Approximate solution of non-linear equations of ytterbium (III) chemical adsorption process within zinc oxide würtzite nano-matrices using EHPM and BPES

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ABSTRACT

Knowledge of the kinetics of doping elements adsorption within hosting edifices is of great importance in the development of chemistry and materials science. In this paper, the Enhanced homotopy perturbation method (EHPM) is applied along with the Boubaker polynomials Expansion Scheme (BPES) to the problem of adsorption and desorption behaviors of Ytterbium inside würtzite ZnO matrices. The approximate analytical expressions of the non-steady-state concentrations as results of reactions mechanisms inside würtzite ZnO Matrices, is derived for the given values of the relevant parameters. Influence of initial concentration of Yb(III), initial pH of solution and temperature on the adsorption of Ytterbium are taken into account. The obtained results are compared to the available analytical results and are found to be in good agreement. Theoretical considerations are discussed in order to illustrate the ability and reliability of the methods. Comparison of NHPM results with those of BPES revealed both techniques are effective and convenient.   © 2012 Trade Science Inc. - INDIA

INTRODUCTION

In the last decades, several studies have been carried out on semiconductors doped with rare earth elements[1-11]. Rare earth (RE) doped semiconductors have long been the topic of research owing to their prominent and desirable optical and magnetic properties[3-8]. Typically trivalent rare earth elements have very stable emissions, due to the 4-*f* electrons which are deeply buried and hence well shielded from the outer shells. This property of the rare earth elements enables their incorporation into various hosts with different lattices. The sharpness of many lines in the emission spectra of RE doped semiconductor enables, in principle to in-

vestigate interactions in a solid by optical means with a degree of accuracy similar to that usually possible with free atoms or ions. Modification in the main physical properties of the ZnO films due to the introduction of very small impurities in the molecular matrix having a noticeable effect on surface morphology of ZnO sprayed thin films has been reported[12-20].

In the present work, comparative solutions to the differential equations systems governing the kinetics of Ytterbium adsorption within particular hosting edifices are presented. These partial differential equations are often very complicated to be solved exactly and even if an exact solution is obtained, the required calculations may be too complicated to be practical. In the last three

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decades, many attempts to yield numerical and analytical solution have been performed. Wazwaz[21] used early modified decomposition method for solving nonlinear equations, while He[22-25], Momani et al.[26] and Saadati et al.[27] applied variational iteration methods to Helmholtz equation as well as some autonomous ordinary differential systems. Homotopy perturbation method HPM solutions to the modified Camassa-Holm and Degasperis-Procesi equations, diffusion inverse problem system equation and Fokker-Planck equation have been recently proposed by Yildirim et al.[28], Ozis et al.[29], Wang [30], Song[31] et al. and many others[32-37].

The paper is arranged as follows: In section 2, fundaments to the studied chemical process are presented along with experimental details. Section 3 presents the resolution protocols, namely the enhanced homotopy perturbation method EHPM, and the Boubaker polynomials expansion scheme BPES. In section 4, results and related plots are discussed, detailed and compared to some other results presented in the recent literature. Conclusion is formulated in section 6.

FUNDAMENTS TO THE STUDIED PROCESS

ZnO hosting structures features

ZnO is a good host for incorporating rare earth elements du e to a number of different reasons. First some
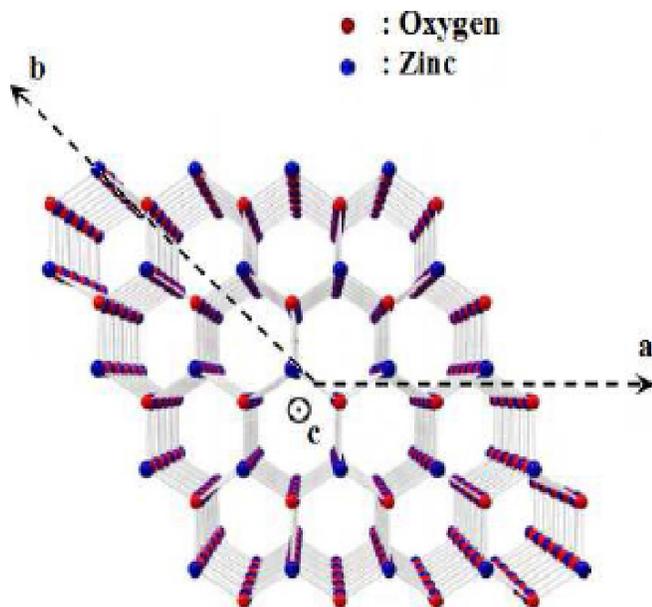
Figure 1 : Würtzite ZnO crystalline structure (c-axis anti-parallel view)

of its properties can be markedly changed by introducing rare earths. Secondly it lends itself readily to investigation, since it is one of the simplest crystalline compounds and can be prepared easily. ZnO crystal has a würtzite lattice, consisting of two interpenetrating hexagonal close packed lattices (Figure 1), one containing the anions (0^{2-}), the other the cations (Zn^{2+}).

When Zn and O atoms combine Zn loses two valence electrons to O, thus eventually due to loss of an outer shell the Zinc atom shrinks in size from 1.33 Å to 0.74 Å, while Oxygen atom increases in size due to addition of an outer shell from 0.64 Å to 1.4 Å[38]. The wide disparity in size between the zinc and oxygen atoms leaves relatively large open spaces thus enabling incorporation of host atoms, i. e. Ytterbium (Figure 2).
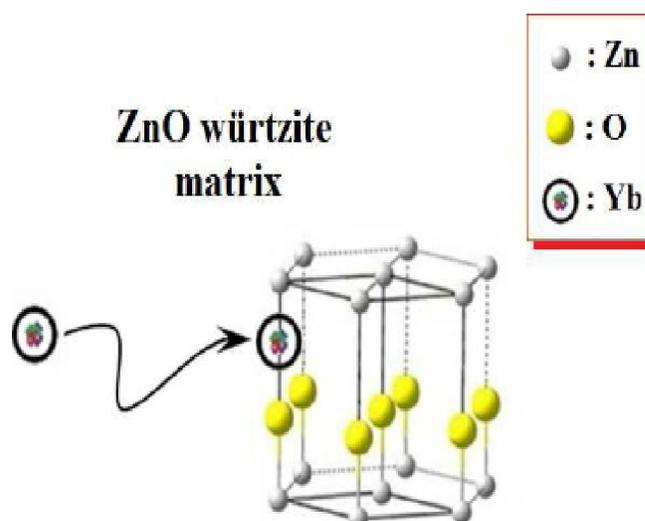
Figure 2 : Ytterbium incorporation inside ZnO crystalline structure

Ytterbium as a guest atom

Ytterbium (Yb) is a chemical element belonging to the group of rare earth metals and that it widely used as a laser-active doping agent in a variety of host materials. Ytterbium atoms have a very simple electronic level structure, with only one excited state manifold ($^2F_{5/2}$) within reach from the ground-state manifold ($^2F_{7/2}$) with near-infrared or visible photons. The Yb^{3+} ions are of interest also as a sensitizer of energy transfer for infrared to visible up conversion and infrared lasers. In Energetically designed devices, pumping, cooling, re-pumping and amplification involve transitions between different sublevels of the ground-state and excited-state manifolds (Figure 3).
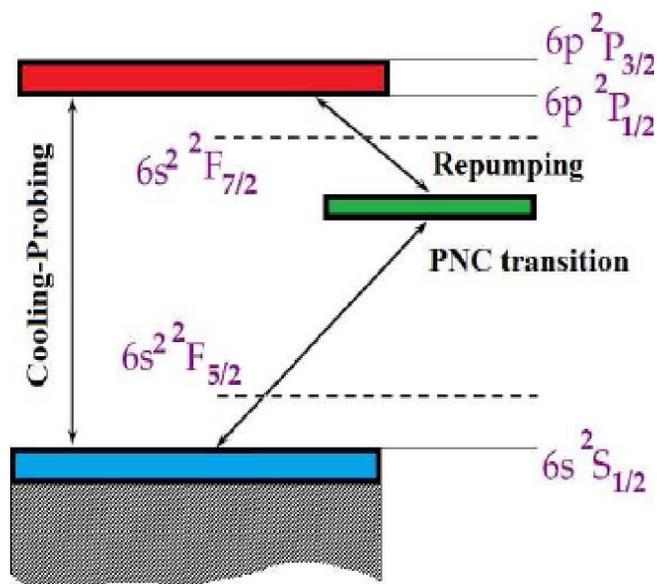
Figure 3 : Ytterbium shell band structure

Ytterbium-doped compounds are promising materials with numerous attractive properties[39]. The broad fluorescence spectrum (compared with i. e. Nd3+) and the millisecond-range upper-state lifetime provide sufficient bandwidth to generate and amplify ultrashort laser pulses.

The mechanism of incorporation of Ytterbium inside ZnO crystalline structure have been studied by Stevens[40], Low[41], Thronely, Lea et al.[42] and many others[43-47], but a big part of the process is still unexplained. Ytterbium cation Yb^{3+} initial configuration, characterized by a single hole in the 4f-shell, is split by spin-orbit coupling into a lower lying ($^2F_{7/2}$) and a ($^2F_{5/2}$) multiplet. Inside a ZnO-like structure, Yb^{3+} is trapped inside a four-negatively-charged nearest neighborhood, thus, ($^2F_{7/2}$) splits into Γ_6 Kramer doublets. This change increases electropositivity and affinity to Oxygen, resulting in a forced cation-cation substitution.

Experimental details

First, Yb-free ZnO thin films were prepared in a substrate temperature domain of 400-500°C using propanol 2(C_3H_8O) : 750 cm^3, water (H_2O) : 250 cm^3, and zinc Acetate ($Z_n(CH_3CO_2)_2$) : 0.1 mole. The precursor mixture was acidified using acetic acid (pH =5). Under solution and gas flow rates of 2 cm^3 min^{-1} and 41 cm^3 min^{-1} respectively, the obtained ZnO thin films thickness was approximately 0.5 μm. Obtained films were doped by mixing the starting solution containing zinc acetate (10^{-2} M), with water and Ytterbium chloride (YbCl$_3$,xH2O, 99.9% purity) in acidified medium at a substrate temperature of the order of 460°C. Doping amounts were 100, 200 and 300 ppm Yttrebium respectively. Figure 4 presents reflectance and transmission spectra of the doped samples (B-C-D), with
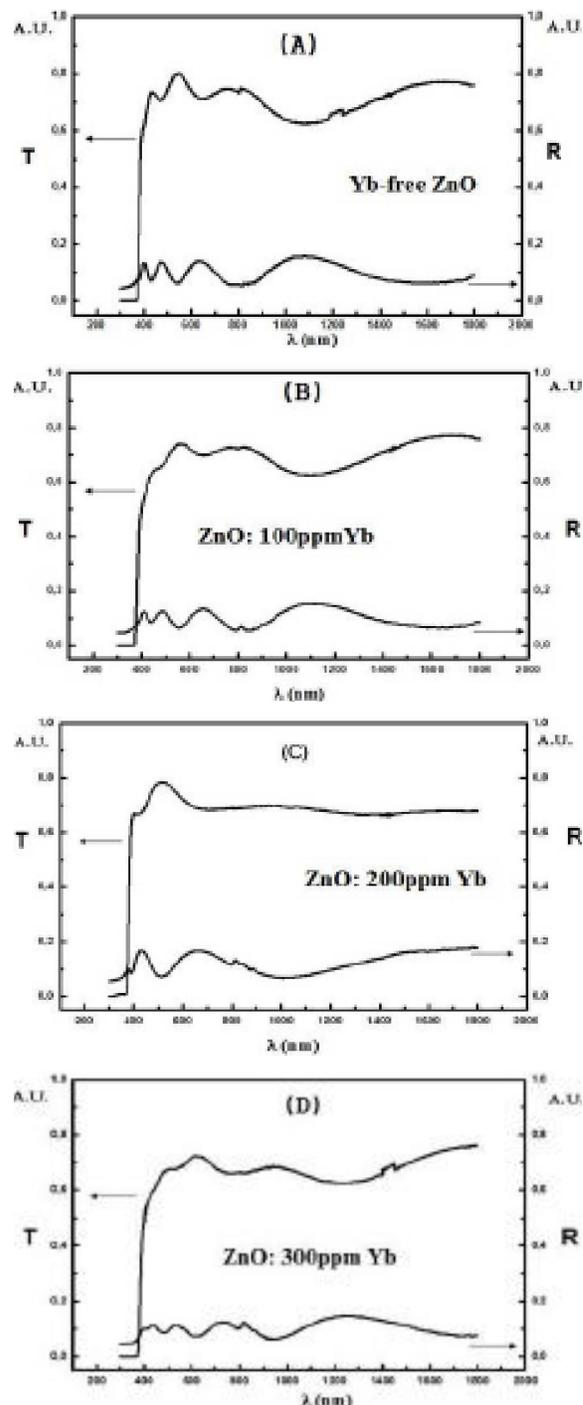
Figure 4 : Reflectance-transmission spectra of the doped samples (B-C-D), (Plots for the un-doped sample (A) are given for comparison purposes).

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reference to an un-doped sample (A). It is noticed that the transmission coefficient increases in the lower part of the visible domain (70%-85%) while the reflectance oscillates in a narrow range (5%-15%).

XRD patterns of the as-deposited ZnO Yb-doped films are shown in Figure 5. Diagram analyses along with 3D imaging results (Figure 6) show that the doped layers (B, C and D) monitor an enhanced preferred orientation of the crystallites with respect to the (200) reflection oppositely to the Yb-free films. In fact the ZnO layers are commonly characterized by the main XRD peaks: (101) (100) and (002) in hexagonal wurtzite system. The Yb-doped ZnO films c-axis oriented (002) plane shows a very high intensity relatively to other orientations. This feature is associated with high optical performance perpendicularly to the plane of the glass substrate.

Model of adsorption chemical kinetics

The relatively simple shell electronic structure of Yt-
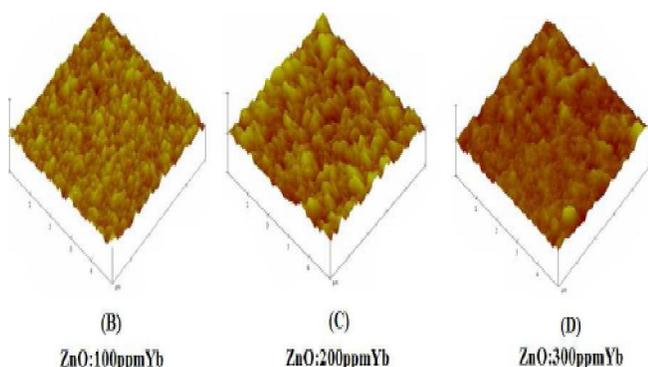
(B)   (C)   (D)
ZnO:100ppmYb   ZnO:200ppmYb   ZnO:300ppmYb
Figure 5 : layers 3D surface topography
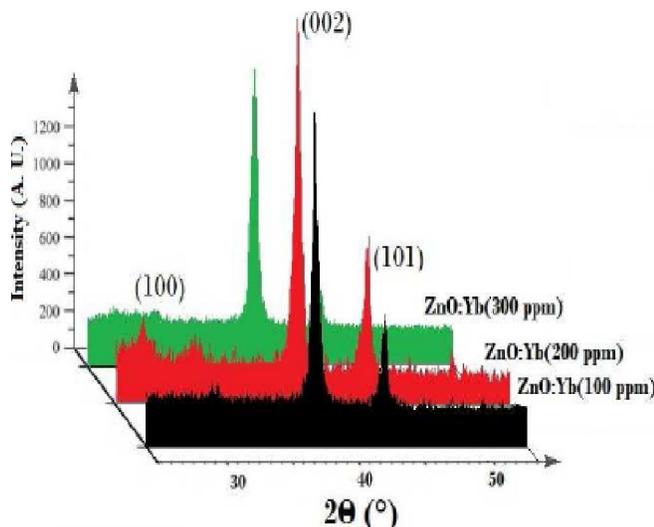
Figure 6 : XRD Diagrams of doped ZnO.

terbium excludes excited-state absorption and also a variety of detrimental quenching processes. In this case, we can expect, in concordance with analyses presented in §2.2, the following simultaneous reactions:

$$2YbCl_{3(l)} \leftrightarrow 2Yb_{(S)}\left[II,4f^{14}\right] + 3Cl_2 \tag{1}$$

$$6ZnO_{(S)} \leftrightarrow 6Zn_{(S)} + 3O_2 \tag{2}$$

$$4Yb_{(s)}\left[II,4f^{14}\right] + 3O_2 \rightarrow 2Yb_2O_{3(S)}$$
$$\left[III,4f^{13}\right] \rightarrow 4Yb_{(s)}\left[III,4f^{13}\right] + 3O_2 \tag{3}$$
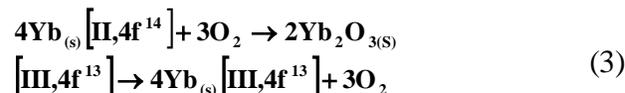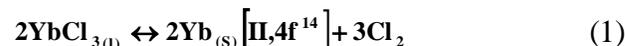
It is noted in these reactions that a divalent Ytterbium is reacting with oxygen to form the sesquioxide in which Ytterbium is trivalent. It was clearly stated by Kossanyi et al.[48] that "*rare earths are incorporated in ZnO as trivalent ions which do not occupy substitutional sites but rather interstitial sites associated with excess of oxygen in the ZnO lattice*".

In fact, for the normal trivalent lanthanide metals there is no change in valence state in forming the sesquioxide. Thus the single difference is due to the energy required to promote a $4f$ electron to the valence band of metallic ytterbium. This energy is estimated to 9.3 kcal/g.-at[49] and is presumed to be fully provided by the experimental setup.

Assuming that the adsorption process can be treated as a pseudo-order reversible reaction with respect to the metal cation[50, 51], Ytterbium incorporation is governed by the following equation:

$$-\frac{d[Yb]_{(S)}}{dt} = \frac{Q}{V}\left(k_f\left[Yb^{3+}\right]_{(l)} - k_r\left[Yb(III)\right]_{(S)}\right) \tag{4}$$

with :

$[Yb]_{(s)}$: Incorporated Ytterbium concentration in the matrix.

$[Yb^{3+}]_{(l)}$: Ytterbium cation concentration in the solution.

$[Yb(III)]_{(s)}$: Trivalent Ytterbium atom in the interfacial area.

Q : Mean interacting interfacial area.

k_f : Forward pseudo-first-order-rate constant.

k_r : Reverse pseudo-first-order-rate constant.

V : ZnO lattice unitary volume.

By introducing the temperature-dependent ratio K_e:

$$K_e = \frac{k_f}{k_r} = \frac{[Yb(III)]_{(S)}^{(Eq.)}}{[Yb^{3+}]_{(l)}^{(Eq.)}} \approx \frac{[Yb(III)]_{(S)}}{[Yb^{3+}]_{(l)}} \tag{5}$$

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assuming:

$$\left[Yb^{3+}\right]_{(l)} = -\varepsilon \frac{d^2\left[Yb\right]_{(S)}}{dt^2} + \left[Yb^{3+}\right]_{(l)}^{(init.)} \tag{6}$$

Where ε is a constant, and finally, by considering boundary conditions, we obtain the system:

$$\begin{cases} -y'(t) = \dfrac{Q}{V}\left(\left(k_f - K_e\right)\left(\varepsilon y''(t)+1\right)\right) \\[2mm] y(t) = \dfrac{\left[Yb\right]_{(S)}(t)}{c_0} \\[2mm] c_0 = \left[Yb^{3+}\right]_{(l)}^{(init.)} \\[2mm] y(0) = 0;\, y'(0) = 0 \end{cases} \tag{7}$$

RESOLUTION OF THE MAIN EQUATION USING EHPM AND BPES

For a given temperature, a first solution to Eq. (7) using the Enhanced Homotopy Perturbation Method (EHPM) as an extended version of the already established analytic homotopy-perturbation method (HPM)[28-37]. As a precursor and fundament to EHMP, HPM was first proposed by the Chinese mathematician He[22-25]. The enhanced form, which is developed in this paper along with a polynomial scheme, has been recently applied to a general form of system of PDEs, in a 4-dimension space:

$$\begin{cases} \dfrac{\partial f_1}{\partial t} + F_1(x,y,z,t,f_1,\cdots,f_n) = g_1(x,y,z,t) \\[2mm] \dfrac{\partial f_2}{\partial t} + F_2(x,y,z,t,f_1,\cdots,f_n) = g_2(x,y,z,t) \\[1mm] \vdots \\[1mm] \dfrac{\partial f_n}{\partial t} + F_n(x,y,z,t,f_1,\cdots,f_n) = g_n(x,y,z,t) \end{cases} \tag{8}$$

with initial conditions:

$$\begin{cases} f_1(x,y,z,t)\big|_{t=t_0} = h_1(x,y,z) \\[2mm] f_2(x,y,z,t)\big|_{t=t_0} = h_2(x,y,z) \\[1mm] \vdots \\[1mm] f_n(x,y,z,t)\big|_{t=t_0} = h_n(x,y,z) \end{cases} \tag{9}$$

where $F_i\big|_{i=1,\cdots,n}$ are non-linear operators, which can depend to all of the functions $f_i\big|_{i=1,\cdots,n}$ and their deriva-

tives, and $h\big|_{i=1,\cdots,n}$ are in-homogeneous terms. A detailed description of the EHPM is given in (Appendix A) and related solution plots are given in Figure 7.

A second solution using the Boubaker polynomials expansion scheme BPES[52-71] is also proposed. The resolution protocol, as detailed in (Appendix B) is based on assigning the following expression to the solution of Eq. (7):

$$y_{BPES}(x) = \frac{1}{2N_0} \sum_{k=1}^{N_0} \lambda_k^{(sol.)} \times B_{4k}(x \times r_k) \tag{10}$$

where B_{4k} are the 4k-order Boubaker polynomials, r_k are B_{4k} minimal positive roots, N_o is a prefixed integer and $\lambda_k^{(sol.)}\big|_{k=1..N_0}$ are unknown pondering real coefficients.

The main advantage of this formulation (Eq. 10) is the evidence of verifying the boundary conditions expressed in Eq. (7), in advance to problem resolution thanks to the properties of the Boubaker polynomials[55-65], besides proposing differentiable and piecewise continuous solutions[56-62]. As evoked earlier, a detailed description of the BPES is given in (Appendix B) and related solution plots are given in Figure 7.

DISCUSSION AND PERSPECTIVES

Figure 7 gathers the solutions obtained for different temperatures.

While investigating the kinetic resolution given by the given methods (Figure 7), a significant temperature gradient is observed while an exponential parabolic time-dependent behavior is recorded. This result is confirmed by the results presented in the relevant literature[72-74].

Concentration profiles are also concordant with precedent results[75, 76]. Additionally, it can be noticed that there is no reaction below a temperature limit (bold line in Figure 7). This feature refers to the energy required to promote a $4f$ electron to the valence band of metallic ytterbium, as stated by Gshneider J_R[49]. It can be that concluded that a minimal energy is required to activate the adsorption process, regardless of the provided doping element amount.

APPENDIX A

For solving system (8), by the EHPM, we con-

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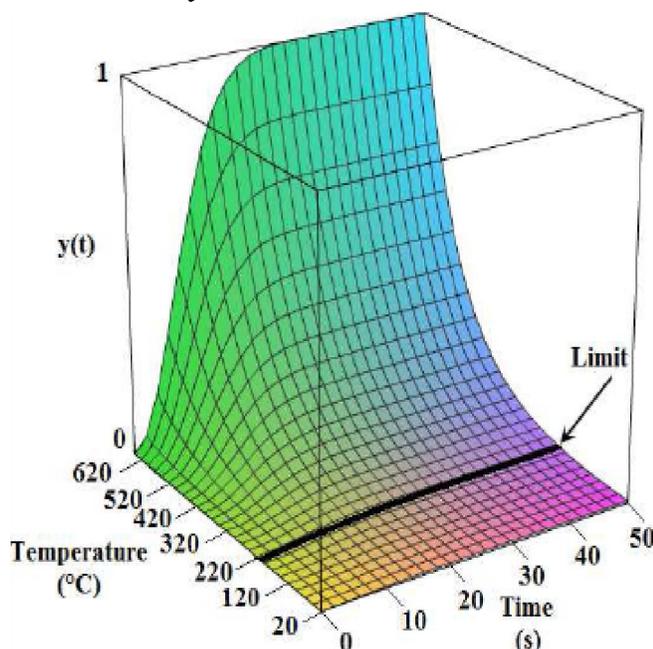
Figure 7 : Solutions plots.

struct the following homotopies:

$$
\begin{cases}
(1-p)(\dfrac{\partial \Phi_1}{\partial t} - \phi_{1,0}) + p \\
\left(\dfrac{\partial \Phi_1}{\partial t} + F_1(x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_1 \right) = 0 \\
(1-p)(\dfrac{\partial \Phi_2}{\partial t} - \phi_{2,0}) + p \\
\left(\dfrac{\partial \Phi_2}{\partial t} + F_2(x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_2 \right) = 0 \\
(1-p)(\dfrac{\partial \Phi_3}{\partial t} - \phi_{n,0}) + p \\
\left(\dfrac{\partial \Phi_n}{\partial t} + F_n(x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_n \right) = 0
\end{cases}
$$

(A.1)

or :

$$
\begin{cases}
\dfrac{\partial \Phi_1}{\partial t} = \phi_{1,0} - p\begin{pmatrix} \phi_{1,0} + F_1 \\ (x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_1 \end{pmatrix} \\
\dfrac{\partial \Phi_2}{\partial t} = \phi_{2,0} - p\begin{pmatrix} \phi_{2,0} + F_2 \\ (x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_1 \end{pmatrix} \\
\vdots \\
\dfrac{\partial \Phi_n}{\partial t} = \phi_{n,0} - p\begin{pmatrix} \phi_{n,0} + F_n \\ (x,y,z,t,\Phi_1,\cdots,\Phi_n) - h_n \end{pmatrix}
\end{cases}
$$

(A.2)

We define here the inverse operator $\tilde{\nabla}$:

$$ \tilde{\nabla} = L^{-1}\int_{t_0}^{t}(.)dt $$

(A.3)

When applied both sides of Eq. (A.1), operator $\tilde{\nabla}$ gives:

$$
\begin{cases}
\Phi_1(x,y,z,t) = \Phi_1(x,y,t_0) + \int_{t_0}^{t}\phi_{1,0}dt - \\
p\int_{t_0}^{t}\left(\phi_{1,0} + F_1(x,y,t,\Phi_1,\cdots,\Phi_n) - h_1\right)dt \\
\Phi_2(x,y,z,t) = \Phi_2(x,y,t_0) + \int_{t_0}^{t}\phi_{2,0}dt - \\
p\int_{t_0}^{t}\left(\phi_{2,0} + F_2(x,y,t,\Phi_1,\cdots,\Phi_n) - h_2\right)dt \\
\Phi_n(x,y,z,t) = \Phi_n(x,y,t_0) + \int_{t_0}^{t}\phi_{n,0}dt - \\
p\int_{t_0}^{t}\left(\phi_{n,0} + F_n(x,y,t,\Phi_1,\cdots,\Phi_n) - h_n\right)dt
\end{cases}
$$

(A.4)

where:

$$
\begin{cases}
\Phi_1(x,y,t_0) = \phi_1(x,y,t)\big|_{t=t_0} \\
\Phi_2(x,y,t_0) = \phi_2(x,y,t)\big|_{t=t_0} \\
\vdots \\
\Phi_n(x,y,t_0) = \phi_n(x,y,t)\big|_{t=t_0}
\end{cases}
$$

(A.5)

Now, let's present the solution of the system (A.4) as the following:

$$
\begin{cases}
\Phi_1 = \Phi_{1,0} + p\Phi_{1,1} + p^2\Phi_{1,2} + \cdots \\
\Phi_2 = \Phi_{2,0} + p\Phi2_{1,1} + p^2\Phi_{2,2} + \cdots \\
\vdots \\
\Phi_n = \Phi_{n,0} + p\Phi_{n,1} + p^2\Phi_{n,2} + \cdots
\end{cases}
$$

(A.6)

where $\Phi_{i,j}\big|_{i=1,..n;j=1,..n}$ are functions to determine.

Now, let's suppose that the initial approximations of the solutions of Eqs. (1) are in the following form:

$$ \phi_{i,0}(x,y,z,t)\big|_{i=1,..n} = \sum_{j=0}^{+\infty}a_{i,j}(x,y)P_j(t) $$

(A7)

where $a_{i,j}\big|_{i=1,..n;j=1,..n}$ are unknown coefficients and $P_j(t)\big|_{j=1,..n}$ are specific functions.

Substituting (A.6) and (A.5) into (A.4) and identifying same powers coefficients of *p* gives:

$$
\left.\begin{aligned}
&\Phi_{i,0}(x,y,t) = f_i(x,y,z) + \sum_{j=0}^{+\infty}a_{i,j}\int_{t_0}^{t}P_j(t)dt \ (\text{for power} : 0) \\
&\Phi_{i,1}(x,y,t) = -\sum_{j=0}^{+\infty}a_{i,j}\int_{t_0}^{t}P_j(t)dt - \int_{t_0}^{t}\left(F_i(x,y,t,\Phi_{1,0},\cdots,\Phi_{n,0}) - h_i\right)dt \ (\text{for power} :1) \\
&\Phi_{i,2}(x,y,t) = \int_{t_0}^{t}\left(F_i(x,y,t,\Phi_{1,0},\cdots,\Phi_{n,0},\Phi_{1,1},\cdots,\Phi_{n,1})\right)dt \ (\text{for power} :2) \\
&\Phi_{i,j}(x,y,t) = \int_{t_0}^{t}\left(F_i(x,y,t,\Phi_{1,0},\cdots,\Phi_{n,0},\Phi_{1,j-1},\cdots,\Phi_{n,j-1})\right)dt \ (\text{for power} : j)
\end{aligned}\right\}
$$

(A.8)

Finally, if we solve these equations in such a way that $\Phi_{i,1}(x,y,t) = 0$, then Eq. (A.8) results in

$$\Phi_{i,1}(x,y,z,t) = \Phi_{i,2}(x,y,z,t) = \cdots = 0 \qquad (A.9)$$

Hence the exact solution may be obtained as the following:

$$\phi_i(x,y,t)\big|_{i=1,\dots,n} = \Phi_{i,0}(x,y,t) =$$

$$f_i(x,y,z) + \sum_{j=0}^{+\infty} a_{i,j} \int_{t_0}^{t} P_j(t)dt \qquad (A10)$$

It is worthwhile to mention that if $h_i(x,y,t)\big|_{i=1,\dots,n}$ and

$\phi_{i,0}(x,y,t)\big|_{i=1,\dots,n}$ are analytic when t is at the vicinity of t_o, then their Taylor series can hence be defined as:

$$\begin{cases} \phi_{i,0}(x,y,t)\big|_{i=1,\dots,n} = \sum_{j=0}^{+\infty} a_{i,j}(x,y,t)(t-t_0)^n \\ h_i(x,y,t)\big|_{i=1,\dots,n} = \sum_{j=0}^{+\infty} a_{i,j}^*(x,y,t)(t-t_0)^n \end{cases} \qquad (A11)$$

These series can be used in Eqs. (A.11), where

$a_{i,j}(x,y,t)\big|_{i=1,\dots,n;j=1,\dots,n}$ are unknown coefficients to be

computed, and $a_{i,j}^*(x,y,t)\big|_{i=1,\dots,n;j=1,\dots,n}$ have given values.

APPENDIX B

The Boubaker Polynomials Expansion Scheme BPES is a resolution protocol which has been successfully applied to several applied-physics and mathematics problems. The BPES protocol ensures the validity of the related boundary conditions regardless main equation features. The BPES is mainly based on Boubaker polynomials first derivatives properties:

$$\begin{cases} \sum_{q=1}^{N} B_{4q}(x)\bigg|_{x=0} = -2N \neq 0; \\ \sum_{q=1}^{N} B_{4q}(x)\bigg|_{x=r_q} = 0; \end{cases} \qquad (B.1)$$

and:

$$\begin{cases} \sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\bigg|_{x=0} = 0 \\ \sum_{q=1}^{N} \frac{dB_{4q}(x)}{dx}\bigg|_{x=r_q} = \sum_{q=1}^{N} H_q \\ \text{with}: H_n = B'_{4n}(r_n) = \left(\dfrac{4r_n[2-r_n^2] \times \sum_{q=1}^{n} B_{4q}^2(r_n)}{B_{4(n+1)}(r_n)} + 4r_n^3 \right) \end{cases} \qquad (B.2)$$

Several solution have been proposed through the BPES in many fields such as numerical analysis, theoretical physics, mathematical algorithms, heat transfer, homodynamics, material characterization, fuzzy systems modeling and biology.

For solving system (7), by the BPES, the following expression is set:

$$u(x) = \frac{1}{2N_0} \sum_{k=1}^{N_0} \lambda_k \times B_{4k}(xr_k) \qquad (B.3)$$

where B_{4k} are the 4k-order Boubaker polynomials, $x \in [0,1]$ is the normalized variable, r_k are B_{4k} minimal positive roots,

N_o is a prefixed integer and $\lambda_k\big|_{k=1..N_0}$ are unknown pondering real coefficients.

Thanks to the properties expressed by Equations (B.1) and (B.2), boundary conditions are trivially verified in advance to resolution process. The system (7) is hence reduced to:

$$\begin{cases} -\dfrac{1}{2N_0} \sum_{k=1}^{N_0} \lambda_k \times \dfrac{dB_{4k}(xr_k)}{dx} - \dfrac{Q}{2VN_0} \\ (k_f - K_e)(\varepsilon \dfrac{1}{2N_0} \sum_{k=1}^{N_0} \lambda_k \times \dfrac{d^2B_{4k}(xr_k)}{dx^2} + 1) = 0 \end{cases} \qquad (B.4)$$

The BPES solution is obtained by determining the non-null set of coefficients

$\tilde{\lambda}_k\big|_{k=1..N_0}$ that minimizes the absolute difference Δ_{N_0}:

$$\begin{cases} \Delta_{N_0} = \left| \left(\dfrac{1}{2N_0} \sum_{k=1}^{N_0} \tilde{\lambda}_k \times \Lambda_k \right) - \left(\dfrac{1}{2N_0} \sum_{k=1}^{N_0} \tilde{\lambda}_k \times \Lambda'_k \right) \right| \\ \text{with}: \\ \Lambda_k = \int_0^1 \dfrac{d^2B_{4k}}{dx^2}(x \times r_k)dx \\ \Lambda'_k = \dfrac{Q}{2VN_0}(k_f - K_e)\int_0^1 \left(\varepsilon \dfrac{d^2B_{4k}}{dx^2}(x \times r_k) + 1 \right)dx \end{cases} \qquad (B.5)$$

CONCLUSION

In this work we have tried to give evidence to the efficiency of an enhanced protocol: the Enhanced Homotopy Perturbation Method EHPM and the Boubaker Polynomials expansion Scheme BPES as tools for solving differential equations. These schemes have been successfully applied to the model of adsorption f Yterium inside ZnO würtzite matrix.. Solutions have been plotted in the time-temperature *t-T* planes and favorably compared to some results presented in the recent related literature.

Obtained results can be a sustainable guide for decision making, understanding physicochemical parameters evolution patterns and rationally controlled improvement of the chemical process in adsorption-desorption protocols. It is scheduled to consider the diffusion/dispersion phenomena along with replacement of the steady doping source by a continuous supply. For the BPES resolution, the convergence speed, as a main concern, is under study and evaluation in our research group.

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