. The phase composition of the films was examined with reflection high energy electron diffraction (RHEED) at 65 keV and the presence of V_2O_5 textured polycrystal with preferencial orientation of [100] was found for the range of 35.4–48.9% O_2 partial pressure. Optical characterization of the films was produced with spectroscopic ellipsometry (SE) over the spectral range 250–800 nm.

1. Introduction

Vanadium pentoxide, V_2O_5, is the most stable oxide in V–O system exhibiting a semiconductor-metal transition at ~250°C. V_2O_5 thin films exhibit multicoloured electrochromism, and have high potential for use in electrochromic display devices, colour filters, and other optical devices [1–5]. V_5O_5 thin films can also be used in variable reflectance mirrors, smart windows, and surfaces with tunable emittance for temperature control of space vehicles. Layered crystal structure of V_2O_5 opens a possibility for gentle tuning of their physical characteristics via chemical intercalation of different metals yielding excellent film material for rechargable microbatteries.

Heat treatment of V_2O_5 films results in nanostructurization of material which final chemical composition and geometry are dependent on temperature and atmosphere composition. These vanadium oxide nanophases have enhanced ability for metal intercalation and gas sensitivity and are promising for effective applications in electronic devices.

2. Experimental

Thin films of V_2O_5 were deposited on Si(100) substrates by reactive DC magnetron sputtering of vanadium metal target in (O_2 + Ar) low pressure gasmixture. The phase composition of the films was examined with reflection high energy electron diffraction (RHEED). The presence of V_2O_5 textured polycrystal with preferencial orientation of [100] was found for the range of 32.7–40.8% $O_2/(O_2 + Ar)$ pressure ratio. Typical RHEED pattern of textured film is shown in Fig. 1.

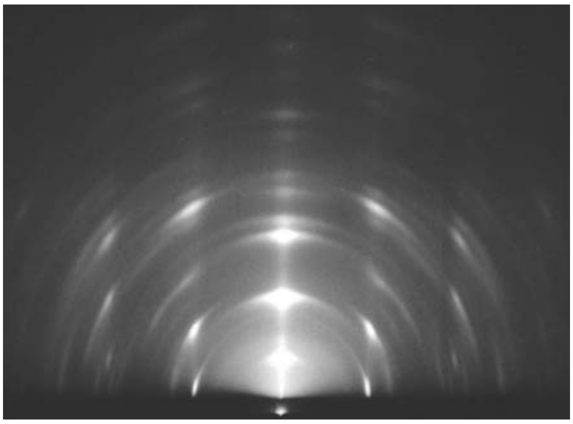

Fig. 1. RHEED pattern observed for V_2O_5 film formed at O_2/Ar ratio 32.7%

The films are polycrystal without pronounced ordering for the range of 40.8–48.9% O_2 partial pressure. Presence of unique V^{5+} valence state for vanadium ions in the film has been confirmed with X-ray photoelectron spectroscopy (XPS). Spectral dependences of refractive index n and extinction coefficient k and film thickness d were determined with using spectral ellipsometer "Spectroscan". Ellipsometric parameters were measured over wavelength range 250–900 nm at incident angle 70° with spectral resolution 2 nm. The V_2O_5 films are transparent in the spectral range 500–900 nm and refractive index dispersion was approximated by Cauchy polynomials:

$$n(\lambda) = a + \frac{b}{\lambda^2} + \frac{c}{\lambda^4}. \quad (1)$$

In the short wavelength spectral range $\lambda < 500$ nm a strong absorption has been detected. Well fitting of experimental curves can be achieved by introduction of two oscillators. Then Lorentz–Drude dispersion model (2) was applied with parameters shown in Table 1:

$$\varepsilon(E) = \varepsilon_\infty - \frac{E_{1D}^2}{E^2 - i\,E_{2D}\,E} + \sum_{n=1}^{m} \frac{A_n E_n^2}{E_n^2 - E^2 + i\,\Gamma_n\,E_n\,E}. \quad (2)$$

Table I. Dispersion parameters for V_2O_5/Si(100) systems

λ = 500–900 nm, Cauchy polynomials					
Sample	Thickness, nm	a	$b \cdot 10^{-4}$	$c \cdot 10^{-10}$	σ
1	43.29	2.45	–6.55	5.54	11.3
2	36.17	2.51	–6.38	5.48	17.5
λ < 500 nm, Lorentz–Drude dispersion model					
Sample	ε_∞	A_n	E_n, eV	Γ_n	σ
1	3.38	1.62	3.07	0.19	39.7
		2.15	4.71	0.35	
2	3.44	1.75	3.12	0.16	53.8
		2.29	4.80	0.31	

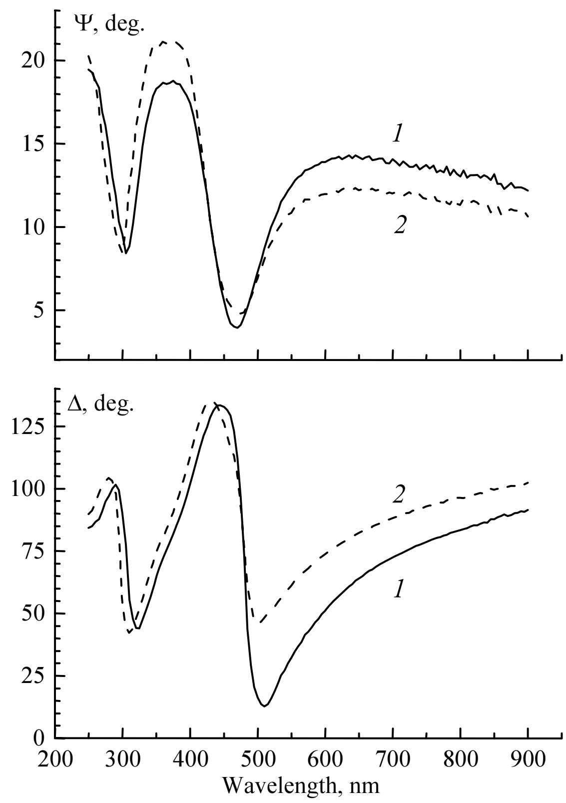

Fig. 2. Dependencies Ψ(λ) and Δ(λ) for system V_2O_5/Si(100). Samples are shown by numbers

In the spectral range λ = 250–500 nm the strong maximums of absorption in V_2O_5/Si(100) films are positioned at photon energy $E_2 \sim 3.1$ and $E_4 \sim 4.7$ eV. These results are well consistent with optical properties of V_2O_5 single crystal determined earlier with spectroscopic methods over a range $E = 2–14$ eV. In all these studies the most intensive absorption peak was observed at $E \sim 2.9–3.0$ eV that is well relates with $E_2 \sim 3.1$ eV determined in our experiments for V_2O_5/Si(100) films. This dominant spectral feature relates to optical transitions from the top part of valence band to the pair of localized conductivity bands. The absorption peak at $E_4 \sim 4.7$ eV is related to the transitions from the top of valence band to upper conductivity band.

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