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Accurate Modelling and Simulation of Boron Diffusion in Textured Solar Cells

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Abstract

The aim of this paper is to develop accurate mathematical models to investigate Boron diffusion in textured solar cells. Most of the papers found in literature have investigated Boron diffusion in planar solar cells. However, texturing affects significantly both Boron diffusion processes and cell performance. Since texturing creates extra defects in the valleys of texturing pyramids, increases the surface area of the cell, and causes significant residual stresses. We are proposing and selecting from literature suitable diffusion models that provide Boron diffusion profiles for textured cells that are in good agreement with experiments found in literature. Numerical results showing the effects of texturing geometry on Boron diffusion for a sample solar cell will be presented, analyzed, and validated. We found that both the magnitude of the Boron diffusion concentrations and the Boron diffusion depths are decreasing with increasing texturing angles. Therefore, the optical efficiency will be significantly affected.

Keywords
Accurate models, numerical simulation, texturing geometry, Boron diffusion, solar cells.

1. Introduction
The aim of this paper is to develop accurate mathematical models for the ion implantation and ion diffusion in textured silicon solar cells (Elizabeth et al. 2021), (Johannes et al. 2021, Jurgen at al. 2019), (Netsor at al. 2010), (Song and Meixiang 2018). Firstly, we are including the effects of the texturing geometry on ion implantation by improving the equations of the standard Pearson IV model. The existing standard Pearson IV model does not include the effects of texturing on ion implantation. The standard Pearson IV model has been widely used by semiconductor community to investigate ion implantation in planar solar cells (Elizabeth et al. 2021), (Johannes et al. 2021), (Jurgen at al. 2019), (Hanane et al., 2016), (Fa-Jun et al., 2014). This model needs to be improved for textured solar cells (El Boukili 2019). Secondly, we are including the effects of texturing geometry in the equations of ion diffusion in textured solar cells through Poisson's equation (El Boukili 2019). This will significantly improve the accuracy of the ion diffusion profiles in textured solar cells. In recent literature, researchers are using the same mathematical models for planar and textured solar cells (Hanane et al., 2016), (Fa-Jun et al., 2014). This is not accurate. The experimental results found in literature for ion diffusion are proving that many extra effects are caused by texturing. These effects are not present in planar solar cells. First, texturing will increase the planar surfaces of the solar cell and introduce extra defects at the valleys and at the tips of the texturing pyramids. This will reduce the ion implanted dose and then the diffusion profiles of the dopants as Boron. Our motivation in this research is an attempt to add little improvement to the existing mathematical models used in literature for ion implantation and diffusion in textured solar cells. The existing models are not accurately considering the effects texturing. This research is needed by the community of solar cells to help predict accurately the performance of the recent textured solar cells and reduce their cost to market. The problem we are trying to solve in this research is how to model mathematically the effects of the texturing geometry on ion implantation and diffusion. This is not a piece of cake. and it is still a big challenge. As far as we know, no one is working on these issues.

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We have three objectives in this paper. The first objective is to include the texturing angle θ in Pearson IV model used for ion implantation. The second objective is to include this same angle θ in the ion diffusion equations through Poisson's equation. The third objective is to investigate, analyze and optimize the effects of this angle θ and Pearson IV model on the diffusion of Boron under different temperatures and diffusion times. We define the texturing angle θ as the angle between the incident ions and the normal **n** to a given face of a pyramid on the front surface of a textured solar cell, see Figure 1. In this paper, we are considering periodical pyramids and front sided texturing. However, the models we are proposing are suitable for random pyramids and double-sided texturing. Each pyramid has four faces. We are considering an arbitrary face.

2. Literature Review

One of the innovative steps in the fabrication processes of the modern solar cells is texturing. It is applied to reduce the reflection losses by more than 10% and improve the optical absorption of the front or rear surface of the planar solar cells (Elizabeth et al. 2021), (Johannes et al. 2021), (Jurgen at al. 2019), (Netsor at al. 2010), (Song and Meixiang 2018). However, according to literature, the optimization of the texturing geometry is still a challenge (Johannes et al. 2021), (Ngwe et al. 2018), (Xinyu et al. 2017), (Fa-Jun et al., 2014).

Among the fabrication processes of recent crystalline solar cells we use: ion implantation and ion diffusion (Wegierek and Pastuszak 2021), (Jayer et al. 2021), (El Boukili 2019), (Bothe 2005), (Ohrdese 2011), (Zimbardi 2012). (Rohatgi 2012); (Pawlak 2012); (Benick 2009); (Ohrdes 2011); (Zimbardi 2012); (Coletti 2012); (Meier 2010).

In literature, the standard Gauss probability density function C(x) or the standard Pearson IV probability density function F(x) are used to model mathematically the ion implantation in planar or textured solar cells (Fa-Jun et al., 2014). In our previous work (El Boukili 2019), we have modified these two densities C(x) and F(x) to consider the effects of the texturing angle, θ, on these standard Gauss and Pearson IV probabilities. We have proposed the following probabilities $C(x,\theta)$ and $F(x,\theta)$ that are more accurate than C(x) and F(x) for textured solar cells:

$$C(x,\theta)=\frac{\phi\cos(\theta)}{\sqrt{2\pi\sigma}}\exp\left[-\frac{(x-R)^2}{2\sigma}\right] \tag{1}$$

$$F(x,\theta)=\phi\cos(\theta)E\exp\left[F\times G\right]. \tag{2}$$

Where,

$$E=\left|b+cs+ds^2\right|^{\frac{1}{2d}} \tag{3}$$

$$F=-(\frac{c}{2d}+a)\frac{2}{\sqrt{4bd-c^2}} \tag{4}$$

$$G=\arctan(\frac{2ds+c}{\sqrt{4bd-c^2}}) \tag{5}$$

The coefficients *a, b, c*, d, are calculated from the four moments of C(x) as follows:

$$a=c \tag{6}$$

$$b=\frac{4\beta-3\gamma^2}{10\beta-12\gamma^2-18}\sigma^2 \tag{7}$$

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$$c = -\frac{\beta + 3}{10\beta - 12\gamma^2 - 18}\gamma\sigma \tag{8}$$

$$d = -\frac{2\beta - 3\gamma^2 - 6}{10\beta - 12\gamma^2 - 18} \tag{9}$$

For more details, you could see (El Boukili 2019). In our previous research paper (El Boukili 2021), we have developed a mathematical model for ion diffusion in textured solar cells (MMDTSC) where we have applied the modified Gauss probability density $C(x,\theta)$ in Poisson's equation. However, Gauss probability density uses only the two first moments: Range and Standard Deviation. The approximation of a real doping profile using Gauss probability density is only accurate to the first order. In this paper, we are applying the modified Pearson IV probability density $F(x,\theta)$ in Poison's equation to get more accuracy in ion implantation and ion diffusion in textured solar cells. Pearson IV model is more accurate than Gauss model since it uses the four moments: Range, Standard Deviation, Skewness, and Kurtosis.

3. Development of an accurate model for diffusion in textured solar cells

The single side or double-sided texturing increase the sun light absorption and the optical efficiency of the planar solar cells, see Figures 1 and 2.

However, ion implantation and diffusion are more challenging in solar cells with textured surfaces than in solar cells with planar surfaces. For example, texturing pyramids cause the buildup of extra defects at the valleys between pyramids and at the types of pyramids. To help the solar cell community understand and optimize the effects of texturing geometry on ion diffusion, we have developed a comprehensive set of ion diffusion models in our previous paper (El Boukili 2021). In our previous paper (El Boukili 2021), we have applied Gauss probability density. In this paper, we are applying Pearson IV probability density in Poisson's equation (10) to get more accuracy in Boron diffusion profiles in textured solar cells. The improved model we are proposing is given by the following six nonlinear partial differential equations (10) to (15) whose unknowns are the functions: $(\varphi, C_A, C_{AI}, C_{AV}, C_I, C_V)$.

$$div(\varepsilon\nabla\varphi) = q.(n - p - C_{net}). \tag{10}$$

$$\frac{\partial C_A(x,t)}{\partial t} = R_A \tag{11}$$

$$\frac{\partial C_{AI}(x,t)}{\partial t} = -div(J_{AI}) + R_{AI} \tag{12}$$

$$\frac{\partial C_{AV}(x,t)}{\partial t} = -div(J_{AV}) + R_{AV} \tag{13}$$

$$\frac{\partial C_I(x,t)}{\partial t} = -div(J_I) + R_I \tag{14}$$

$$\frac{\partial C_V(x,t)}{\partial t} = -div(J_V) + R_V \tag{15}$$

Where

$$C_{net} = -\sum_{i=1}^{N} z_i C_i(x,\theta). \tag{16}$$

The probability density $C_i(x,\theta)$ is the concentration of the dopant number 'i' obtained after a doping process. It is calculated using Pearson IV probability density $F(x,\theta)$ as follows:

$$C_i(x,\theta = F(x,\theta) = \phi\cos(\theta)E\exp\left[F \times G\right] \tag{17}$$

These equations are solved using Finite Volumes method for space discretization and Newton's method to linearize the equations. The following densities $\varphi, C_A, C_{AI}, C_{AV}, C_I, C_V$ represent the: electrostatic potential, unpaired dopant concentration, paired dopant concentration with Interstitials and Vacancies, unpaired Interstitials, and unpaired Vacancies respectively. The other parameters and functions are described in (El Boukili 2021) (Figure 3)

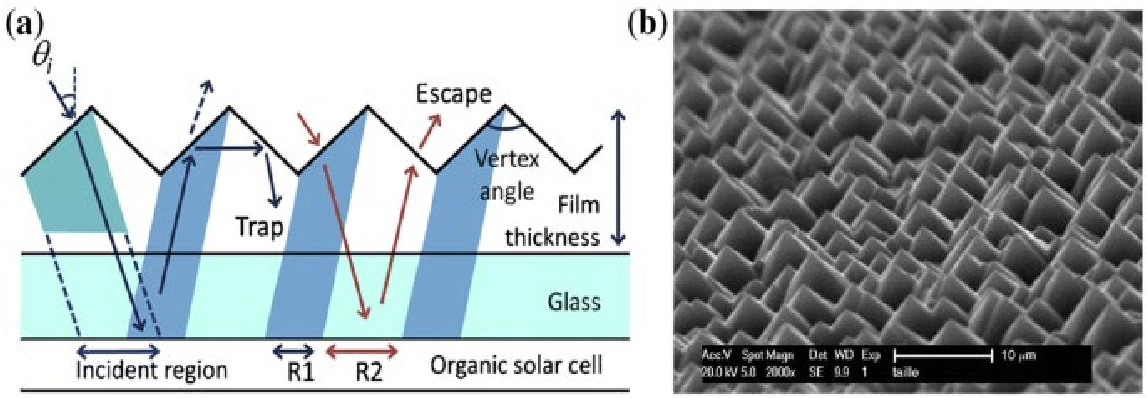

Figure 1. Texturing enhances light absorption by the solar cell. (a) cross section showing texturing angle θ . (b) top view of textured cell.

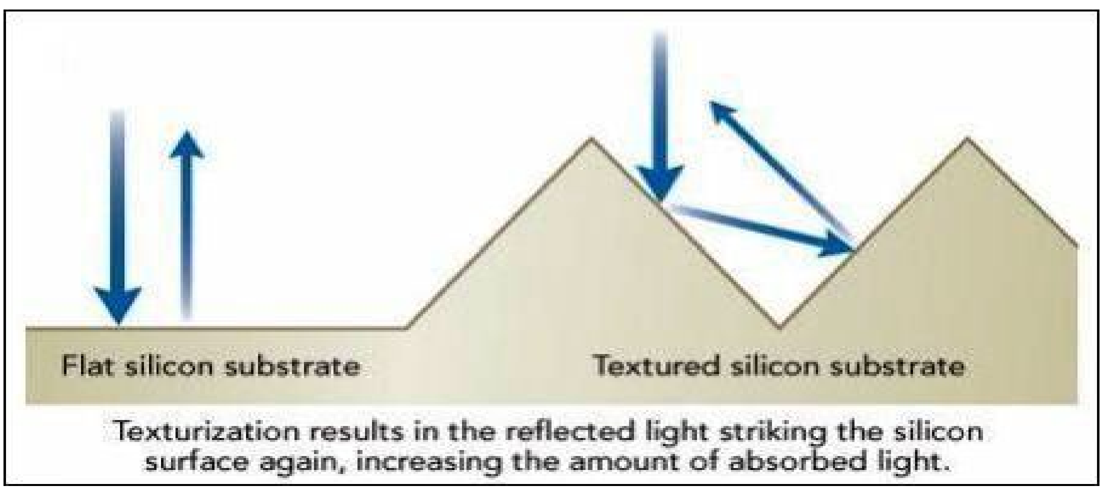

Figure 2. Reflection losses are smaller in textured solar cells

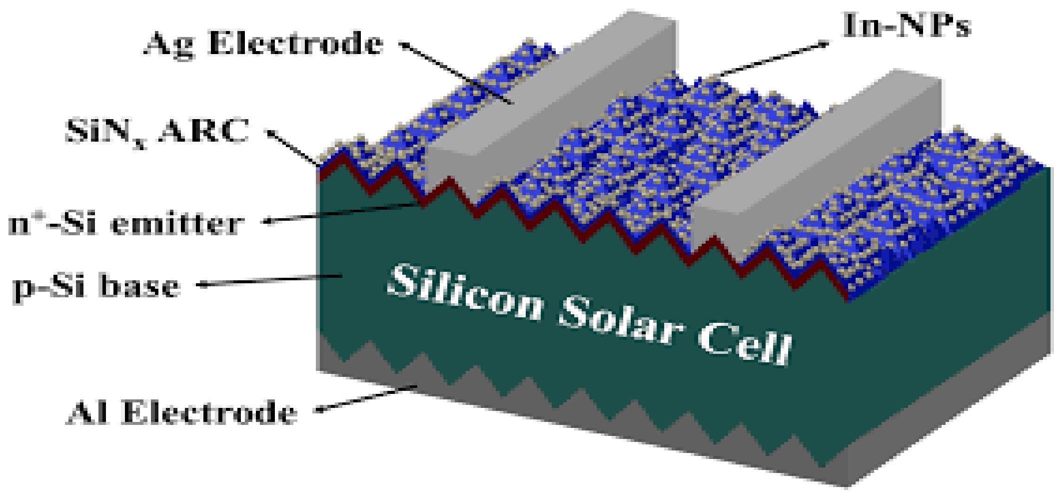

Figure 3. Double-sided textured solar cell with upward pyramids.

5. Results and Discussion

The numerical results presented here are for a solar cell that is textured with identical pyramids of faces (111) as shown in Figure 4. We have investigated the effects of different texturing angles going from 30° to 80° degrees. We have used for all these results Pearson IV model, $F(x,\theta)$, for Boron implantation in the textured solar cell shown in Figure 4. The height of pyramids is 0.12um. The width of the pyramids is 0.05um. The dose of Boron is $2\times10^{15} cm^{-2}$, implant energy is 10 KeV. The depth, y, of the cell is 0.37 um and the length, x, is 0.3 um.

Figure 4 shows the mesh of the solar cell and the Boron diffusion profile on textured solar cell for θ=30°. Figure 5 shows the 1D cut of the Boron diffusion profile at x=0.15 and θ=30° and y between 0 um and 0.15 um. Figure 6 shows the cut of the Boron diffusion profile at x=0.15 and θ=60° and y between 0 um and 0.15 um. Figure 7 shows the cut of the Boron diffusion profile at x=0.15 and y between 0 um and 0.15 um for a planar solar cell. From careful investigations of the Figures 7, 6, and 5, we concluded that the Boron diffusion profiles on textured solar cells have lower maximum values and shallow depths when the texturing angles are large. For θ=30°, the maximum value of the diffused Boron is 1.2e+20 (atom/cm-2) (see Figure 5). For θ=60°, the maximum value of the Boron diffusion profile is 7e+19 (atom/cm-2) (see Figure 6). These 2 values are smaller than the maximum value of the diffused Boron on planar solar cells which is 4e+20 (atom/cm-2) (see Figure 7). The diffusion depth on textured surface for θ=30° is about 0.05 um and on flat surface is about 0.08 um. The Boron diffusion profiles shown in the Figures 5 and 6 are qualitatively in good agreement with the experimental diffusion profiles found in recent literature (Cui et al. 2021) , (Adriano et al. 2020).

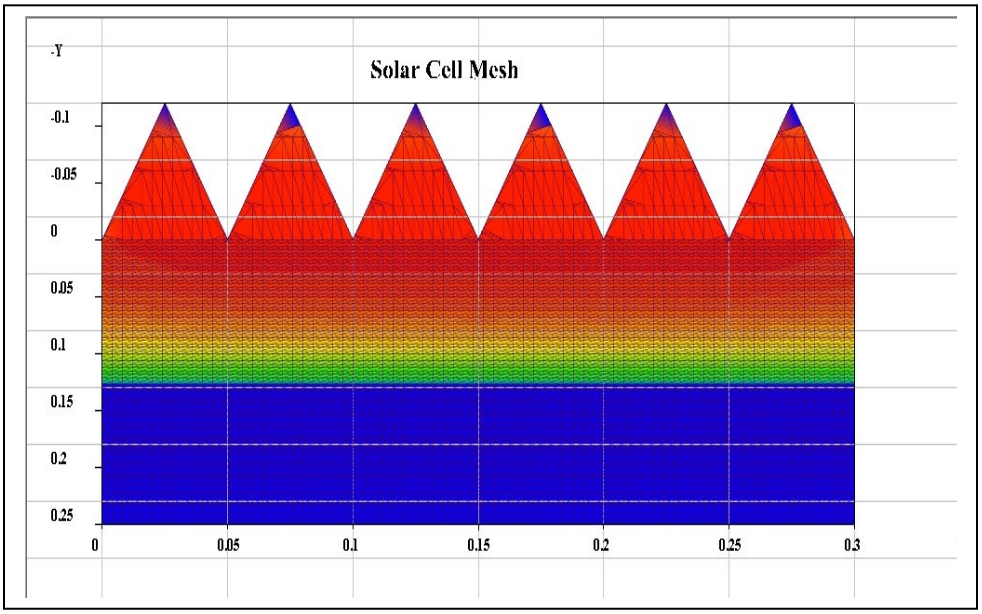

Figure 4. Mesh and Boron diffusion profile for θ=36° using Pearson IV model.

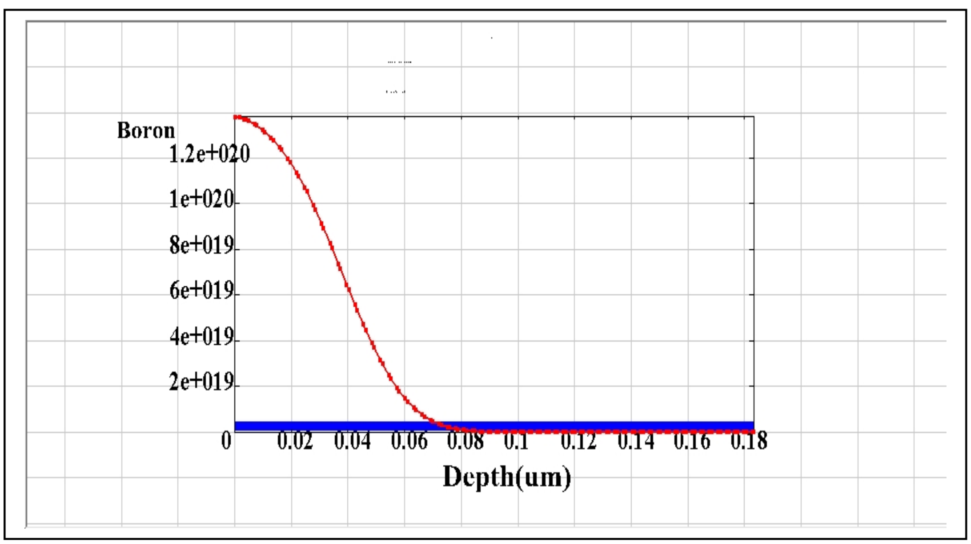

Figure 5. 1D Cut of Boron diffusion profile on textured surface for θ=30°.

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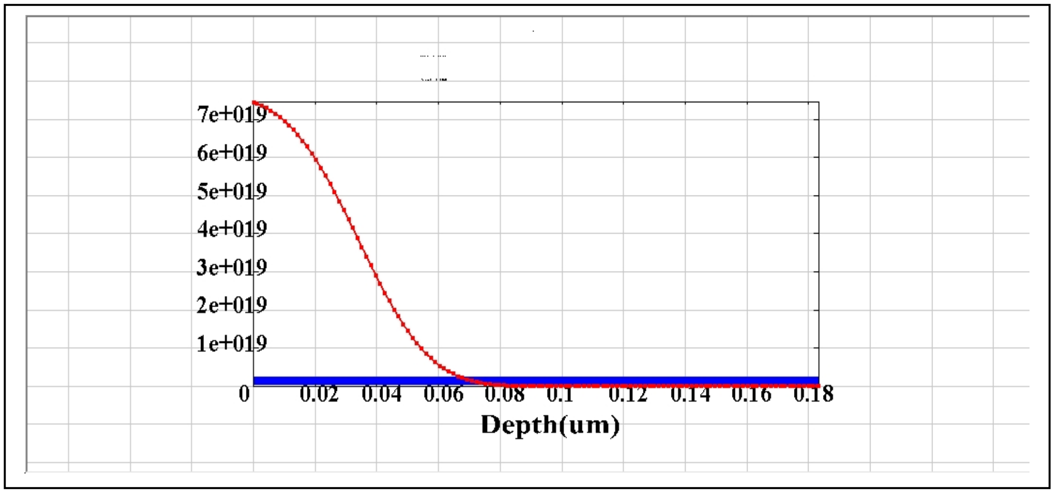

Figure 6. Boron diffusion profile on textured surface for θ =60°.

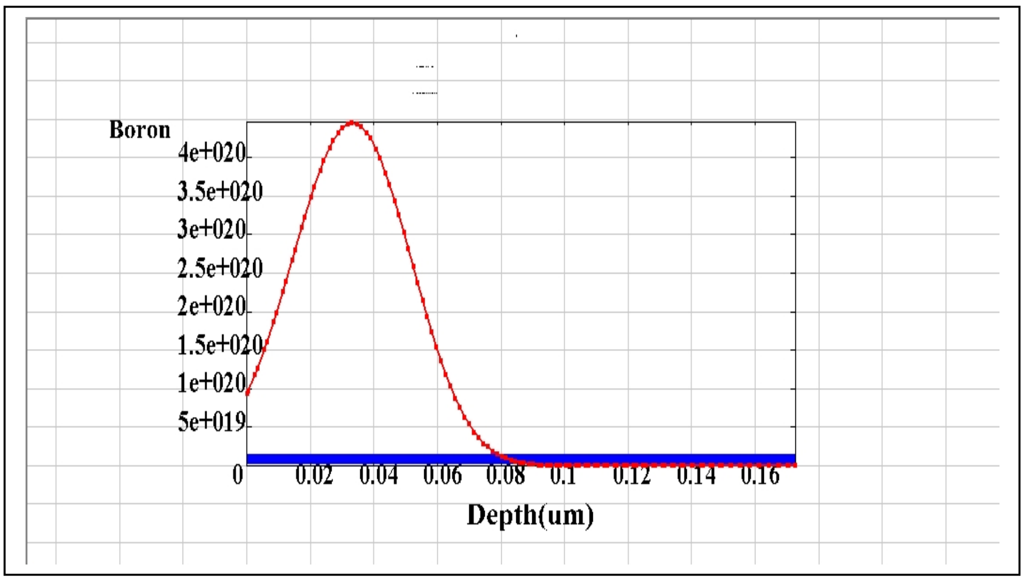

Figure 7. Boron diffusion profile on a planar solar cell.

6. Conclusion

The findings in this research paper are explaining some of the effects of texturing angles on the Boron diffusion profiles in textured solar cells. The simulation results are confirming that the magnitude of the Boron diffusion profiles is decreasing with increasing texturing angles. The diffusion depths are also decreasing with increasing texturing angles. Therefore, the optical efficiency will be significantly impacted. The use of Pearson IV model in implantation and diffusion equations provided Boron diffusion profiles that are in good agreement with experimental profiles found in recent literature. We will study the impact of texturing with random pyramids on the diffusion of Boron in double-sided textured solar cells in our future work.

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Biography

Abderrazzak El Boukili received both the PhD degree in Applied Mathematics in 1995, and the MSc degree in Numerical Analysis, Scientific Computing and Nonlinear Analysis in 1991 at Pierre et Marie Curie University in Paris-France. He received the BSc degree in Applied Mathematics and Computer Science at Picardie University in Amiens-France. In 1996 he had an industrial Post-Doctoral position at Thomoson-LCR company in Orsay-France where he worked as software engineer on Drift-Diffusion model to simulate heterojunction bipolar transistors used in radar applications. In 1997 he had European Post-Doctoral position at University of Pavia-Italy where he worked as research engineer on software development for simulation and mathematical modeling of quantum effects in heterojunction bipolar transistors used in mobile phones and high frequency applications. In 2000 he was Assistant Professor and Research Engineer at the Universit of Ottawa in Ottawa-Canada. During 2001-2002 he was working at Silvaco Software Inc. in Santa Clara, California-USA as Senior Software Developer on mathematical modeling and simulations of vertical cavity surface emitting lasers. Between 2002-2008 he was working at Crosslight Software Inc. in Vancouver-Canada as Senior Software Developer on 3D Process simulation. Since Fall 2008 he is working as Assistant Professor of Mathematics at Al Akhawayn University in Ifrane-Morocco. His research interests are in industrial software development for simulations and mathematical modeling of opto-electronic devices and processes.

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