A Computer Algebra Algorithm for the Symbolic Solution of a Problem involving the diffusion of adatoms on a Circular Wafer when sculpting a Nanopore with an Ion Beam.

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Abstract - Using computer algebra software we obtain the basic diffusion rate corresponding to the concentration of surface adatoms inside a circular nanopore. The method used is the Laplace Transform Technique and calculus of residues. This method can be extended to other more complex problems if considered annihilation at defect and adatom creation by ion impingement effects. This application indicates that computer algebra software for symbolic computation has a very promissory future in mathematical nanotechnology modeling.

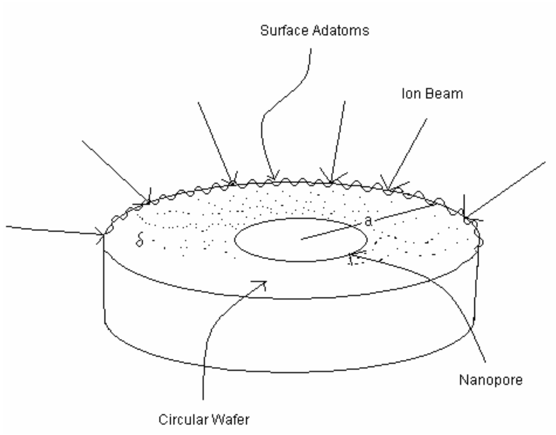
Keywords: Adatoms, diffusion, nanopore, CAS, Laplace Transform, Ion Beam Sculpting.

1. Introduction

Mathematical Nanotechnology modeling is a source of very interesting computational problems. Many of such problems can be solved using software for numerical calculations but there are certain of such problems that demand software for symbolic computations such as computer algebra systems. The object of the present work is to solve certain spatial nanopore sculpting model using computer algebra software. The problem that is chosen to present here can not be solved using numerical software because the solution of the proposed problem is the analytical formula for the basic diffusion rate which is a symbolic expression that can not be determined by pure numerical experimentation. Also, the chosen problem should not be solved by hand using paper and pen because the algebraic manipulations are very tedious. In concrete the problem to solve using computer algebra system is the following: Consider a circular wafer in which certain nanopore needs to be sculpted, the question is: what is the explicit expression for the basic diffusion rate of the adatoms at such configuration and what is the concentration of these surface adatoms inside a nanopore?

2. Mathematical Model

The Physical problem that is considered here is illustrated at the following figure [4], [5].



Where: a: Circular Wafer radius
δ:material diffusion constant
C(r, t): concentration of surface adatoms
α: adatoms creation/annihilation rate

The model we took was a diffusion one. The incident Ion Beam is applied on the boundary of the Circular Wafer causing the appearance of adatoms. These adatoms will make their way throughout the wafer (by diffusion) to finish inside the nanopore. The circular wafer has an associated diffusion constant that will affect the whole process. The final objective is to reduce the nanopore due to the adatoms that adhere to its boundary and It is important to control the quantity that will fall there.

The condition chosen to solve the equation it's an Ion injection model that results in a Neumann's boundary condition.

The explicit equation for adatoms diffusion is the following [6]:

$$\left(\frac{\partial}{\partial t}\mathrm{C}(r,t)\right)-\frac{\delta\left(\left(\frac{\partial}{\partial r}\mathrm{C}(r,t)\right)+r\left(\frac{\partial^2}{\partial r^2}\mathrm{C}(r,t)\right)\right)}{r}-\alpha\,\mathrm{C}(r,t)=0 \tag{1}$$

with the initial condition

$$\mathrm{C}(r,0)=0 \tag{2}$$

and with the Neumann's condition

$$\lim_{r\to a}\frac{\partial}{\partial r}\mathrm{C}(r,t)=Q_0\,\mathbf{e}^{(-\gamma t)} \tag{3}$$

where *C(r, t)* represents the concentration of surface adatoms

The question here is analytically to solve the equation (1) with the conditions (2) and (3) using symbolic computation assisted by CAS.

3. Methods

We use Laplace transform technique and apply the Bromwich integral and the residue theory to calculate the Laplace inverse transform [1]. We implement such strategy using CAS. Unfortunately the actual CAS do not incorporate directly the inverse Laplace transform by mean of residue theory and then is necessary introduce such residue theory by hand. In concrete the procedure is the following:

- Apply the Laplace transform with CAS to equation (1) with (2) and reduce (1) to an ordinary differential equation for the Laplace transform of *C(r, t)*.
- Solve such ordinary equation with the Neumann's condition (3) using CAS
- Implement in CAS the Bromwich integral and the necessary calculus of residues to obtain the inverse of the Laplace transform to obtain the analytical solution of (1) and verify the result.
- Extract from the solution, the explicit form of the basic diffusion rate of the concentration of surface adatoms in a circular wafer with a Neumann's condition injection model.

The application step by step of this method is presented in full detail at the Appendix.

4. Results

The solution of the equation (1) with the initial condition (2) and the Neumann's condition (3) that is obtained using computer algebra software is given by the following long formula

$$\mathrm{C}(r,t) = -\frac{Q_0\, J_0\!\left(\sqrt{\frac{\gamma+\alpha}{\delta}}\, r\right)}{e^{(\gamma t)}\, J_1\!\left(\sqrt{\frac{\gamma+\alpha}{\delta}}\, a\right)\sqrt{\frac{\gamma+\alpha}{\delta}}} - \frac{Q_0\, e^{(t\alpha)}}{-\frac{a\alpha}{2\delta} - \frac{a\gamma}{2\delta}} + \left(\sum_{n=1}^{\infty}\left(\frac{2\, J_0\!\left(\frac{\alpha_n r}{a}\right) a\,\delta\, Q_0\, e^{\left(\frac{\left(\alpha a^2 - \alpha_n^{\ 2}\delta\right) t}{a^2}\right)}}{(\alpha a^2 - \alpha_n^{\ 2}\delta + \gamma a^2)\, J_0(\alpha_n)}\right)\right) \tag{4}$$

where J_m is the Bessel function of order m of the first kind and α_n are the roots or zeros of J_0, called $J_0(\alpha_n) = 0$ [2], with *n* an integer from 1 to ∞.

We extract from (4) two expressions (one from the second and one from third term) to analyze stability.

$$e^{(t\alpha)} \tag{5}$$

$$e^{\left(\frac{\left(\alpha a^2-\alpha_n{}^2\delta\right)t}{a^2}\right)} \tag{6}$$

It is important to keep controlled the rate of diffusion of adatoms.
Expression (5) and (6) are temporal models, and the first one doesn't have spatial considerations.

At the other side, equation (6) does consider spatial implications giving the possible circular wafer critical radius.

5. Analysis of results

The right hand of equation (4) has three terms. The first term is clearly dismissed.
Stability analysis on the other two terms has to be made. Both terms express the rate of diffusion of adatoms, but only the third one gives reason of spatial properties such as the critical radius of the circular wafer.
We can then consider various situations:

1. When $\alpha<0$, we obtain a decreasing exponential function in (5) leaving us equation (6) to calculate the critical radius. Expression (7) shows us the critic radius condition. Clearly, if we want to obtain a real solution, the diffusion's constant has to be a negative number, producing a non-valid result.

$$a<\sqrt{\frac{\alpha_n{}^2\delta}{\alpha}} \tag{7}$$

This means that there is no critical condition for the circular wafer radius.

2. When $\alpha>0$, we obtain from (5) an exponential growth of surface adatoms, risking the final goal of the process (to shrink the nanopore, but not to close it).

These results are owed because we took a Neumann's condition injection model.
We conclude that it's more suitable to use Dirichlet's condition injection models and for this case the critical radius of the wafer is given by (7).

6. Discussion and conclusions

It is useful to say now, that the solution that was obtained, also can be determined by hand using paper and pen, without use CAS; but in all case CAS is a very useful tool to obtain such solution. From the other side, when annihilation at defects and adatom creation by ion impingement effects are included at the nanopore sculpting model, then in such cases the procedure of brute force by hand with paper and pen is very hard to implement and then is necessary to use some CAS that permits symbolic or analytical manipulations of the equations of the model.

Also is necessary to remark here that the numerical computer software that provides numerical solutions to boundary problems with partial differential equations including non-linear equations, can not proportionate explicit formulas of the solutions.

Finally is opportune to recognize that nanopore sculpting models that were considered are all linear models and the actual CAS is not able to solve in general non-linear models; but it is possible, yet in the case of non-linear problems to have approximate analytical or symbolic solutions using such CAS which is an alternative with respect the numerical software [3].

7. References

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8. Appendix

Using CAS the application of the Laplace Transform to both sides of (1) and taken account (2) we have:

$$s\,\mathrm{P}(r,s) - \frac{\delta\left(\left(\frac{\partial}{\partial r}\mathrm{P}(r,s)\right) + r\left(\frac{\partial^2}{\partial r^2}\mathrm{P}(r,s)\right)\right)}{r} - \alpha\,\mathrm{P}(r,s) = 0 \tag{A1}$$

where

$$\mathrm{P}(r,s) = \int_0^\infty \mathrm{C}(r,t)\,\mathbf{e}^{(-st)}\,dt \tag{A2}$$

The Laplace transformed Newman's condition that results from (3) is

$$\frac{\partial}{\partial r}\mathrm{P}(r,s) = Q_0\,\mathbf{e}^{(-\gamma\,t)} \tag{A3}$$

The solution of (A1) with the condition (A3) and with the condition that C(r, s) must to be finite at r= 0, can be obtained using computer algebra and the result is

$$\mathrm{P}(r) = -\frac{Q_0\, J_0\left(\sqrt{-\frac{s-\alpha}{\delta}}\; r\right)}{J_1\left(\sqrt{-\frac{s-\alpha}{\delta}}\; a\right)\sqrt{-\frac{s-\alpha}{\delta}}\;(s+\gamma)} \tag{A4}$$

The explicit form of C(r, t) can be determined if we can realize the inverse Laplace transform of both sides of (A.4). Such inverse transform can be calculated as the complex contour integral [2]

$$\mathrm{C}(r, t) = \frac{1}{2}\left(\frac{1}{\pi\, i}\int -\frac{Q_0\, \mathrm{BesselJ}\left(0, \sqrt{-\frac{s-\alpha}{\delta}}\; r\right) e^{st}}{\mathrm{BesselJ}\left(1, \sqrt{-\frac{s-\alpha}{\delta}}\; a\right)\sqrt{-\frac{s-\alpha}{\delta}}\;(s+\gamma)}\, ds\right) \tag{A5}$$

where the contour integral is realized over certain closed path that encloses all the poles of the P(r , s). As we can see such poles are at s= -γ.at s= α and at

$$s_n = \frac{\alpha\, a^2 - {\alpha_n}^2\, \delta}{a^2} \tag{A6}$$

where α_n are the zeroes of the Bessel function J_0 and n goes from 1 to infinity. Applying the residue theorem to the integral in (A5) we obtain that

$$\begin{aligned}\mathrm{C}(r, t) = &-\frac{Q_0\, J_0\left(\sqrt{\frac{\gamma+\alpha}{\delta}}\; r\right)}{\mathrm{e}^{(\gamma\, t)}\, J_1\left(\sqrt{\frac{\gamma+\alpha}{\delta}}\; a\right)\sqrt{\frac{\gamma+\alpha}{\delta}}} - \frac{Q_0\, \mathrm{e}^{(t\, \alpha)}}{-\frac{a\, \alpha}{2\, \delta} - \frac{a\, \gamma}{2\, \delta}} \\ &+ \left(\sum_{n=1}^{\infty}\left(\frac{2\, J_0\left(\frac{\alpha_n\, r}{a}\right) a\, \delta\, Q_0\, \mathrm{e}^{\left(\frac{\left(\alpha\, a^2 - {\alpha_n}^2\, \delta\right) t}{a^2}\right)}}{(\alpha\, a^2 - {\alpha_n}^2\, \delta + \gamma\, a^2)\, J_0(\alpha_n)}\right)\right)\end{aligned} \tag{A7}$$

Given that all poles are of the first order we can calculate the residues using CAS and we obtain the result that the equation (4) shows.

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