Information System for Design of Thin Multilayer Film Processes Parameters Management based on Diffusion

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Abstract

This designing investigates the diffusion phenomena within multilayer films, emphasizing the crucial role of mathematical modeling and computational simulation techniques. By considering the transitions between adjacent layers, our approach incorporates advanced modeling methods and software frameworks, including integral transformations, to accurately depict diffusion processes. Theoretical insights are validated through experimental data analysis and solution identification based on the theory of state control of multicomponent systems. Our results reveal close agreement between modeled and experimental aluminum concentration distributions, particularly as the duration of multilayer formation approaches completion. Furthermore, our findings suggest practical applications, including enhancing the efficiency of experimental studies and exploring properties of emerging nanomaterials. This study underscores the synergy between theoretical modeling and experimental validation, offering insights into complex transport phenomena and paving the way for advancements in materials science and engineering.

Keywords

Multilayer Films, Computational Simulation, Software Frameworks, Data-Driven Analysis, Complex Diffusion Mechanisms

1. Introduction

Addressing the complexities inherent in investigating diffusion within multilayer films demands advancements in modern modeling techniques, computation algorithms software frameworks, enabling accurate depiction of phenomena while accounting for transitions between adjacent layers [1, 2]. Integral transformations stand out among the efficacious methods employed to comprehensively tackle these challenges, serving to derive solutions for diverse boundary value problems in mathematical physics concerning homogeneous structures. This encompasses diffusion scenarios across various environments, thereby facilitating their mathematical representation.

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Moreover, alongside the indispensable role of advanced modeling techniques and software, sophisticated computational approaches play a crucial role in tackling the challenges of studying diffusion within multilayer media. Leveraging cutting-edge methodologies in computer programming and software architecture, these approaches elevate the capabilities of mathematical methods, such as integral transformations, to unprecedented levels of precision and efficiency. This symbiotic relationship between mathematical modeling and computational innovation not only enhances our ability to accurately represent diffusion phenomena within multilayer structures but also paves the way for new avenues of exploration and analysis [3, 4].

Furthermore, the integration of modern modeling techniques with state-of-the-art computational tools facilitates a deeper understanding of diffusion processes across diverse material compositions and environmental conditions. Through harnessing the power of numerical simulations and data-driven analyses, researchers can unlock insights into previously inaccessible complex diffusion mechanisms. This multidisciplinary approach empowers scientists and engineers to not only address fundamental questions in materials science and engineering but also devise innovative strategies for optimizing the performance and functionality of multilayer films across various technological applications.

In this article, the authors endeavor to amalgamate complex mathematical models with best practices in software development to address the challenge of computer simulation of diffusion transport processes within multilayer nanofilms.

2. Disogning Methidology and Physics Problem Formulation

In this conceptual framework, mutual diffusion occurs between adjacent layers of the multicomposite at each interface. The mechanisms governing this mutual transfer are influenced by the variable gradients and rates of concentration change at the interface boundaries between layers. By integrating changes in concentrations and their gradients over time into the boundary and interface conditions, it becomes feasible to model the mechanisms of this additional mutual transport alongside the fundamental transport equations.

When devising a mathematical model for diffusion transfer within oxide films, the consideration of a multilayer configuration is essential. Assuming that the diffusion of atoms of constituent components (such as aluminum, molybdenum, and silicon) primarily governs system mixing, concentration profiles for such a multilayer system can be derived from the Fick equations. These equations incorporate boundary conditions at the outer layers and account for contact conditions between successive layers. This methodological approach results in a mathematical model that comprehensively describes the diffusion transfer process within a planar multilayered medium.

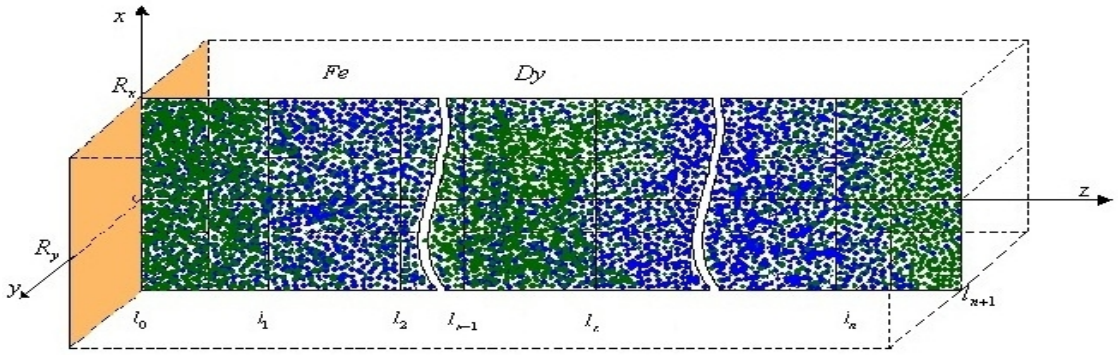

Figure 1: Schema of multilayer nanofilm

$$\frac{\partial}{\partial t}C_k(t,x,z)+\gamma_k^2 C_k = D_0\frac{\partial^2 C_k}{\partial x^2}+D_{z_k}\frac{\partial^2 C_k}{\partial z^2}; \qquad (1)$$

Within domain ($j=\overline{1,2}; k=\overline{1,n}$)

$$t>0, x\in(0,R), z: z\in\bigcup_{k=1}^{n+1}(l_{k-1},l_k); l_0\geq 0; l_{n+1}=\infty$$

Here:

Ck represents diffusion concentrations; Dk represents diffusion coefficients; ■k2 define mass distribution coefficient (at first attempt $\gamma_k^2=0; k=\overline{1,n+1}$) .

The initial and boundary condition of proposed model are:

$$C_k(t,x,z)\big|_{t=0}=C_{0_k}(x,z)\equiv C_{0_k}(z), \qquad (2)$$

$$\left[\alpha_{11}^0\frac{d}{dz}+\beta_{11}^0\right]C_1(t,x,z)\big|_{z=l_0}=C_{l_0}(t,x); \qquad \frac{\partial C_{n+1}}{\partial z}\big|_{z=\infty}=0; \qquad (3)$$

$$\left[\left[\alpha_{j1}^k\frac{\partial}{\partial z}+\beta_{j1}^k\right]C_k-\left[\alpha_{j2}^k\frac{\partial}{\partial z}+\beta_{j2}^k\right]C_{k+1}\right]_{z=l_k}=0, \qquad (4)$$

With boundary conditions across variable x

$$\frac{\partial C_k}{\partial x}\big|_{x=0}=0; \qquad C_k\big|_{x=R}=C_{1_k}(t,z). \qquad (5)$$

Here:

$\alpha_{ij}^k,\beta_{ij}^k;\ k=\overline{0,n};\ i,j=\overline{1,2}$ are coefficients which determines boundary and contact conditions on the multilayer media.

$D_k, k=\overline{1,n+1}-$ diffusion coefficients in direction of z axis;

D_0- diffusion coefficient in direction of x axis;

$\Delta l_k=l_k-l_{k-1}; k=\overline{1,n+1}$ – thikness of k-th layer; $l=l_{n+1}-l_0$ – media thickness.

Solution of the formulated mathematical problem can be found by applying Fourier transforms following algorithm detail described at [5].

$$C_k(t,x,z)=\int_0^t\int_0^R W_{l_0,k}(t-\tau;x,\varsigma;z)C_{l_0}(\tau,\varsigma)d\varsigma d\tau$$
$$+\sum_{k_1=1}^{n+1}\int_0^t\int_0^r\int_{l_{k_1-1}}^{l_{k_1}} \mathrm{H}_{k,k_1}(t-\tau;x,\varsigma;z,\xi)\cdot C_{0_k}(\varsigma,\xi)\cdot\delta_+(\tau)\sigma_{k_1}d\varsigma d\xi d\tau+\sum_{k_1=1}^{n+1}\int_0^t\int_{l_{k_1-1}}^{l_{k_1}} W_{R_{k,k_1}}(t-\tau;x;z,\xi)\cdot C_{1_{k_1}}(\tau,\xi)\sigma_{k_1}d\xi d\tau. \quad (6)$$

Ehe following functions are used here

- Cauchy's function

$$\mathrm{H}_{k,k_1}(t;x,\varsigma;z,\xi)=\frac{2}{R}\sum_{m=0}^{\infty}\varepsilon_{k,k_1}^m(t,z,\xi)\cdot\cos\eta_m\xi\cdot\cos\eta_m x \quad (7)$$

- Green's functions

$$W_{l_0,k}(t,x;z,\xi)=\frac{2}{R}\sum_{m=0}^{\infty}W_{l_0,k}^m(t-\tau,z)(-1)^m\frac{\cos\eta_m\xi}{\eta_m} \quad (8)$$
$$W_{R_{k,k_1}}(t;x,\varsigma;z,\xi)=\frac{2}{R}\sum_{m=0}^{\infty}e^{-D_0\eta_m^2t}D_0(-1)^{m+1}\eta_m\varepsilon_{k,k_1}^m(t;z,\xi)(-1)^m\cdot\cos\eta_m x$$

3. Computer identification of parameters

According to the results of experimental data and using the solution identification methodology were carried out using the theory of state control of multicomponent systems [5].

The identified diffusion coefficients distributions correspond to experimental data, are used as input parameters of the obtained mathematical solution of model (1)-(5) for modeling and analysis of concentration distributions for aluminum component of nanofilms media.

In fig. 2 the distributions of diffusion coefficients for the constituent components of nanofilm (aluminum) are presented, reproduced using the methods of optimal control of the state of multicomponent transport systems, the analytical solution of model and the data of experimental observations [6]. Both heat and corrosion resistance of result alloys are determined by the level of aluminum, which ensures the formation of protective surface oxides. Let us consider the results of computer modeling and parameters identification of aluminum concentration distributions in each of the five points.

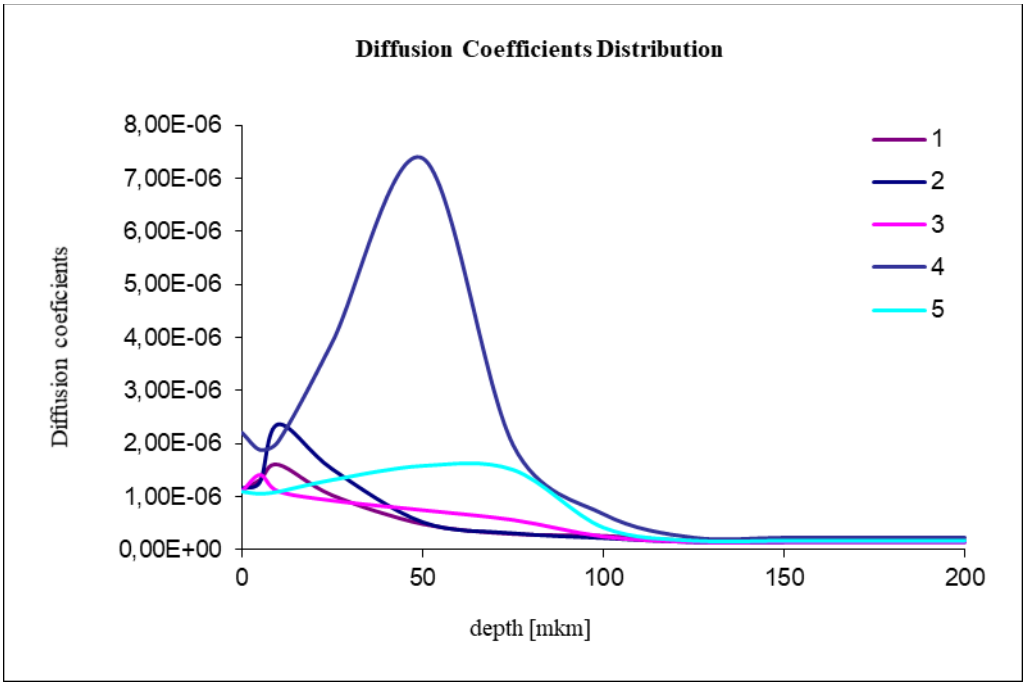

Figure 2: Diffusion coefficients distribution in Aluminum sample at five different points

Special software framework was developed for numerical modeling of concentration distributions in aluminum using the obtained distributions of diffusion coefficients. To achieve good accuracy and high performance, multi-threaded parallelization [7] were used for the modular software architecture, following software engineering best practices [8]. The individual results of numerical modeling are shown in the figures below.

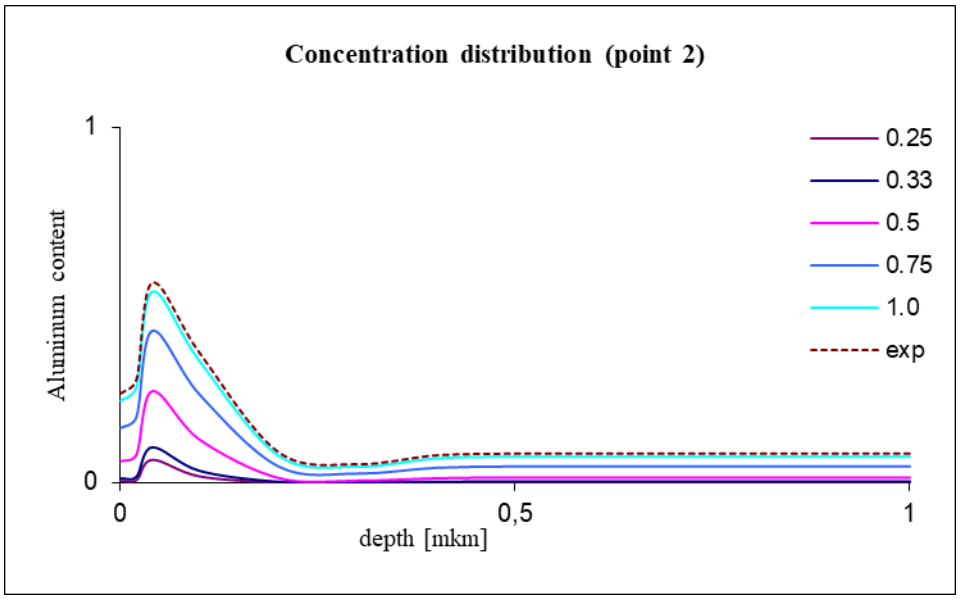

Figure 3: Concentration of aluminum in film (point 2)

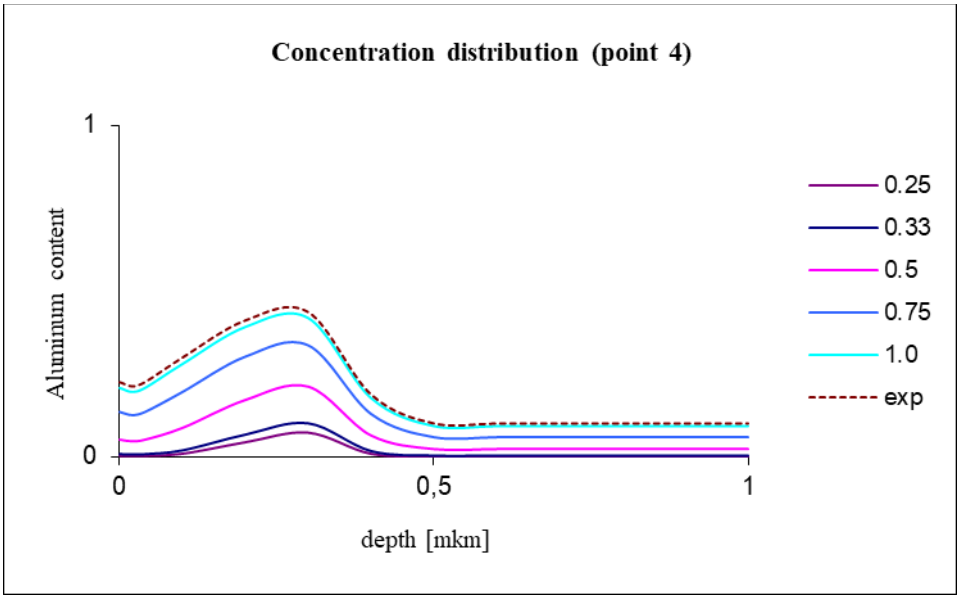

Figure 4 : Concentration of aluminum in film (point 4)

In fig. 3-5 show the results of numerical modeling and use traces of experimental observations (exp) reflecting the aluminum content. Presented distributions were constructed for different formation times of technological multilayer of nanofilm: the given time equal to (1T) corresponds to the experimental time (20 days). The duration of the formation of the technological multilayer of the nanofilm due to the molecular diffusion of the specified components is divided into 5 periods, which include the formation of the protective multilayer from the initial period (0.25 T) to the final period (1 T).

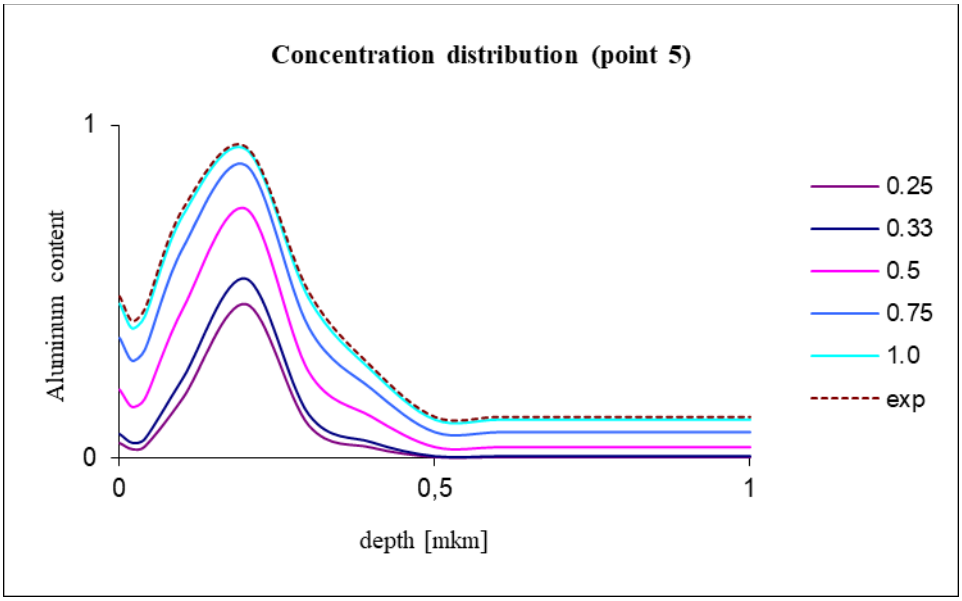

Figure 5: Concentration of aluminum in film (point 5)

As can be seen on the plots, distribution characteristic is in complete correlation with aluminum content at a depth after 100 μm at the reduced time of 0.25T and 0.33T, which

corresponds to one third of the experiment duration. In addition, content is close to zero. The notable increase in aluminum content are for time from 0.33T to 0.75T.

The profiles obtained by modeling aluminum concentration distributions are well agreed with the corresponding experimental profiles in the cases of multilayer formation time reaching the period of completion of the formation of the nanofilms protective multilayer. The maximum deviation is around 2-5%, which points on the reliability of the mathematical model and the proposed simulation software. Consequentially, the obtained results have options for practical use. Such simulations can be used to improve the efficiency of experimental studies of transport in multicomponent multi composites and to study the properties of new nanomaterials

Conclusions

The convergence between modeled and experimental aluminum concentration distributions underscores the efficacy of our approach, particularly as the duration of multilayer formation approaches the completion phase of the nanofilm's protective layer. With maximum deviations are in small range, and our findings attest to the reliability of both the mathematical model and the simulation software employed. These results not only validate our methodology but also signal its potential for practical utilization.

Moving forward, the implications of our information systems software extend beyond mere validation; they open doors to practical applications. Using leveraging simulations, we can enhance the efficiency of experimental investigations into transport phenomena within multicomponent composites. Furthermore, our approach offers a systematic means of studying the properties of emerging nanomaterials, thereby contributing to advancements in materials science and engineering.

As we continue to refine and expand upon these methodologies and control systems of designing, we are poised to make significant strides in our understanding of multilayer film dynamics and the development of novel nanomaterials with tailored properties for diverse applications.

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