

A Numerical Solution for the Coverage-Dependent Surface Diffusion equation in ultra-thin film

Kadhim R. Khalaf and Fatima. H. Saeed

Department of Physics , College of Education for pure sciences, University of Basrah / Basrah-Iraq

Abstract

The ultra-thin film is nanoscale layers of material that play an important role in functionalizing surfaces to building devices. This theoretical study deal with systems of metal growth on weakly interacting substrates. The adatoms particles assemble into dispersed islands and grow in size until they affect each other and eventually form a continuous layer that covers the whole substrate surface. The surface diffusion of an adatom occurs in a certain time interval, as a film grows, between its adsorption and its final position of the film. In most deposition models, the subsurface and bulk diffusion features are neglected so that the film morphology is only determined by the surface dimension. And to simplify our mathematical treatment, we are going to assume that, the surface diffusion of adatoms is homogenous in both dimensions. So, the surface diffusion equation will be solved in one dimension. The coverage diffusion coefficient includes the effect of adsorbate lateral interactions. To demonstrate this, Fick's second law equation was numerically solved using different forms of coverage-dependent surface diffusion coefficient. The surface diffusion of Potassium on rubidium K/Ru(011) has been studied as an example for coverages up to one monolayer. The coverage dependence of the diffusion coefficient is determined by analysis of the concentration profiles by using (MOL) finite difference numerical method. The coverage profiles and time of coverage depend on the diffusion coefficient formula.

Keywords: Ultra-thin film growth, Coverage dependent diffusion coefficient, Fick's second law equation, (MOL) finite difference method

Date of Submission: 08-01-2022

Date of Acceptance: 22-01-2022

I. Introduction

Reducing the dimensions of the material and making it Within the nano-range leads to changes in the properties of the material because quantum phenomena will prevail at these small measurements[1]. For technological purposes and for the production of nanometer electronic devices that make surfaces such as films, their depth is (10-100 nm). The high layer of surface atoms that are near to or falling on the surface can be considered the surface ,where it can be said that (2-10) of the layers of atoms or recent particles can be considered the surface which is within the borders of (0.5-3 nm) [2]. The diffusion of particles on solid surfaces is a complex subject as it needs to understand the many fundamental interactions that occur between particles and the surface[3] . Because of the significant technological development in the field of surface diffusion , practical research on the diffusion of an adatom on metal surfaces and the composition of a single layer of the ultra-thin film is involved in the installation of nanoelectronics devices [4]. dominator the amount of adatom to the surface of the material at certain temperatures has allowed the production of an ultra-thin film that leads to precise devices. That more thin membranes are nanolayers of materials used to functionalize surfaces or to act as building blocks in more complex devices ,in recent years ,thin metal films have become vital within modern devices ,for example, nanoelectronics [5]. The process of building an ultra-thin film layer of metal on a surface of another metal contributes to protecting tools from corrosion and storing information in hard drives ,or to integrating them with other components to build light-emitting diodes (LED) transistors ,solar cells, and batteries, as well as integrating 2D materials into integrated circuits ,and this contributes to the launch of a new generation of nanoelectronics devices, along with futuristic technologies such as quantum computers[1,5] The importance of lateral interactions between adatom in surface diffusion will be discussed through coverage-dependent diffusion coefficient as surface initial coverage and coverage values at different times provide information on the type of interactions between adsorbates on the surface whether they are attractive or repulsive interactions[6]. A coverage-dependent diffusion coefficient is an effective tool for measuring surface diffusion in general and the effect of adsorbates reactions on prevalence in particular[7]. Our theoretical study is focused on building a theoretical model after solving the coverage-dependent diffusion equation and using numerical methods in the solution and then applying it in a theoretical simulation of ultra-thin film used in nanoelectronics ,we will use the one-dimensional Second Fick's diffusion equation where the diffusion coefficient is coverage-dependent .Then we solve the second Fick's diffusion equation in one dimension with

numerically cartesian coordinates to coverage using finite differences and lines method (MOL) to calculate the appropriate coverage of each distance of (x) values for one layer in one dimension, with a note the role of lateral interactions between adatom except attraction or repulsive as well as the lack of interaction between atoms, we take the form of distributing adatom in the primary case when they take the form of gaussian and observe the change in the shape of coverage as time progresses until reaching a coverage equally surface with one layer where this process is performed at a constant temperature and at different times

Adatom Diffusion

Particles that reach or near the surface not only interact with each other but also interact with the surface, so the reaction barrier between particles (atoms or molecules) and the surface changes [8]. In light of this, the mechanical which through it the surface to change the reaction barrier is not easy because the surface will not be merely a level space with two dimensions. The basic units of surface construction such as atoms or particles do not spread continuously on it because the surface has some crease (Corrugation) and this depends on the nature of the direction and composition of the surface grid, and in any case, the real surfaces contain different types of surface compositions such as islands and Steps as well as defects [9,10]. Surface Conditions that enhance interaction depend on particles and surface [11]. Surface diffusion studies can reveal the exact details of interactions between conjoined particles. Surface diffusion measurements when covering low provide information about the possibilities of conjoined surface, while measurements at high coverage can investigate the potential of basic conjoiners. Studies of thermal absorption caused by lasers have found that the surface spread based on coverage of a particular metal surface is due to interactions between the nearest neighbor except those interactions were repulsive or attraction between the conjoined on the surface and this depends on the nature of the conjoined material and the atoms of the substrate. It was found that the surface diffusion of carbon dioxide, CO_2 on Ru (001) is due to the interactions of the nearest repulsion neighbor in the layer, CO_2 . Similar (LITD) measurements found that the diffusion of both Xe and Kr on the surface of Pt (111) is due to attractive interactions between adsorbates on the surface [12]. Figure 1 shows the direct interaction between the adatom to the surface.

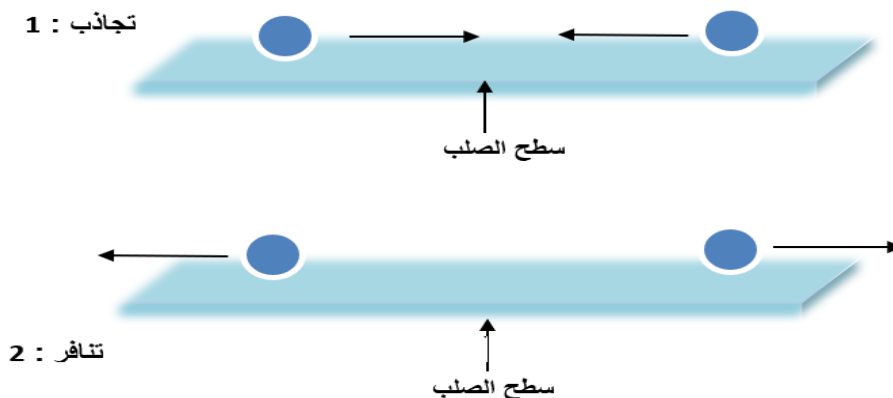


Figure .(1) The types of interactions between adatom [2].

Surface Diffusion of adatoms.

In surface science, surface diffusion is one of the most widely studied processes in nanotechnology and further study is still needed to understand the processes that occur for each system [7]. For atoms diffuse on a particular surface, the atomic density of these atoms covering the surface can be linked to $\theta(x, t)$ per unit of space and time unit with mass flow rate, $\bar{j}(x, t)$ through the continuity equation without a source of atom generation on the surface,

$$\frac{\partial \theta(x, t)}{\partial t} = -\bar{\nabla} \cdot \bar{j}(x, t) \quad (1)$$

It can be replaced $\bar{j}(x, t)$ (in equation (1)) using Fick's first law of deployment.

$$\bar{j}(x, t) = -D(\theta(x, t))\bar{\nabla}\theta(x, t) \quad (2)$$

Where $D(\theta(x, t))$ Represents a constant proportionality between the mass flow rate $\bar{j}(x, t)$, The steep in the concentration of adatom. $\bar{\nabla}\theta(x, t)$ is called diffusion coefficient, so the diffusion equation for this condition is given in relation,

$$\frac{\partial \theta(x, t)}{\partial t} = \bar{\nabla} \cdot [D(\theta(x, t))\bar{\nabla}\theta(x, t)] \quad (3)$$

This partial differential equation describes the total behavior of adatom on the surface resulting from the random movement of each atom ,and after this equation is resolved we obtain the topical density of the moving atoms [13].

In this paper ,it will be treated (the spread of fixed surface concentration) where the surface is covered with a certain type of adatom as in the following form (2), As we know ,surface diffusion is a many-body phenomenon [14].

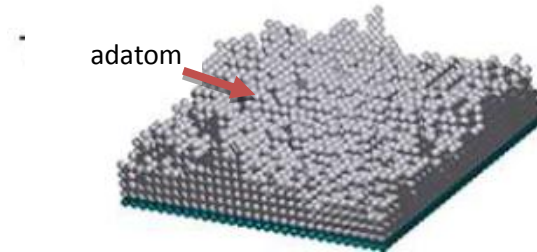


Figure (2) : shows a surface covered with a certain type of adatom.

These adatoms on the surface will afflict from diffusion as time progresses until they reach the final redistribution coverage of adatom to the surface from the most concentrated to the least concentrated area , which is affected by lateral interactions between them or between them and substrate atoms .Which implicitly occurs in the definition of a coverage-dependent diffusion coefficient equation.

Using Fick's equation at a constant total concentration (3) that takes the following shape in two dimensions[7].

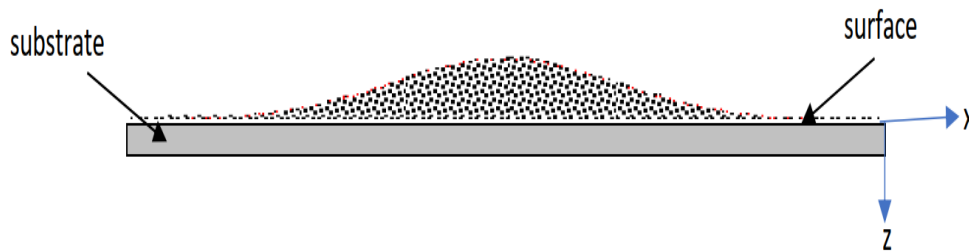


Figure (3): represents diffusion adatom on a surface towards the surface and depth [7].

$$\frac{\partial \theta(x,z,t)}{\partial t} = \frac{\partial}{\partial t} \left[D_s(\theta(x,z,t)) \frac{\partial \theta(x,z,t)}{\partial x} \right] + D_z \frac{\partial^2 \theta(x,z,t)}{\partial z^2} \quad (4)$$

D_s Surface diffusion coefficient, D_z Diffusion factor towards depth z . Although

$D_s(\theta(x,z,t)) \gg D_z$ for every $t \geq 0$ In other words ,there is no diffusion towards depth z .The equation of diffusion in one dimension becomes as follows

$$\frac{\partial \theta(x,t)}{\partial t} = \frac{\partial}{\partial x} \left[D(\theta(x,t)) \frac{\partial \theta(x,t)}{\partial x} \right] \quad (5)$$

This equation can only be solved after knowing the formula of $D(\theta)$, which is determined by the nature of the interaction between neighboring adsorbed according to certain circumstances or using the results of practical experiments ,as well as determining the boundary and initial conditions for it. In general ,this equation is difficult to solve by the analytical method ,so we will resort to numerical methods and finite differences to solve it and we will use the method of lines (MOL) where we avoid the convergence conditions required by other methods.

The Numerical Solution for Nonlinear Diffusion equation

When looking at equation ,(3) we note that it represents a nonlinear partial differential equation ,because the Diffusion coefficient is coverage-dependent $D(\theta)$. But if the diffusion coefficient does not depend ,it becomes a linear partial differential equation that can be solved by analytical methods Ref,[15]. many numerical methods have been used to solve such equations and study them on a large scale as numerical methods of solving non-linear problems are still a very important tool in investigating many non-linear phenomena [16] ,Some of them are mothed [17-20] .

Assuming $D(\theta(x,t)) = D(\theta)$ and we performing the differentiation on the right-hand side of (5) we get

$$\frac{\partial \theta(x,t)}{\partial t} = \frac{\partial D(\theta)}{\partial \theta} \left(\frac{\partial \theta}{\partial x} \right)^2 + D(\theta) \frac{\partial^2 \theta}{\partial x^2} \quad (6)$$

Equation (6) will be solved for the spatial interval $[a,b]$ which is the dimensions of the length of the surface of the thin film ,and under the following boundary conditions:

$$\theta(a, t) = \alpha(t), \quad \theta(b, t) = \beta(t), \quad t > 0 \tag{7}$$

Which give the Coverage at both ends of the surface as functions of time, and the initial condition is :

$$\theta(x, 0) = \theta_0(x), \quad x \in [a, b] \tag{8}$$

This determines the concentration distribution of adatom along with the spatial interval at the beginning of the diffusion.

We will use an important and widely numerical method subject to the boundary conditions (7) and the initial condition (8) which is the method of lines (MOL). one of the finite difference methods used to solve partial differential equations only numerically nonlinearly. Originally introduced in 1956 by Liskovetz for partial differential equations of the elliptical type and parabolic and hyperbolic pieces.[16]. Since then ,this method has been applied in many different cases and is still actively used to this day[21,22,23].

Method (MOL) first segments the equation (6) in space form ,(4) resulting in an initial value issue for a system consisting of standard grade ODEs.

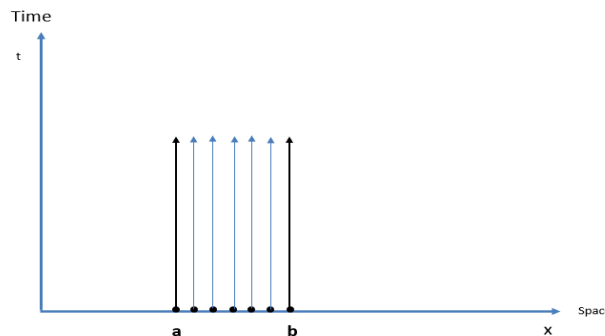


Figure (4) :Site segmentation , θ values are given along black lines and represent (BCS) and at black dots are given (IC) initial conditions. And we have to find the values of θ along the lines of Blue.

The issue of initial values is resolved using some approximate numerical methods .When using the explicit Euler method and when D is a constant quantity ,the stability requirement of the method when $0 < \frac{D\Delta t}{(\Delta x)^2} < \frac{1}{2}$, where D is the diffusion coefficient, Δx is the amount of change in length, and Δt is the amount of change in time.

Instead of segmenting the equation (6) for the site ,we will break it down for time first as in figure (5) and timeline $t \geq 0$ divided into a period of equal size by the mesh-points

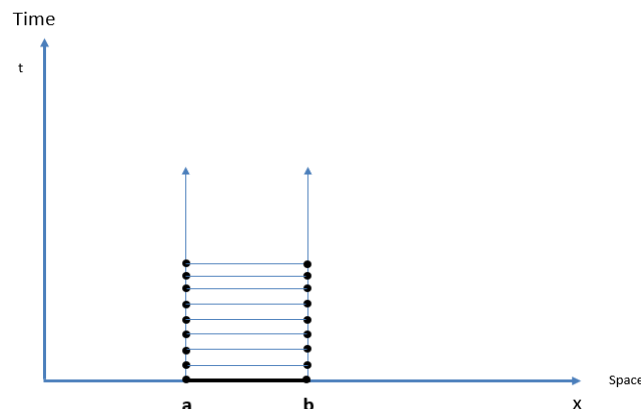


Figure (5) :represents the fragmentation of time. given θ values along the black line and represents the initial conditions (IC) and at black points are given the boundary conditions (BCs) . And we have to find the values of θ over the blue lines.

The equation by which time is calculated at each point is given as follows:

$$t_n = n\Delta t, \quad n = 0,1,2 \tag{9}$$

Where Δt represents the size of the network period, the equation (6) is distributed on a mesh (9) using an implicit time derivative approximation chart:

$$\frac{\theta_n - \theta_{n-1}}{\Delta t} = \partial_\theta D(\theta_n) \left(\frac{d\theta_n}{dx}\right)^2 + D(\theta_n) \frac{d^2\theta_n}{dx^2} \tag{10}$$

Where: $\theta_{n-1} = \theta_{n-1}(x)$, $\theta_n = \theta_n(x)$ Approximation of the values of both $\theta(x, t_{n-1})$, $\theta(x, t_n)$ respectively. Equation (6) is a second-order ordinary differential equation.

equation (10) can be written in the form,

$$\frac{d^2\theta_n}{dx^2} = f(\theta_n, v_n; \theta_{n-1}), \tag{11}$$

Where $v_n = \frac{d\theta_n}{dx}$, represents coverage gradient and f is a function that is nonlinear that we can express as follows,

$$f(\theta_n, v_n; \theta_{n-1}) = \frac{\phi(\theta_n, v_n; \theta_{n-1})}{D(\theta_n)}, \tag{12}$$

$$\phi_n(\theta_n, v_n; \theta_{n-1}) = \frac{\theta_n - \theta_{n-1}}{\Delta t} - \partial_\theta D(\theta_n) v_n^2 \tag{13}$$

Equation (11) and boundary conditions $\theta_n(a) = \alpha(t_n)$, $\theta_n(b) = \beta(t_n)$, The definition of the issue of the two-point convoluted boundary value (TPBVP) of an unknown function is θ_n , So if the function, θ_{n-1} .Known to the researcher, the problem can be resolved using numerical analysis techniques.

To solve the equation (11) numerically, we start from the initial distribution of adatom, θ_0 By applying the boundary conditions, we get the distribution of coverage for adatom, θ_n at time, t_n . Where $n=1, 2, 3, \dots$, We will use the finite Differences Method (FDM) with Newton's method of solution. Newton or Newton-Ravson's method is reliable and rapidly repetitive and quadratic[24].

Implementing Newton's method requires finding partial derivatives of the function.

$f(\theta_n, v_n; \theta_{n-1})$. For, θ_n, v_n , so we're going to adopt some shortcuts and symbols to simplify the explanation of the method:

$$f_n = f(\theta_n, v_n; \theta_{n-1}), \quad \phi_n = \phi(\theta_n, v_n; \theta_{n-1}).$$

And to denote partial derivatives f_n by:

$$q_n = q(\theta_n, v_n; \theta_{n-1}), \quad p_n = p(\theta_n, v_n). \text{ We get:}$$

$$q_n = \frac{\partial f_n}{\partial \theta_n} = \frac{1}{D(\theta_n)} \left(-f_n \frac{\partial D(\theta_n)}{\partial \theta_n} + \frac{\partial \phi_n}{\partial \theta_n} \right) \tag{14}$$

$$p_n = \frac{\partial f_n}{\partial v_n} = \frac{1}{D(\theta_n)} \frac{\partial \phi_n}{\partial v_n} \tag{15}$$

where:

$$\frac{\partial \phi_n}{\partial \theta_n} = \frac{1}{\Delta t} - \frac{\partial^2 D(\theta_n)}{\partial \theta^2} \cdot v_n^2 \tag{16}$$

$$\frac{\partial \phi_n}{\partial v_n} = -2 \frac{\partial D(\theta_n)}{\partial \theta} \cdot v_n \tag{17}$$

These equations will be useful when calculating matrix inverse elements of Newton's finite difference method [16].

Applying the finite difference method.

The method is chosen to solve the equation (11) and taking into account the application of boundary conditions, $\theta_n(a) = \alpha(t_n)$, $\theta_n(b) = \beta(t_n)$ Which we've expressed as functions of time at points (a, b) [25]. The application of the finite difference method includes dividing the interval [a, b] into N of mesh-points and equally, where

$$1, \dots, N; \quad \Delta x = \frac{b-a}{N-1} \tag{18}$$

The equation (18) determines a regular network over the time interval [a,b]. The equation (11) on the grid can be segmented in to equation (18) using the finite difference method (FDM) with the central difference of the second derivative approximation which takes the following formula:

$$\frac{\theta_{n,i+1} - 2\theta_{n,i} + \theta_{n,i-1}}{\Delta x^2} = \frac{1}{D(\theta_n)} \left[\frac{\theta_{n,i} - \theta_{n-1,i}}{\Delta t} \right] \frac{\partial_\theta D(\theta_{n,i})}{D(\theta_{n,i})} v_{n,i}^2 \quad i = 2,3, \dots, N-1 \tag{19}$$

Where ($v_{n,i}$) expressed as follows:

$$v_{n,i} = \frac{\theta_{n,i+1} - \theta_{n,i-1}}{2\Delta x} \tag{20}$$

That's valuable. $\theta_{n-1,i}$, $v_{n,i}$, $\theta_{n,i}$ In equations (19) and (20) it refers to the exact values of bringing both $\theta_{n-1}(x_i)$, $v_n(x_i)$, $\theta_n(x_i)$ respectively. And then we put $x = x_i$ everywhere in the equations of (12-17) and then we replace the exact values at grid points with each of their almost $\theta_{n-1,i}$, $v_{n,i}$, $\theta_{n,i}$ The equation (19) applies to inner mesh-points. At the boundaries, the necessary boundary conditions must be applied:

$$\theta_{n,i} = \alpha(t_n), \quad \theta_{n,N} = \beta(t_n) \tag{21}$$

Solving the nonlinear system by Newton method.

Equation (19) together with the boundary conditions equation (21) forms a nonlinear system of N from algebraic equations to N of unknown functions $(\theta_{n,i}, i = 1, 2, \dots, N)$. To solve this nonlinear system, we will apply Newton's repetition method. And insert a vector - column, G_n . Who writes in the form following:

$$G_n = [G_{n,1}, G_{n,2}, \dots, G_{n,N}]^T \tag{22}$$

Where:

$$G_{n,1} = \theta_{n,1} - \alpha(t_n), \quad G_{n,N} = \theta_{n,N} - \beta(t_n), \tag{23}$$

In light of this, the matrix, $G_{n,i}$. Be as follows:

$$G_{n,i} = \theta_{n,i+1} - 2\theta_{n,i} + \theta_{n,i-1} - \Delta x^2 f_{n,i} \tag{24}$$

Note that the function, $f_{n,i}$. is expressed as follows

$$f_{n,i} = f(\theta_{n,i}, v_{n,i}; \theta_{n-1,i}), \quad i = 2, 3, \dots, N - 1, \tag{25}$$

The equation (18) and the boundary conditions equation (20) can be written as one equation:

$$G_n(\theta_n) = 0 \tag{26}$$

Where:

$$\theta_n = [\theta_{n,1}, \theta_{n,2}, \dots, \theta_{n,N}]^T \tag{27}$$

Newton's repetition of the equation system (26) is:

$$\theta_n^{(k+1)} = \theta_n^{(k)} - (L_n^{(k)})^{(-1)} G_n(\theta_n^{(k)}), \quad k = 0, 1, 2, \dots \tag{28}$$

Where, $L_n^{(k)}$. It's a matrix inverse, G_n . For θ_n evaluated At, $\theta_n^{(k)}$. Inverse Matrix, G_n . Be as follows :

$$L_n^{(k)} = \frac{\partial G_n}{\partial \theta_n}(\theta_n^{(k)}) \tag{29}$$

So the inverse elements of the matrix, $L_n^{(k)}$. Equal:

$$L_{n(1,1)}^{(k)} = 1, \quad L_{n(N,N)}^{(k)} = 1 \tag{30}$$

In light of this, the inverse elements of Newton's repetition matrix will take the following form:

$$\left. \begin{aligned} L_{n(i,i-1)}^{(k)} &= 1 + \frac{1}{2} \Delta x p_{n,i}^{(k)}, \\ L_{n(i,i)}^{(k)} &= -2\Delta x^2 q_{n,i}^{(k)}, \\ L_{n(i,i+1)}^{(k)} &= 1 - \frac{1}{2} \Delta x p_{n,i}^{(k)}, \end{aligned} \right\} \tag{31}$$

Newton's repetition of $p_{n,i}^{(k)}$ & $q_{n,i}^{(k)}$ Given as follows:

$$q_{n,i}^{(k)} = q(\theta_{n,i}^{(k)}, v_{n,i}^{(k)}; \theta_{n-1,i}), \quad p_{n,i}^{(k)} = p(\theta_{n,i}^{(k)}, v_{n,i}^{(k)}), \quad i = 2, 3, \dots, N - 1 \tag{32}$$

The arrays described in equation (31) were resolved by the MATLAB program.

Coverage-dependent surface diffusion coefficient model.

Diffusion processes are some of them fast and others are slow, depending on the form of the diffusion coefficient function, which plays an important role in a wide range of applications and takes several forms of functions, such as the force law, $D = u^m$, $m = 1, 2$, and the exponential forms that have been used at the center of our study [26]. In general, we have used the basic form of coverage-dependent diffusion coefficient to explain the role of lateral interactions in the diffusion process, which show their effect on activation energy, E_{diff} . Activation energy, which is implicitly included in the diffusion coefficient, requires theoretical software to calculate it and is difficult to provide, in which case it has been provided by the research literature. They appear in the coverage-dependent diffusion coefficient that takes the following general form:

$$D(\theta) = D_0 \exp\left(-\frac{E_{diff}}{KT}\right) \tag{33}$$

Where $D(\theta)$ Is the coverage-dependent diffusion coefficient, D_0 It is a pre-exponential factor, E_{diff} . The activation energy, K constant Boltzmann, T , temperature [6,7]. The diffusion coefficient used to explain the diffusion adsorbates and the role of lateral interactions in this process are known as follows :

$$D(\theta) = A \exp B \theta^{3/2} \tag{34}$$

Where (θ) , Coverage, B is the force of interaction between adatom, A is a pre-exponential factor and has different values depending on the nature of the interaction between adatoms, B values are zero in the absence of an interaction between adatom and are negative for the state of attractive interaction and positive when the force of interaction between adatom is repulsive. Each case has a clear effect on the distribution of the density of adatom as time progresses [7].

Dipole-Dipole interaction model.

The coverage-dependent diffusion coefficient model is designed in this case on the assumption that activation energy for diffusion is determined by relying on the following equation :

$$E_{diff} = E_0 - \beta\theta^{3/2} \tag{35}$$

Where E_{diff} is the activation energy and E_0 the activation energy in the absence of adatom and β is the energy of interaction between neighbors adatom, adatoms, and surface, and θ is coverage .where the dependence on, $\theta^{3/2}$ originates from the first term of dipole-dipole interaction expression. varies as a ratio of r^{-3} , r is the distance between neighboring adsorbates. In two dimensions, for mobile adsorbates at homogeneous lateral distribution, the average distance between adsorbates is proportional $1/\theta^{1/2}$ therefore the coverage dependence of the interaction is proportional to $\theta^{3/2}$ [6,7]. This description is correct for dissonance when a particle spreads on the surface [27] .The effect of removing polarization in high coverage and strong interactions is neglected . [6]

The general form of the coverage-dependent diffusion coefficient is defined by equation (34) and after compensating the equation (35) in equation (33) we get:

$$D(\theta) = D_0 \exp\left(-\frac{E_0}{KT}\right) \exp\left(\frac{\beta\theta^{3/2}}{KT}\right) \tag{36}$$

After assuming that $B = \frac{\beta}{K_B T}$ and $A = D_0 \exp\left(-\frac{E_0}{KT}\right)$ We will obtain the model used for the coverage-dependent diffusion coefficient described in equation (34) and it should be emphasized that the B reaction factor is shown in the numbers referred to in the text ,as well as the pre-Exponential A coefficient ,depending on surface temperature as this method is valid for a wide range of different models of coverage-dependent diffusion coefficient .The activation energy that implicitly enters in the diffusion coefficient as described in equation (35) requires theoretical software to calculate it and is difficult to provide, in which case it is provided by the research literature .The temperature is constant for all cases T=175 K obtained from research sources, B is the force of interaction between adatom and ranges in value from(0-01) [6]. The coverage-dependent diffusion coefficient changes with the change in coverage ,as it varies in the state of repulsion and attractive interaction between adatom, but in the absence of an interaction, it remains constant, relying only on the pre-exponential factor A only ,which is clearly from the equation(34). This will be explained to different values of the strength of the interaction and in all cases the interactions of attraction or dissonance or non-interaction between adatom. Figure (6): shows the coverage-dependent surface diffusion coefficient as a function of surface coverage when there is no interaction between adatom where B=0. As figure (7) shows, the change in the surface diffusion coefficient is dependent on coverage as a function of the surface coverage of the attractive interaction state where B=-10. Figure (8) represents the coverage-dependent surface diffusion coefficient form as a coverage function for repulsive interaction between adatom.

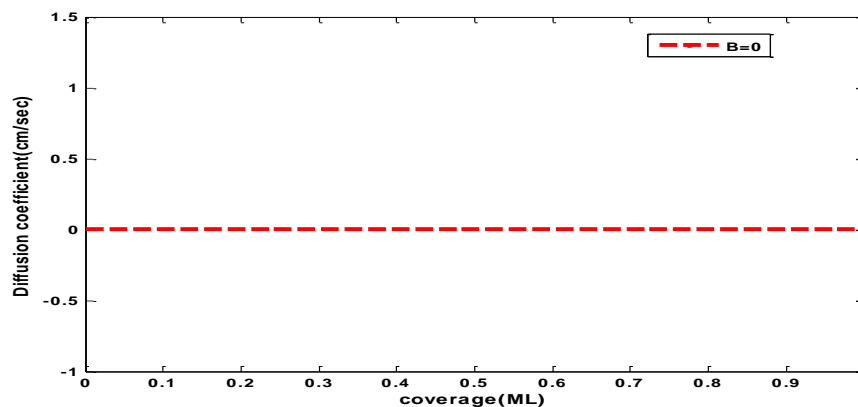
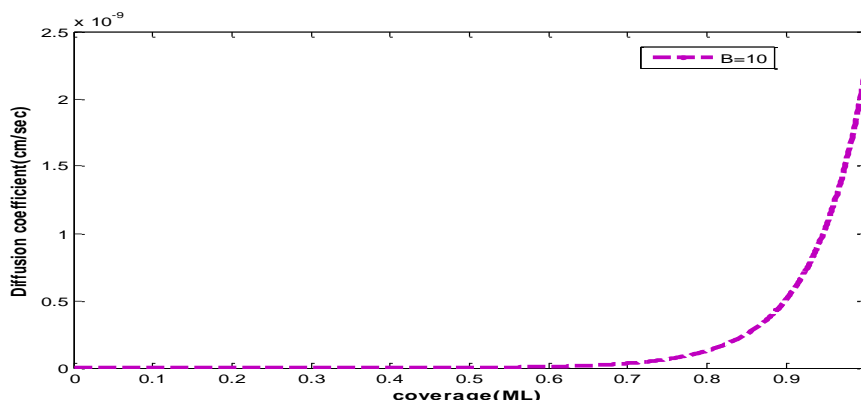


Figure (6) :shows the shape of the surface diffusion coefficient as a coverage function where B=0



Figure(7): represents the surface diffusion coefficient as a coverage function where B=10

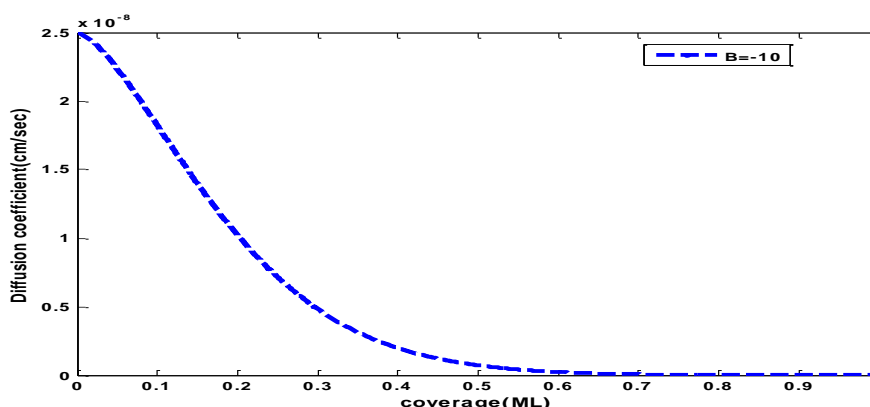


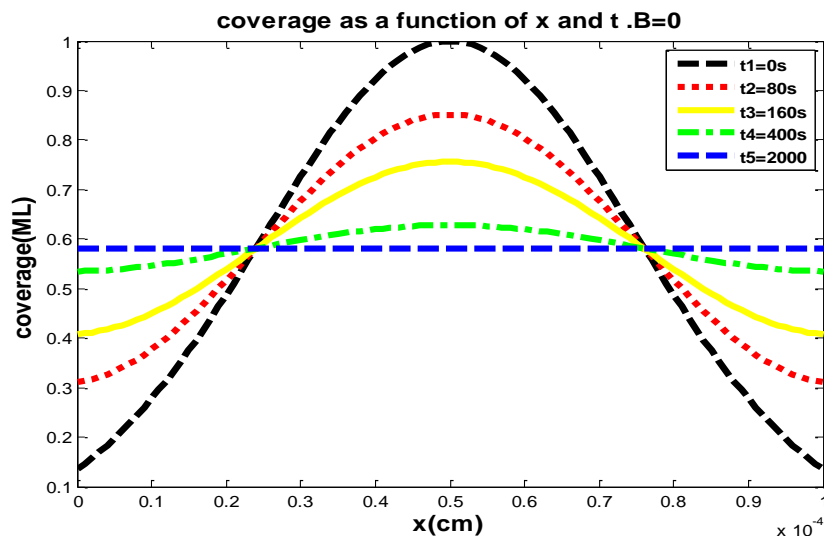
Figure (8) Changes the surface diffusion coefficient as a cover function B =-10

II. Results and discussion

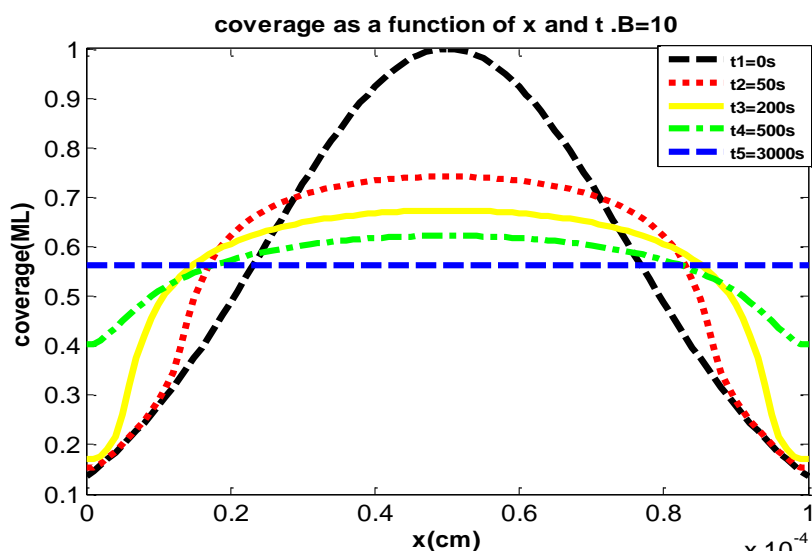
After using the numerical method by which the partial non-linear differential equation represented by the equation (3) was solved over the specified spatial interval $x \in [a,b]$. Using different values of B, boundary conditions (7) initial conditions (8) and using two different forms of the surface-bound atom density distribution function, which is the gaussian and flat gaussian shape were obtained a theoretical model of coverage-dependent diffusion in one dimension in the direction of (x) and to obtain a layer ultra-thin film used within nanoelectronics after obtaining the parameters of the equation from research sources that represent the practical application of diffusion such as Potassium on rubidium K/Ru(011) as shown in the drawings below.

We conclude from this model used that is suitable for different systems where the necessary information is available with the conjoined and surface, and different values can be used for the force of interaction B, as we have used the power of interaction B=(10,-10) to provide it in research sources.

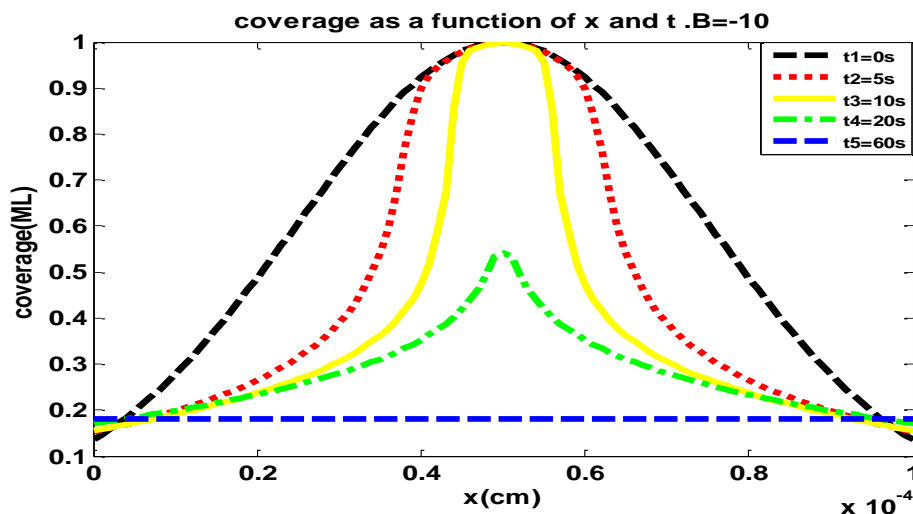
The form of the primary distribution function of the density of atoms attached to the surface is related to the width of the sample and can take the form of caustic distribution and Carve Fitting has adapted the practical results from the source [6]. The shape of the density of atoms conjoined at the initial conditions where $t = 0$ is indicated in the shapes represented by the black dotted line.



Figure(9): represents the density of the distribution of adatom for the system in case no interaction at $B=0$



Figure(10): diffusion of adatom for the distance of a system In the case repulsive interaction between adatom where $B=10$.



Figure(11): represented diffusion of adatom for the system in the case attractive interaction between adatom at $B=-10$.

Figure (9) shows the state of diffusion adatom on the surface as time progresses, as the shape represents the spread of conjoined atoms on a surface at a certain temperature and the absence of interaction between adatom at different times $t=0, 80, 160, 400, 2000$ s, and the pre-exponential factor used for this state was $A = 1.2 \times 10^{-10}$, and The strength of interaction between conjoined atoms $B=0$ [6]. The form of coverage of atoms attached to the surface with the interaction of repulsion between adsorbates when the value of the strength of the reaction is $B=10$ and has a temperature of 175k and different times $t=0, 50, 200, 500, 3000$ s when the pre-exponential factor for this state is equal to $A=1 \times 10^{-13}$. The density of the distribution of conjoined atoms on the surface can be expressed in form (10). The form of coverage adatom on the surface when there is an interaction between atoms of the type of attraction takes a more dramatic form than the absence of interaction between atoms as well as the state of the interaction of dissonance as described in the form (11) which represents the spread of conjoined by the presence of the force of attraction between them where $B=-10$ at the same temperature as the previous two cases and at different time $t=0, 5, 10, 20, 60$ s where the pre-exponential factor for the state of attraction interaction $A=2.5 \times 10^{-8}$.

References

- [1]. M. H. AL-Musaoui, **Theoretical study of Ion-diffusion in Heterostructure**, University of Basrah, Iraq, (2020).
- [2]. Qasim S. K. Al – Shook, **Effect of an Adsorbed Atom on Resonant Charge Exchange in Atom Scattering off Solid Surface**, The College of Education – University of Basrah in Iraq, (2010).
- [3]. Musa Kadhim. S. **Theoretical Study in the Molecular Chemisorption for Diatomic Molecule on Transition Metal Surfaces**, The College of Education-University of Basrah, Iraq, (2006).
- [4]. Hisham Yousif Al-Mhdi, Dr. J.M. Al-Mukh, **The Chemisorption of Cobalt atom on Noble Metal Surfaces: Konda Effect**, University of Basrah, Iraq, (2008).
- [5]. Gervilla Palomar, Víctor. **Metal film growth on weakly-interacting substrates: Multiscale modeling**. Diss. Linköping University Electronic Press, (2020).
- [6]. Verhoef, R.W, and M. Asscher. **Diffusion on surfaces using laser diffraction :effect of adsorbate lateral interactions**. surface science, (1997).
- [7]. Fatima Al-Saeed. Shaker I. Easa. Jenan M. Al-Mukh. **Theoretical study in Doping process: Ion implantation and Diffusion**, University of Basrah, Iraq, (2005).
- [8]. Kroger, J. et al. **Surface state electron dynamics of clean and adsorbate-covered metal surfaces studied with the scanning tunnelling microscope**. Progress in Surface Science 80.1-2 (2005): 26-48.
- [9]. Borisov, A. G., et al. **Atoms interacting with a metal surface with adsorbates: local and non-local effects on the charge transfer**. Surface science 350.1-3 (1996): 26-48.
- [10]. H. Lu-bing, D. Hui-qui and H. Wang-Yu. **Transcations of Nonfunous Metals**, Society of China, (2006).
- [11]. B. S. Patricia L Ynn Maazouz, **Reaction Dynamics and Charge Transfer in the Scattering of state- Selected Ions on surface**, Ph. D. Thesis University of Notre Dame, Indiana, (2004).
- [12]. Westre, E.D, Brown, D.E, Kutzner, J.& George, S.M, **Surface diffusion of potassium on Ru(110)**, Surface Science, (1993).
- [13]. Yu. B. Gaididei, V.M. Loktev, A.G. Naumovets, A.G. Zagorodny, **Adatom interaction effects in surface diffusion**, Bogolyubov Institute for Theoretical physics of the National Academy of Sciences of Ukraine, (2012).
- [14]. Naumovets, A.G. **Collective Surface diffusion: An experimentalists View**. Physica A:Statistical Mechanics and its Applications, 357-2, (2005).
- [15]. Mohammad. H. Khalaf, Fatima. H. Saeed. **Theoretical Study of Dopant impurities Diffusion in Multi-quantum Well Heterostructure**. Journal of Basrah Researches ((Sciences)) Vol. (46). No.2 (2020).
- [16]. Farago. Istvan, et al. **A numerical approach to solving unsteady one-Dimensional nonlinear Diffusion equations**, (2020).
- [17]. Liskovets, Oleg Anisimovich. **The method of straight lines**. Differentsial'nye Uravneniya 1.12 (1965): 1662-1678.
- [18]. Zafarullah, A. "Application of the method of lines to parabolic partial differential equations with error estimates." Journal of the ACM (JACM) 17.2 (1970): 294-302.
- [19]. Thomée, Vidar. **Galerkin finite element methods for parabolic problems**. Vol. 25. Springer Science & Business Media, 2007.
- [20]. Larson, Mats G., and Fredrik Bengzon. **The finite element method: theory, implementation, and applications**. Vol. 10. Springer Science & Business Media, 2013.
- [21]. Zafarullah, A., **Application of the Method of Lines to Parabolic Partial Differential Equations With Error Estimates**, Journal of the ACM 17, 2, 294–302, (1970).
- [22]. Schiesser, W., **The Numerical Method of Lines, Integration of Partial Differential Equations**, 1991. <https://www.elsevier.com/books/the-numerical-method-of-lines/schiesser/978-0-12-624130-3>
- [23]. Ramos, J., A conservative, **piecewise-analytical, transversal method of lines for reaction-diffusion equations**, International Journal of Numerical Methods for Heat & Fluid Flow 29, 4093–4129 (2019).
- [24]. Filipov, S. M., Gospodinov, I. D. and Farag' o, I., **Replacing the finite difference methods for nonlinear two-point boundary value problems by successive application of the linear shooting method**, Journal of Computational and Applied Mathematics 358, 46–60 (2019).
- [25]. Filipov, S. M., Gospodinov, I. D. and Farag' o, I., **Shooting–projection method for two–point boundary value problems**, Applied Mathematics Letters 72, 10–15 (2017).
- [26]. Filipov, S. M., Gospodinov, I. D. and Farag' o, I., **Shooting–projection method for two–point boundary value problems**, Applied Mathematics Letters 72, 10–15 (2017).
- [27]. Farbman, I., M. Asscher, and A. Ben-Shaul. **Effects of adsorbate lateral repulsion on desorption and diffusion kinetics studied by Monte Carlo simulations**. The Journal of chemical physics 104.14 (1996): 5674-5682.