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Statistical and Mathematical Modeling of DC Electrical Properties of Titanium Oxide thin Films as Function of Film Thickness and Temperature

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ABSTRACT

Ti films of different thickness ranging from 12.3 to 246.2 nm were deposited, using resistive heat method and post-annealed at different temperatures (300, 373, 473 and 573 K) with a flow of 5 cm^3 s^{-1} oxygen. The resistivity of sample was measured by Four Point Probe instrument, while a Hall Effect measurement system with a magnetic field strength of 2500 Gauss was used for Hall Effect investigation. Resistivity, carrier concentration, hall coefficient and mobility of samples were obtained at different thicknesses and temperatures and then mathematical model and behavior functions of these properties were obtained as function of film thickness and annealing temperatures.
KEYWORDS: Modeling, Resistivity, Hall coefficient, mobility and concentration carriers.

INTRODUCTION

Modeling and simulation are useful instruments for good perception of sciences and access to different states with low-cost. Many researchers have reported of Modeling application in nanocomposite and polymer [1 and 2] medicine (growth and controlling of cancer) [3and 4], nano science and technology [5 and 6] and so on.

TiO_2, in thin films and nanocrystalline form, has been a subject of considerable interest in the last few years as a low-cost material in photocatalysis, in photovoltaics, or as gas sensors and other applications. Further more structure and properties (e. g. Electrical properties) of the titanium oxide thin films are function of film thickness and annealing temperature, strongly.

In this work, DC electrical properties of titanium oxide thin films prepared by PVD method and post annealing at different thickness and annealing temperature measured by Khojier et al. [7], were investigated and then behavior function of resulted electrical properties was obtained by mathematica code.

MATERIAL AND METHOD

Titanium films of different thickness ranging from 12.3 to 246.2 nm were deposited on glass substrates (18 × 18 × 1 m cut from microscope slide) by resistive evaporation from tungsten boats at room temperature (a nominal deposition rate of 0.3 nm s^{-1} was used). The purity of titanium was 99.98%. An Edwards (Edwards E19 A3) coating plant with a base pressure of 2×10^{-6} mbar was used. Prior to deposition, all glass substrates were ultrasonically cleaned in heated acetone then ethanol. Post-annealing of the Ti films were performed at three different temperatures of 373, 473 and 573 K in oxygen environment with a flow rate of 5 cm^3 s^{-1}(the atmosphere air of the annealing tube (furnace) was flushed with argon gas several times before introducing oxygen and heating the samples). The resistivity of sample was measured by Four Point Probe instrument, while a Hall Effect measurement system with a magnetic field strength of 2500 Gauss was used for Hall Effect investigation.

Different functions were fitted on experimental data. Table curve and mathematica code were used for this work. Thickness was independent variable and resistivity, hall coefficient, carrier concentration and mobility were dependent variables. Linear, Quadratic, Cubic, Logarithmic, Exponential, Power and S functions were checked and the best function was selected (table 1). In addition, this observed that behavior function for a quantity as function of thickness at different annealing temperatures is was same but the constants were different, thus we reached to the behavior function as function of thickness and annealing temperature at thickness of 10-500 nm and annealing temperature of 300-600 K.

Theory

The presentation of different factors to better perception of table 1 and suitable selection of function is required for this purpose.

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Table, 1, The results of selected functions from investigation of various functions

Properties (T_a)	Function	Model	R %	R^2 %	R_A %	F	*Sign 0-0.05*
ρ(300 K)	S	Exp(4.00+(1.6x10^{-8})/d)	99.4	99.8	98.6	422	0.000
ρ(373 K)	S	Exp(4.15+(1.7x10^{-8})/d)	99.7	99.3	99.2	856	0.000
ρ(473 K)	S	Exp(4.30+(1.8x10^{-8})/d)	99.9	99.8	99.8	3970	0.000
ρ(573 K)	S	Exp(4.45+(1.9x10^{-8})/d)	99.8	99.7	99.6	1897	0.000
R_H(300 K)	Power	Exp(-27.500-0.660lnd)	99.4	98.9	98.6	439	0.000
R_H(373 K)	Power	Exp(-27.354-0.656lnd)	97.3	94.6	93.7	106	0.000
R_H(473 K)	Power	Exp(-27.154-0.650lnd)	98.3	96.6	96.1	172	0.000
R_H(573 K)	Power	Exp(-26.954-0.645lnd)	97.6	95.2	94.4	119	0.000
μ(300 K)	Exp.	Exp(-2.23-3.00x10^{-6}d)	99.2	98.4	98.1	307	0.000
μ(373 K)	Exp.	Exp(-2.27-3.07x10^{-6}d)	98.6	97.0	96.5	192	0.000
μ(473 K)	Exp.	Exp(-2.32-3.17x10^{-6}d)	98.2	96.3	95.7	158	0.000
μ(573 K)	Exp.	Exp(-2.37-3.27x10^{-6}d)	98.4	96.6	96.4	189	0.000
n(300 K)	Power	10^{19}xExp(13.6+0.68lnd)	99.4	98.9	98.7	448	0.000
n(373 K)	Power	10^{19}xExp(13.0+0.65lnd)	97.4	94.8	93.9	110	0.000
n(473 K)	Power	10^{19}xExp(12.0+0.60lnd)	98.3	96.7	96.1	174	0.000
n(573 K)	Power	10^{19}xExp(11.0+0.55lnd)	97.6	95.2	94.4	120	0.000

The quantity (R) (called the linear correlation coefficient):

The strength and the direction of linear relationship which are between two variables, is measured by R. This value represents linear correlation coefficient.

$$R = \frac{Sxy}{\sqrt{Sxx}\sqrt{Syy}}$$

$$Sxy = \sum xy - n\overline{xy}$$

According to the statistical researches, R^2, which represents the coefficient of determination, is used in the statistical model to predict next outcomes based on the other related information. It determines how efficient future outcomes are predicted by the model. R-squared value varies from 0 to 100. When the R-squared is 100 is means that movement in the index entirely explains all movement of a security. When R-squared is between (85, 100) interval, it tell us the performance patterns of fund have been in line with the index. Low R-squared, lower than 70, indicates the fund does not act much similar with the index[8].

$$R^2 = \frac{SSreg}{SST}$$

$$SSreg = \sum \left(\hat{y} - \bar{y}\right)^2$$

$$SST = \sum \left(y - \bar{y}\right)^2$$

F-ratio:

A new statistic, called the F-ratio is computed by dividing the MSreg by MSE. The F-ratio can be thought of as a measure of how different the means are relative to the variability within each sample. The larger this value, the greater the likelihood that the differences between the means are due to something other than chance alone, namely real effects. How big this F-ratio needs to be in order to make a decision about the reality of effects is the next topic of discussion. This is illustrated below:

$$F = \frac{MSreg}{MSE}$$

Significance, or P-value, is the probability that an effect at least as extreme as the current observation has occurred by chance. Other than that, we can say that when we assume that the null hypothesis is true, the probability of n obtaining test which at least one of that was observed is presented by P-value. Generally the null hypothesis is rejected when the P-value is the less than acceptable level α (Greek alpha), normally is 0.5 or 0.01. The result is statistically significant, if the null hypothesis is rejected by the model.

For example, **P** or Sig= 0.000, there greater than 99.9% certainty that the difference did not occur by chance.

RESULT AND DISCUSSION

S function as form of $\rho = \exp\left(a + \frac{b}{d}\right)$, was the best function with minimum error for resistivity (table 1), where d is thickness and a and b are constants. Resistivity at all of temperatures (300-600 K) had this form, while *a* and *b* increased by increasing of annealing temperature as follow (fig. 1):

$$a = 4.05 + (T - 300) \times 15 \times 10^{-4}$$

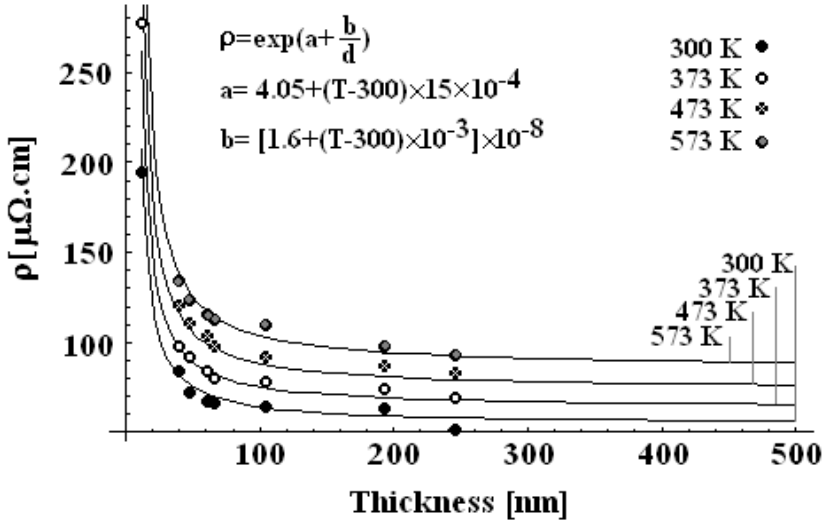

Fig. 1, Variation of resistivity as function of thickness at different annealing temperatures. (d) is thickness, (a) and (b) are constant, points and curves are experimental data and model functions, respectively.

Fig. 2 and 3 showed behavior function and experimental data for hall coefficient and carrier concentrations of titanium oxide thin films, respectively. Power functions as form of $R_H = \exp(a + b \ln d)$ and $n = 10^{19} \times \exp(a + bLnd)$ were the best function with minimum error for hall coefficient and concentration of carriers (table 1), where d is thickness and a and b were constants.

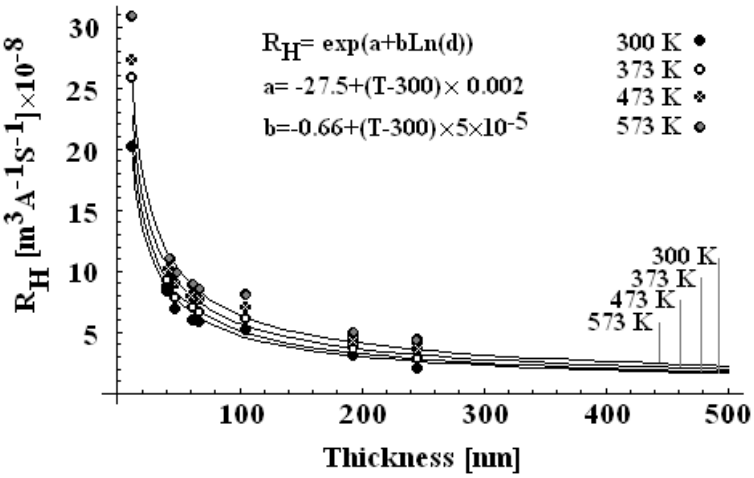

Fig. 2, Variation of hall coefficient as function of thickness at different annealing temperatures. (d) is thickness, (a) and (b) are constant, points and curves are experimental data and model functions, respectively.

A and b varied as form of follow:

For hall coefficient:

$$a = -27.5 + (T - 300) \times 0.002$$

$$b = -0.66 + (T - 300) \times 5 \times 10^{-5}$$

And for carrier concentration:

$$a = 13.73 - (T - 300) \times 10^{-2}$$
$$b = 0.68 - (T - 300) \times 5 \times 10^{-4}$$

Exponential function as $\mu = \exp(a + bd)$ form was the best function for mobility (fig. 4), where d is thickness and a and b varied as form of

$$a = -(2.23 + (T - 300) \times 10^{-4})$$
$$b = -(3 + (T - 300) \times 10^{-3}) \times 10^{6}$$

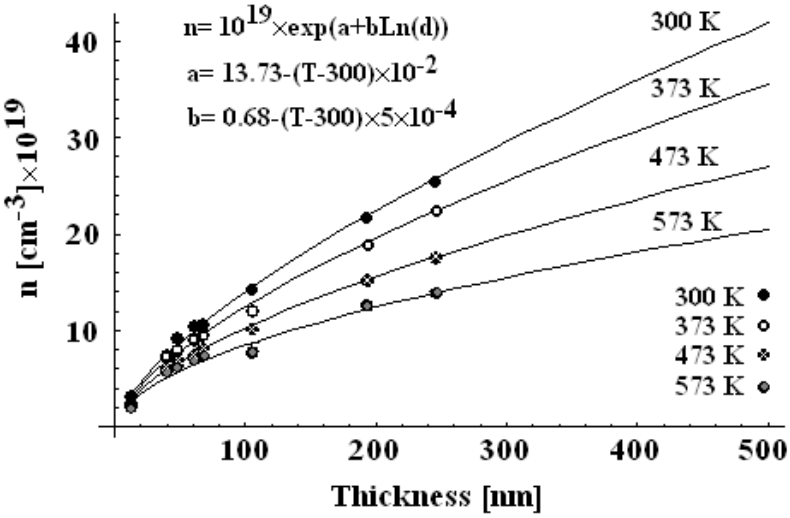

Fig. 3, Variation of concentration of carriers as function of thickness at different annealing temperatures. (d) is thickness, (a) and (b) are constant, points and curves are experimental data and model functions, respectively.

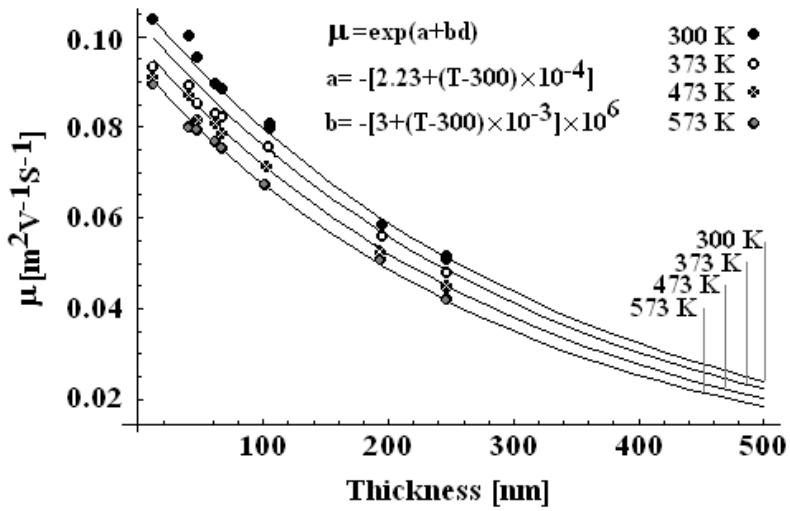

Fig. 4, Variation of mobility as function of thickness at different annealing temperatures. (d) is thickness, (a) and (b) are constant, points and curves are experimental data and model functions, respectively.

Conclusion

Mathematical model for DC electrical properties (resistivity, concentration of carriers, hall coefficient and mobility) of titanium oxide thin film produced by PVD method and post annealing at different thickness and annealing temperature were obtained. For this work, Linear, Quadratic, Cubic, Logarithmic, Exponential, Power and S functions were checked and the best function was selected. The result showed the behavior functions of a property as function of thickness, at different annealing temperature are same with different constants.

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