Applying multi-objective genetic algorithm (MOGA) to optimize synthesis parameters of dielectric Sol-Gel coatings for microelectronics

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Abstract*. This study optimized the parameters of silicon dioxide coating formation using a genetic algorithm. The coatings were prepared via the sol-gel method. Experiments were conducted using a face-centered central composite design, with the following input parameters: the ratio of silicon organic compounds in the initial sol, spin-coating rotation speed, and annealing temperature. The output characteristics included coating thickness, refractive index, and leakage currents of the sol-gel coatings. The influence of coating formation parameters on these characteristics was evaluated. The coating process optimization was performed using a genetic algorithm with the objective of minimizing leakage currents for sol-gel coatings of specified thickness.*

I. Introduction

The advancement of microelectronics, driven by the demand for device miniaturization and enhanced reliability, necessitates the improvement of dielectric coatings. While the sol-gel method offers flexibility in tailoring material properties, it faces challenges in optimizing multiple interdependent parameters. Traditional approaches based on factor screening prove insufficiently efficient. The application of genetic algorithms provides an effective solution to these problems, reducing both time and costs associated with such research [1]. The use of genetic algorithms in developing new sol-gel materials will enable efficient solutions for microelectronics. Previous studies [2–4] have demonstrated the successful optimization of process parameters using genetic algorithms. The present research employed the MOGA (Multi-Objective Genetic Algorithm) module of ANSYS DesignXplorer to optimize the parameters of sol-gel coating formation for microelectronic applications.

II. Determination of optimal parameters for sol-gel coating formation

In order to examine how the initial concentration ratio of methyltriethoxysilane (MTES) to tetraethyl orthosilicate (TEOS) affects the properties of the resulting sol-gel coatings, a series of film-forming solutions was prepared with different MTES:TEOS mass ratios (5:3, 4:3, and 1:1). The film-forming solutions were prepared as follows: specified quantities of methyltriethoxysilane ($CH_3Si(OC_2H_5)_3$) and tetraethyl orthosilicate ($Si(C_2H_5O)_4$) were mixed with a solvent and catalyst. During this process, the solution temperature increased due to hydrolysis and polycondensation reactions. The obtained solutions were subsequently aged at ambient temperature (22±2) °C for 2–3 days to ensure complete maturation.

To study the effect of deposition conditions, the prepared film-forming solution was applied to KDB-4 grade silicon wafers. The spin-coating process typically consists of four stages: solution application, spreading, excess solution removal, and solvent evaporation. The deposition parameters were optimized using an Apogee Cee 200X spin coater (Cost Effective Equipment, USA), which enables liquid solution deposition on flat substrates at rotational speeds ranging from 10 rpm to 12,000 rpm. Following deposition, the wafers were transferred to a programmable SNOL 8.2/1100 muffle furnace for air annealing. Three annealing temperatures were selected for investigation based on their ability to produce homogeneous coatings: 250°C, 325°C, and 400°C [5-8]. The thermal treatment protocol featured a constant heating rate of ≈3.5°C/min, followed by a 60-minute isothermal hold at the target temperature.

Refractive indices and thicknesses of the fabricated samples were measured with an LEF-757 laser ellipsometer (Institute of Semiconductor Physics, Russia) by taking five-point measurements across each wafer followed by data averaging, while current-voltage characteristics were evaluated using a Semishare E6 four-point probe station (Semishare, China) coupled with a GSM7-20H10 parametric analyzer (Good Will Instrument, China).

The study investigating the influence of initial composition and processing parameters on sol-gel coating properties was conducted using the Ansys DesignXplorer module. A central composite experimental design was implemented for three factors (P1–P3): where P1 represents the initial methyltriethoxysilane to tetraethyl orthosilicate ratio, P2 is the spin-coating rotational speed, and P3 denotes the annealing temperature. According to the experimental design, tests were performed for 15 input parameter combinations (see Table 1). The following output parameters characterizing the sol-gel coatings were determined: coating thickness (h), leakage currents (I1, I2, I3) at 50 V, 100 V, and 150 V respectively, and refractive index (n). Thus, the research object model consisted of response functions relating output parameters (h, I1, I2, I3, n) to input factors (K, ω, T). For response surface generation, a nonparametric regression method implemented in the DesignXplorer module of ANSYS Workbench was employed [9].

Table 1. Experimental Design and Results

N	*P1* *K*	*P2* *ω, rpm*	*P3* *T, °C*	*h,* *nm*	*I1,* *nA*	*I2,* *nA*	*I3,* *nA*	*n*
1	*1*	*3000*	*325*	*333.56*	*3.7*	*44.1*	*219.8*	*1.291*
2	*1.3*	*3000*	*325*	*328.70*	*2.5*	*27.0*	*147.7*	*1.303*
3	*1.67*	*3000*	*325*	*324.17*	*4.4*	*58.5*	*211.4*	*1.35*
4	*1.3*	*3000*	*250*	*296.42*	*2.6*	*29.1*	*163.8*	*1.354*
5	*1.3*	*3000*	*400*	*284.43*	*2.5*	*27.3*	*139.2*	*1.392*
6	*1.67*	*1500*	*400*	*782.47*	*3.1*	*49.8*	*144.6*	*1.395*
7	*1*	*4500*	*400*	*178.29*	*3.2*	*47.5*	*207.1*	*1.398*
8	*1*	*1500*	*400*	*714.28*	*2.7*	*42.8*	*184.7*	*1.402*
9	*1.3*	*1500*	*325*	*726.70*	*2.1*	*20.6*	*99.6*	*1.407*
10	*1.67*	*4500*	*400*	*235.81*	*4.1*	*55.0*	*198.2*	*1.407*
11	*1*	*4500*	*250*	*194.97*	*4.8*	*46.6*	*239.5*	*1.409*
12	*1.67*	*1500*	*250*	*764.16*	*3.3*	*52.2*	*171.5*	*1.412*
13	*1.3*	*4500*	*325*	*164.03*	*2.3*	*24.6*	*112.0*	*1.413*
14	*1.67*	*4500*	*250*	*223.81*	*4.0*	*54.2*	*171.2*	*1.413*
15	*1*	*1500*	*250*	*713.35*	*5.0*	*50.8*	*215.3*	*1.414*

The influence of input parameters on the output parameters that define sol-gel coatings was assessed. The centrifuge rotation speed has the greatest impact on the film thickness and refractive index values. The extent of leakage currents is primarily determined by the initial ratio of MTES to TEOS. Figure 1 illustrates the relationship between the leakage current I1 and the initial ratio of MTES to TEOS – P1, as well as the centrifuge rotation speed P2.

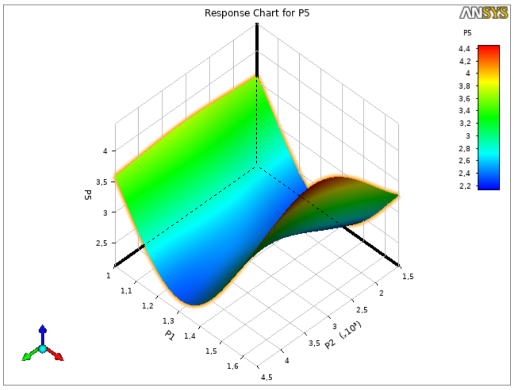

Fig. 1. Leakage current I1 as a function of sol-gel coating formation parameters

The optimization of sol-gel coating formation parameters was performed using the multi-objective genetic algorithm (MOGA) with an initial population size of 100 individuals and 100 individuals per iteration.

Multi-objective optimization was performed using the following criteria: minimization of leakage currents and maximization of refractive index values. The optimization results are presented in Table 2, with experimentally obtained parameter values shown in parentheses. The maximum relative error of the genetic algorithm predictions for output parameters did not exceed 10%.

Table 2. Optimization results

P1 K	*P2 ω, rpm*	*P3 T, °C*	*h, nm*	*I1, nA*	*I2, nA*	*I3, nA*	*n*
1,28	*2977*	*378*	*300*	*2.4*	*26.1*	*141.9*	*1.356*
			(309)	*(2.2)*	*(25.1)*	*(139.5)*	*(1.331)*

III. Conclusion

This study employed the multi-objective genetic algorithm (MOGA) from the DesignXplorer module to determine optimal parameters for producing sol-gel coatings that satisfy essential criteria for dielectric coatings in microelectronics applications, specifically achieving target thickness values while maintaining minimal leakage currents.

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