Mathematical Modeling of Droplet Formation, Evaporation, and Film Growth to Study Crystallite Size and Film Thickness of Spray Pyrolysis Deposited TiO$_2$ Thin Films

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The pure TiO$_2$ thin films were successfully deposited onto a glass substrate by using modified spray pyrolysis system. The TiO$_2$ thin films were deposited at temperature 350°C using Titanium trichloride precursor solutions of concentration 0.075 M, 0.1 M, and 0.125 M. Also, TiO$_2$ thin films with precursor solutions of concentration 0.1 M were deposited at different deposition temperature 350°C, 400°C, and 450°C. The prepared samples were further annealed at 500°C for 2 h to improve crystallinity. The XRD study revealed that the deposited TiO$_2$ thin films were polycrystalline and showed anatase phase with pre-dominant (101) peak. The crystallite size calculated from XRD was found to increase with increase in precursor solution concentration. The mathematical model to calculate crystallite size and film thickness were developed and the predicted results were compared with experimental results. The experimentally calculated crystallite size and thickness was in good agreement with the predicted results. The details of mathematical model and calculations TiO$_2$ thin films for were discussed in detail.

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I. INTRODUCTION

The spray pyrolysis (SP) is one of the cheapest chemical methods to prepare material thin films using gas phase or liquid phase deposition condition [1]. Several reports on SP show that the pinhole free, homogeneous and crystalline films with well-controlled nanostructures and compositions can be deposited on various substrates having complex geometry [2]. There are several processes parameter associated SP such as precursor solution flow rate, volume, concentration, density, viscosity, compressed air flow rate, temperature of deposition etc, which affects the quality and physiochemical properties of deposited material thin film. Because of these merits, SP is extensively used to deposit various metals, semiconductors, ceramics, sulfides, and metal oxide materials [3, 4].

Titanium dioxide is a non-toxic, wide band gap (3.2 eV) semiconductor. In contrast to other semiconductors with similar band gaps (e.g. ZnO), it does not photo-degrade upon excitation. The material has many unique physiochemical properties with its extraordinary chemical stability [5]. Because of this, it is used as a photo-catalyst to split water, anti-foggy coating on glass, anti-bacterial coating on various substrates, and coating on self-cleaning surfaces. TiO$_2$ can be prepared using nontoxic precursors which are easily available. Thin films of TiO$_2$ nanostructures are used as a promising in several emerging fields including gas sensor, humidity sensor, photovoltaic, photocatalyst, etc. For the performance of TiO$_2$ as photoanode in solar cell or as a sensor, crystallite size and film thickness matter a lot. Hence, it is necessary to estimate or predict the effect of process parameter of SP on to the crystallite size and film thickness of TiO$_2$ films.

The mathematical modeling of the spray pyrolysis system with air assisted ultrasonic and electrostatic atomizer is successfully reported in literature. Lado Filipovic et al. [6] explained spray pyrolysis with two different models: First model focused on droplet formation and their transformation in ambient air atmosphere, considering the several forces involved during the said process. Second model emphasis on the film growth phenomenon of SnO$_2$ species using Arrhenius expression but it is not elaborating the vaporization of the droplet in thermal region. A. Nakaruk and C. C. Sorrell [7] also explained conceptual model regarding the bonding evaluation during formation of TiO$_2$. This model focused on the processes involved in transportation of droplet and film deposition. S. M. Navid Khatami et al. [8] formulated mathematical model for the vaporization and film growth of mixed oxide thin film using spray pyrolysis technique. Till a date, very few reports are available on mathematical modeling of TiO$_2$ thin films deposited by SP technique, which explains in detail the process of film formation and estimation of crystallite size and film thickness.

In the present work, modified spray pyrolysis system is used for TiO$_2$ thin films. The modified system is well assisted with various parameters such as effect of substrate temperature, concentration of precursor solution, distance between nozzle and substrate, atmosphere, and solution to carrier gas flow ratio to controlled initial droplet velocity and size. The prepared films were characterized using various techniques. The mathematical modeling for TiO$_2$ thin films by SP is developed, and the predicted and experimental results of crystallite size and film thickness were computed.

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II. MATHEMATICAL MODELING

A. Spray pyrolysis process

The whole spray pyrolysis process is followed by four fundamental processes, as discussed below.

1. Atomization of the precursor solution i.e. droplet initial velocity and size atomization

Various nanostructures using spray pyrolysis can be obtained by the knowledge of droplet size and its terminal velocity. Therefore, the appropriate droplet size selection is one of the key factors in spray pyrolysis technique.

\[
\langle D_i \rangle = 10^{-3} \left[ \frac{\sqrt{\sigma \rho} d_n}{\rho_a V_a} \left( 1 + \frac{1}{AFR} \right)^{1/2} + 6 \times 10^{-5} \left( \frac{\eta_f}{\rho_a \sigma} \right)^{0.25} d_n \left( 1 + \frac{1}{AFR} \right)^{1/2} \right],
\]

where \( \sigma \) is surface tension of the precursor solution, \( \eta_f \) is coefficient of viscosity of the precursor solution, \( \rho \) is the density of the carrier air, \( d_n \) is the diameter of the nozzle, \( V_a \) is the carrier air velocity and \( AFR \) is the air to fluid flow ratio.

2. Droplet transport in ambient air

After spray formation, the droplets traveled in ambient air experience different forces like gravitational force, stokes force or drag force (due to ambient air), and thermophoretic force near the substrate. The equation of motion for a droplet can be obtained considering all these forces during their journey from nozzle to substrate. Therefore, the net force acting on droplet during the motion will be

\[
F_{\text{total}} = F_g - F_S - F_T.
\]

The droplet size distribution can be controlled by optimizing atomizer; it is difficult to measure actual size of the droplet, because the size of the atomized droplets is not uniform. Using holographic technique one can measure effect of air to fluid flow (AFR) on droplet density and its size distribution [9, 10]. However, droplet size distribution greatly depends on type and size of spray nozzle [11]. The size of the droplets is not uniform over the cone angle of the spray nozzle. Hence, the average droplets size becomes an important factor for further modeling. Theoretically, several mathematical functions have been used to describe droplet size distributions over spray cone [12, 13]. The semi-empirical formula for mean droplet diameter is Sauter mean diameter formulation. The Sauter mean diameter for air blast atomizer with respect to nozzle parameters was correlated by Viriato Semibo et al. [14] and is

\[
\langle D_i \rangle = 10^{-3} \left[ \frac{\sqrt{\sigma \rho} d_n}{\rho_a V_a} \left( 1 + \frac{1}{AFR} \right)^{1/2} + 6 \times 10^{-5} \left( \frac{\eta_f}{\rho_a \sigma} \right)^{0.25} d_n \left( 1 + \frac{1}{AFR} \right)^{1/2} \right].
\]

Here, \( F_g \) is the gravitation force on a droplet having mass \( m_d \), \( F_S \) is the Stokes force on a spherical droplet, and \( F_T \) is the thermophoretic force. The thermophoretic force acts on droplet only when the droplet is in thermal zone, slightly above (nearly 10 mm) the substrate. The evaporation of the droplet occurs in thermal zone causes change in diameter. Before reaching in thermal zone, let us assume that the droplet has constant mass \( m_d \) and radius \( r_d \). Therefore, in above Eq. (2) the forces can be converted to droplet acceleration as

\[
a(t)_{\text{total}} = g - \frac{F_S}{m_d} - \frac{F_T}{m_d},
\]

where \( a(t) \) is the droplet time dependent acceleration and \( m_d \) is the mass of the spherical droplet. The mass \( m_d \) of the droplet can be represented as

\[
m_d = \frac{4}{3} \rho_d r_d^3.
\]

The equation for the droplet acceleration can be derived by substituting the values of Stokes and thermophoretic forces and the droplet mass \( m_d \) into Eq. (3). Therefore, the expression for acceleration becomes [6]

\[
a(t)_{\text{total}} = \left[ g - \frac{27 \eta_k K_d \nabla T_a}{4 \rho_d r_d (2 K_a + K_d) r_d^2} \right] - \frac{9 \eta_k}{2 \rho_d r_d^2} V(t),
\]

where

\[
F_S = 6 \pi \eta_k r_d V(t)
\]

and

\[
F_T = \left( \frac{3 \eta_k r_d^5}{\rho_a} \right) \times \left( \frac{3 K_a}{2 K_a^2 + K_d} \right) \nabla T_a.
\]
The equation can be solved for displacement of the droplet by using Euler's characteristics equation and the displacement is

\[
d(t) = \frac{1}{B} (V_0 - V_t)(1 - e^{-Bt}) + V_t t,
\]

where \( t \) is the time required for the droplet to reach the substrate.

3. Droplet transportation in thermal zone; Decomposition/evaporation of the precursor solution

The evaporation of the droplet occurs forcefully due to the existence of a temperature gradient, in the thermophoretic region. The droplet undergoes evaporation before or after it reaches on the surface of the heated substrate. Therefore, the deposition temperature is significantly affecting the evaporation of the droplet. In air assisted spray deposition, the evaporation changes the diameter of the droplet \( D_p \) with time \( t \) is proportional to droplet surface area, and is given by [16]

\[
D_p^2 = D_i^2 - 8t \left( \frac{C_AD_{AB}}{C_p} \right) \ln \left( 1 - \frac{x_{A\infty}}{x_A} \right),
\]

where \( D_i \) is initial droplet diameter, i.e., Sauter mean diameter, \( C_A \) is the molar concentration of species A in the vapor phase, \( C_p \) is the molar concentration of species A in the liquid phase, \( D_{AB} \) is the binary diffusivity of vapor A in gas B, and \( x_A \) and \( x_{A\infty} \) are the mole fractions of species A at the droplet surface and far from the droplet, respectively.

The final diameter after chemical reaction is derived from the one-droplet to one-particle principle in spray pyrolysis [17]:

\[
D_f = D_p \left( \frac{C_{TiO2}M_{TiO2}}{\rho_{TiO2}} \right)^{1/3}.
\]

Here, \( D_f \) is the final particle diameter, \( D_p \) is change in initial droplet diameter near thermal zone, \( C \) is concentration of initial precursor, \( M_s \) is molecular weight of the generated particle, and \( \rho_p \) is the density of the generated particle.

In steady state, the rate of evaporation of a single droplet is expressed using mass conservation equation, hence known as pseudo-steady state evaporation is proposed [17]. The precursor solution evaporation rate is determined by the decreasing droplet mass \( m_d \) in terms of vapor concentration at the droplet surface and in surrounding air as:

\[
\frac{dm_d}{dt} = \frac{2\pi D_v D_p M_s}{N_A} (n_v - n_a) \phi,
\]

where \( D_v \) is the diffusion coefficient of solvent vapor in air and can be define as \( D_v = \frac{1.13 \times 10^{-5} T^{1.5}}{P} \), \( D_p \) is initial droplet diameter in thermal zone, \( N_A \) is Avogadro’s number having value 6.0221413 \times 10^{23} \text{ mol}^{-1} \text{ }, M \) is the molecular weight of fluid, and \( n_v \) and \( n_a \) are the vapor concentrations at the droplet surface and in the surrounding air, respectively.

The vapor concentration can be expressed in terms of partial pressure as \( n_v = \frac{x_v P_f}{R T} \) and \( n_a = \frac{x_a P}{R T} \), where \( x_v \) is the molar fraction of the solvent.

The parameter \( \phi \) in Eq. (8) is the Knudsen correction, which calculates the effect of transport when the size of droplet is of the order of the mean free path of molecules in air (\( \lambda \) nearly 68 nm) [18]:

\[
\phi = \frac{2 \lambda}{D_p + 5.22 \lambda} + 3.42 \lambda.
\]

Therefore, parameters \( D_p \), \( n_s \) and \( n_a \) are depends on the substrate surface temperature \( T \) and thermal zone air pressure \( P_a \).

The pyrolysis of the precursor solution involves physical and chemical processes occur in thermophoretic region. Evaporation, diffusion, and drying are the physical processes, while chemical reaction, nucleation, coagulation, and decomposition are the chemical processes. A chemical reaction for the given titanium trichloride and doubled distill water precursor solution can be:

\[
2\text{TiCl}_3 + \text{H}_2\text{O} \rightarrow \text{TiO}_2 + 4\text{H}_2 + 3\text{Cl}_2.
\]

The decomposition rates of precursors are depends up on the evaporation rate and activation energy of the \( \text{TiO}_2 \). The evaporation rate is also depends up on activation energy [17]. Therefore, the kinetic equation can be represented as

\[
\frac{dx_R}{dt} = Ae^{-E_a/RT} f(x_R).
\]

Here, \( dx_R/dt \) is the reaction rate, \( R \) is molar gas constant (8.3144621 J mol^{-1} K^{-1}), \( x_R \) is the fraction of precursor reacted [\text{TiCl}_3], \( A \) is the pre-exponential factor, \( E_a \) is the activation energy, and \( f(x_R) \) is the function of fraction of precursor reacted for normal grain growth model: \( f(x_R) = (1 - x_R)^n \), where \( n = 1.25 \) [8] is a function of reaction order.

4. Film growth

The films growth depends upon the rate of the arrival of the vapor flux on substrate. When the vapor flux arrival rate is low, the grain diffuses across the substrate slowly without condensation. This results in the growth of a smooth uniform film. While, for high arrival rate, the film growth rate increases due to increase in the cohesive force between the droplet and substrate surface. Such a growth mechanism is known as Liedenfrost aerosol vapor phase deposition. In Liedenfrost aerosol deposition, evaporation of the droplet must occur in thermal zone just above the substrate [19].

The growth of the thin films in spray pyrolysis deposition is followed by vapour deposition and crystal formation. L. Filipovic et al. [6] and R. Ayouchi et al. [20]
TABLE I. Modified spray pyrolysis parts and their specifications.

<table>
<thead>
<tr>
<th>System part</th>
<th>Specifications</th>
<th>Parameter optimizes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air assisted spray nozzle</td>
<td>Made up of glass and consists of the solution tube covered by inserted glass gas tube to pass pressured carrier air/gas.</td>
<td>Droplet size and velocity</td>
</tr>
<tr>
<td>Reactor chamber</td>
<td>Cylindrical chamber of dimension: Cylinder radius = 25 cm Height of cylinder = 60 cm</td>
<td>Atmosphere at the time of deposition (air, different gases)</td>
</tr>
<tr>
<td>Substrate heater</td>
<td>Iron disc of diameter 13.5 cm, thickness 3 cm Heating coil of power 2000 W Maximum temperature of 700 ± 5°C</td>
<td>Substrate temperature, evaporation rate, and film growth on substrate</td>
</tr>
<tr>
<td>PID controller</td>
<td>Make: Devanshi, Model No. VT 4826 SSR rating: 48 V, 65 A Thermocouple: K type I/P: 230 V, 50 A, AC O/P: 30 V or 40 V, 70 A, AC</td>
<td>Substrate temperature</td>
</tr>
<tr>
<td>Peristaltic pump</td>
<td>Model No: PP-10-EX Flow range: 0.1 mL h⁻¹ to 1000 mL h⁻¹ No. of steps: 1400 No. of channels: 1 No. of rollers: 6 Tube size: ID; 1 mm to 4 mm, WT; 1 mm</td>
<td>Solution rate and time of flow</td>
</tr>
<tr>
<td>Air compressor</td>
<td>Model: NS.12 Displacement : 4.2 CFM R.P.M. 650</td>
<td>Carrier air flow control</td>
</tr>
</tbody>
</table>

experimentally show that the film growth rate and crystal formation is directly proportional to spray time and exponentially varies with substrate temperature [6]. Obtained results by them are in good agreement with the Arrhenius expression [21]. According to Arrhenius relation the growth rate is given by

\[ K = \frac{dh}{dt} = A_l e^{-E/K_BT}, \]  \hspace{1cm} (11)

where \( K \) is the rate of reaction, \( A_l \) is the growth rate coefficient (= \( 3.1 \times 10^{-6} \) m s⁻¹), \( T \) is substrate temperature, \( h \) is the thickness of the film, \( t \) is deposition time, and \( K_B \) is the Boltzmann constant (= \( 1.3806 \times 10^{-23} \) m² kg s⁻² K⁻¹). Based on the experimental procedure, the following parameters were used to solve Eq. (11): time \( t = 20 \) min, deposition temperature \( T = 350^\circ C, 400^\circ C, 450^\circ C \), and corresponding activation energy \( E = 0.339 \) eV, 0.326 eV, and 0.313 eV, respectively [22]. The growth rate coefficient \( A_l \) is same for all deposition temperature.

In summary the initial droplet size \( D_i \) is derived from Sauter mean diameter for air blast atomizer, the final droplet diameter \( D_f \) is predicted from the Eq. (7). The thicknesses of the films are predicted from the growth rate Eq. (11). The thickness of the films are depends on the deposition temperature and the concentration of the precursor solution. For spray pyrolysis several dilute precursor solutions are used hence above predicted model can be suitable for both single and mixed oxides.

B. Modified spray pyrolysis system

The schematic diagram of modified spray pyrolysis system is as shown in Fig. 1. The modified spray pyrolysis system consists of air assisted spray nozzle, carrier gas, reaction chamber, PID temperature controller, substrate heater, peristaltic pump etc. their specifications given in Table I.
FIG. 2. XRD pattern of spray pyrolysis deposited TiO$_2$ films (a) for various precursor concentrations and (b) for different deposition temperature annealing at 500°C for 2 h.

FIG. 3. SEM image of the spray deposited TiO$_2$ thin films for different deposition temperature.

III. EXPERIMENTAL METHODOLOGY

A. Deposition of TiO$_2$ thin films to study particle size

The titanium dioxide (TiO$_2$) thin films were deposited onto glass substrate by using spray pyrolysis technique. The concentration of the precursor solution titanium trichloride (TiCl$_3$) varied from 0.075 M to 0.125 M. The substrate temperature was 350°C during deposition. The other optimized parameters kept constant and are as follows:

Solution Flow rate = 1 mL min$^{-1}$

Carrier air flow rate = 7.5 lpm

Gun to substrate distance = 30 cm

The deposited films were annealing at 500°C for 2 h for further oxidization of the films [22].

B. Deposition of TiO$_2$ thin films to study thickness

0.1 M precursor solution of TiCl$_3$ was prepared by dissolving 1 mL of titanium trichloride (TiCl$_3$) in to 77.3 mL of doubled distilled water solution. The prepared precursor solution was sprayed at different substrate temperature 350°C, 400°C, and 450°C. The other optimized parameters kept constant and are as follows:

Solution Flow rate = 1 mL min$^{-1}$

Carrier air flow rate = 7.5 lpm

Gun to substrate distance = 30 cm

The deposited films were annealing at 500°C for 2 h for further oxidization of the films.

The deposited TiO$_2$ thin films were characterized by XRD for the particle size determination and the thickness of the deposited films were estimated from gravito-metric method.

IV. RESULTS AND DISCUSSION

A. Structural properties

The TiO$_2$ thin films were deposited for three precursor solution concentration 0.075 M, 0.1 M, and 0.125 M. The X-ray diffraction data were obtained by means of Philips PM 11730 diffractometer using Cu Kα radiation with a
wavelength, $\lambda = 1.5418$ Å. From XRD micrograph, the anatase crystalline structure of TiO$_2$ is observed for film annealed at temperature 500°C. The crystallite size of TiO$_2$ is calculated using the Scherrer’s equation (Cullity 1956) [23]:

$$D = \frac{0.9\lambda}{\beta \cos \theta}$$  \hspace{1cm} (12)

where $D$ is the average crystallite size, $\lambda = 1.5418$ Å (X-ray wavelength), and $\beta$ the peak FWHM, and $\theta$ the diffraction peak position. X-ray patterns of the deposited films are shown in Fig. 2(a, b). The deposited films are polycrystalline in nature with anatase TiO$_2$ crystalline phase. The anatase TiO$_2$ crystalline planes oriented along (101), (112), (200), (105), (211), (204), (220), (216), etc. The prepared films exhibited tetragonal crystall structure with space group $I4_1/amd$, unit cell parameters $a = 3.7852$ Å, $c = 9.5139$ Å from JCPDS data (#21-1272). With the increase in precursor solution concentration as well as deposition temperature, the peak broadening decreases, this shows increase in crystallinity in the film [24]. The experimentally calculated crystallite size for all samples is shown in Table II.

### B. Microstructural properties

The surface micrographs of pure TiO$_2$ thin films synthesized at different deposition temperature and annealed at 500°C for 2 h in air atmosphere are shown in Fig. 3. The micrographs of all sample shows web like structure with nano- and micropores. The webs are inter linked with each other having variable diameter and the agglomerated particles are surrounded by the web. Density of the web increases with the increase in deposition temperature. The diameters of nano- and micropores was observed to reduce with the increase in deposition temperature. The morphology of the film depends up on substrate temperature and precursor solution.

### C. Film thickness

The thicknesses of the samples are estimated from the weight difference method. The weights of substrate before and after deposition are measured using weighing balance (model No. CAS-44 Sr. No. 1503883). The difference between the weights gives the mass of deposited material. The area of the film is easily estimated and the density of the deposited material is known. By calculating mass,
density, and area of deposition, thickness of the films are estimated by using relation;

\[ t = \frac{\Delta m}{A \rho}, \]  

(13)

where \( \Delta m \) is the change in mass, \( A \) is area of the film, and \( \rho \) is density of the deposited material. The density of the deposited material is 3.890 g m\(^{-3}\) and the deposited area of the samples is \( 2.5 \times 10^{-4} \text{ m}^2 \). These two parameters are almost constant for all samples. The experimentally calculated and theoretically predicted films thicknesses are shown in following Table III.

From the above observation in Tables II and III, and Fig. 4, the crystallite size and thickness of the films measured experimentally and predicted from model are slightly different but their variation with concentration and deposition temperature having similar nature. The difference in the values may be due to the effect of post treatment to the deposited films.

V. CONCLUSION

The pure TiO\(_2\) thin films are successfully deposited using \textit{in-situ} modified spray pyrolysis system, the effect of titanium trichloride precursor solution concentration and different deposition temperature on structural properties of the film is estimated. The XRD study revealed that the deposited TiO\(_2\) thin films have polycrystalline anatase phase with pre-dominant (101) peak. The crystallite size of the film material is found to increase with increase in precursor concentration and deposition temperature. The experimentally calculated crystallite size and thickness are comparable with the predicted values. Thus, the mathematical model developed could potentially apply to estimate particle size and thickness of the different metal oxides and sulfides thin films.

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Appendix: Precursor solution properties

Surface Tension of precursor solution (\( \sigma \)) = 38.9285 dynes cm\(^{-1}\)
Viscosity of precursor solution (\( \eta_p \)) = 0.00084787 dynes s cm\(^{-2}\)
Air viscosity (\( \eta_a \)) = 2.2 \times 10^{-4} \text{ dynes s cm}^{-2}
Nozzle diameter (\( d_n \)) = 0.023 cm
Density of carrier air (\( \rho_a \)) = 0.001181 g cm\(^{-3}\)
Density of precursor solution (\( \rho_l \)) = 0.9735 g cm\(^{-3}\)
Carrier air velocity (\( V_a \)) = 10095.299 cm s\(^{-1}\)
Thermal conductivity of air (\( K_a \)) = 0.025 W m\(^{-1}\) K\(^{-1}\)
Gas constant (\( R \)) = 8.3144621 m N K\(^{-1}\) mol\(^{-1}\)
Mean free path (\( \lambda \)) = 68 nm
Molar fraction of solvent (H\(_2\)O) (\( x_w \)) = 0.9985
Molar fraction of solute (TiCl\(_3\)) (\( x_R \)) = 0.0015
Surrounding air pressure (\( P_a \)) = 1.0 atm
Saturation vapor pressure (\( P_g \)) = 0.023094 atm
Diffusion coefficient of solvent vapor (\( D_a \)) = 8.68 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}
Molecular weight of water (\( M \)) = 18 g mol\(^{-1}\)
Boltzmann constant (\( K_B \)) = 1.38 \times 10^{-16} \text{ erg K}^{-1}
Molar concentration of Ti in the vapor phase (\( C_A \)) = 0.0023672 M
Molar concentration of Ti in the liquid phase (\( C_p \)) = 0.075 M, 0.1 M, 0.125 M
Binary diffusivity of vapor Ti in gas O\(_2\) (\( D_{AB} \)) = 2.4 \times 10^{-2} \text{ cm}^2 \text{ s}^{-1}