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Modification of the Ion Angular Distribution in Plasma Sheath: Modeling Approach under COMSOL Multiphysic

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Abstract: System for in-situ control of the ion angular distribution function (IADF) in plasma reactor is modeled. Typical IADF depends on the pressure, bias and excitation frequency. It is formed due to an ion transport mechanism under the different physical properties of the plasma and sheath domains. The opportunity to control IADF independently on process parameters is achieved by novel design. It is proposed to modify and actually control the IADF by biased grid(s) which are built-in into a substrate holder. A grid bias is generating the time varying E-field within sheath – providing spatially resolved lateral component of the E-field, thus it is influencing the ion path. Developed 2D/3D sheath model (SM) is used to investigate the ion transport at the substrate surface.

Keywords: IADF, sheath, modeling, plasma.

1. Introduction

This contribution deals with a modeling of a system that enables *in-situ* modification and control of the IADF at the surface of a silicon wafer. The initial application of the approach is aiming at the first to the implementation in the semiconductor technology. *In-situ* control and modification of the IADF at the substrate surface will have an impact on etch and/or deposition profile variation, thus having and impact on critical dimensions of the profile and its variation. The deposition conformality (sidewall coverage) may be affected as well as in plasma based deposition techniques. Another potential implementations are for surface structuring without a need to involve additional steps for a pattern transfer (that is litho- and resist processing), for example, in MEMS technology and nanotechnology providing specific structural initial and *in-situ* conditions to enable controlled self-assembling and growth. For example, a surface roughness control or in-*situ* film properties tailoring might find applications in a plasma-aided nanofabrication, preparation of the bio-semiconductor interfaces, etc. It is known, that impact angle has effect on film structure and its growth. The ion-milling is used to control clustering of nanostructured, columnar thin films.[1] Nanostructured AlN is attractive for the future nanodevice applications – it is possible to direct the growth process by DC toward quasi-3D columnar structures.

Although, it is remaining still essentially unclear, at the nano-processing scale, how to select the most effective control parameters and conditions to tailor individual nanostructures (a morphology, shape and sizes of various structures) to be optimal for new advanced technologies and devices.[2] For example, amazing observations by large number of researchers in nanotubes (NT) growth in low temperature plasma revealed that NT alignment is perfectly the same as that of the electric field in sheath.[2] Though, this effect still is not explained conclusively, one explanation that helps clarify the basic understanding of this phenomenon is related to the ion fluxes at the surface. These are the most responsive to electric fields. Applying an external electric field parallel to the substrate surface – carbon NT can be actually bent.[3] Selective manipulation of the ions fluxes can be instrumental in maintaining a steady growth with a predetermined shape[4], also reshaping of caved cylindrical nanorods into conical spike-like microemitter structures[5], the alignment of the gallium-zinc oxide nanorods[6], etc. Obviously, there are significant application opportunities for industry in approaching the ion flux distribution control for post-processing, coating with nanofilms, functionalization, doping, and many other technologies.

2. Formulation of the proposed approach

In the plasma reactors, the wafer is supported by electrode, which is typically coupled to an RF generator through a blocking capacitor and an impedance matching unit. A plasma sheath occupies a narrow domain between the plasma and the surface of the wafer. Classic textbook on plasma physics and sheath theory can be found elsewhere.[7]

Typical IADF of ions arriving to the wafer surface will depend on the gas pressure and electrode potential in respect to the plasma potential. The IADF in low pressure plasma domain is isotropic with energy, that is only slightly above the background gas kinetic energy ($T_i>T_g$). However, the ions are reaching surface with a significant normal velocity component and small lateral component (Figure 1). This is due to the difference in the physical properties of the plasma and sheath domains and thus the ion transport through subdomains. The normal component within sheath is increased due to the sheath potential and will depend also on the applied frequency. The characteristic IADF in plasma etch processing is illustrated in Fig. 1-b. More information on IADF properties can be found elsewhere.[8,9]

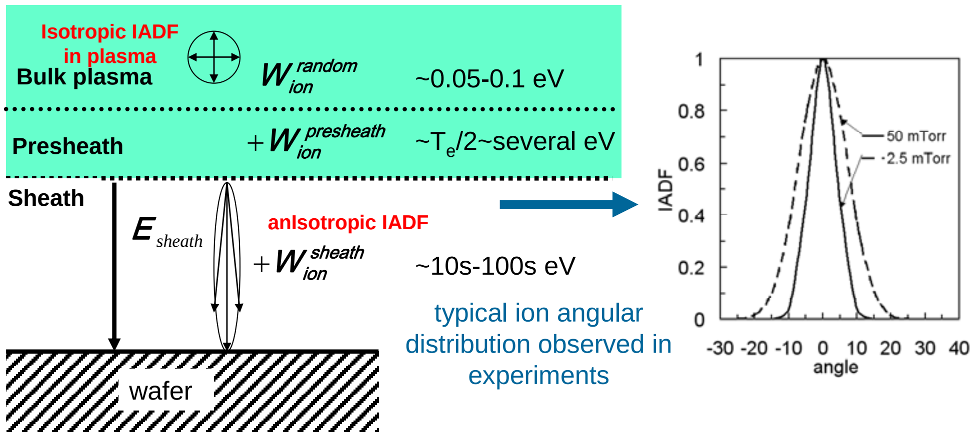


Figure 1: Typical structure (a) of the plasma-wall interface and production of the angular distribution of the ions within sheath. Characteristic IADF at low pressures (b).

Besides the primary process conditions (chamber pressure, bias and frequency of the RF electrode) the IADF illustrated in Figure 1-b can be modified by applying the external electric field. Increase of the lateral component of the E-field would be the most effective way. To generate lateral E-field we introduced a "grid system" (Figure. 2) into holder, which is underlying the silicon wafer.

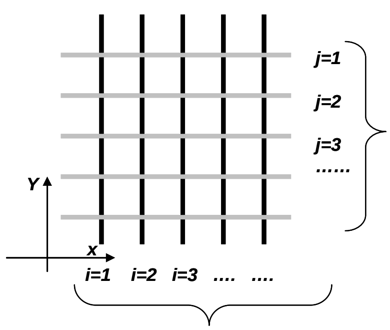


Figure 2: Grid structure used in model in so-called "cross-wire-bias" configuration.

The individual conductors of the grid are supposed to be biased in specific fashion.[10] Here, we will consider simple cases without going into more complex biasing schemes. Because of the presence of the biased grid (applied potentials V^i and V^j to individual conductors) the electric field will be created with component lateral to a surface (Figure 3.). Such transient potential on grid will enable generation of a time varying electric fields in sheath, thus changing path of the ions over processing time. The ion path will create specific pattern of ion flux focusing on the top of the wafer. The IADF will vary in dependence on the {x,y} coordinate on the wafer (this will be predetermined by a grid configuration) and will change also over time domain. In the simplest case, the IADF might have form of the bi-angular distribution function (Figure 4-b,c) or some more complex form.

The real image of the IADF in 3D will look more complex. The impact of the ion flux onto the surface structuring can be determined only by simulation or experiment. Furthermore, the initial IADF is not necessarily the same at every point on the surface of the wafer, and can vary across the surface of the wafer. Thus, a local modeling cell (sheath model, SM) should be fed by a full scale reactor plasma model (axial 2D). And, speaking in terms of technologist, the most valuable information will be “how the modification of the IADF will affect etch or deposition process at the surface of the wafer?” That means, certain surface chemistry should be considered and a feature profile simulator has to be available to complete such feasibility study. In this model we will deal with local sheath model, assuming we have available yet plasma model within reactor and feature profile evolution model. Block scheme of such model for complete evaluation of the IADF control is shown in Figure 5.

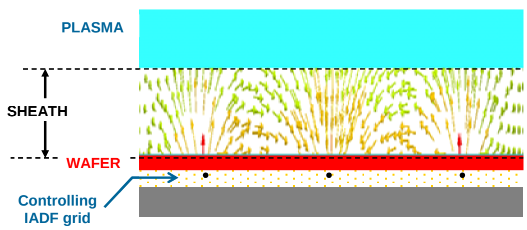


Figure 3: Simulated electric field in sheath by 2D model.

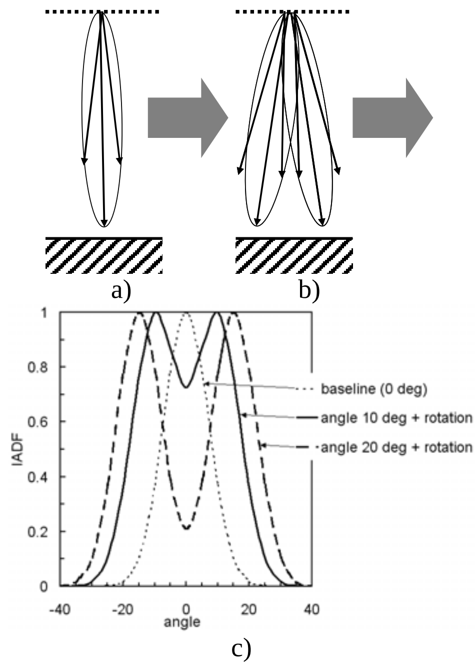


Figure 4: Typical angular distribution of the ions in sheath (a) and suggested modification of the distribution for simulation tests (b); plot (c) shows curves transition from mono-angular IADF to bi-angular IADF.

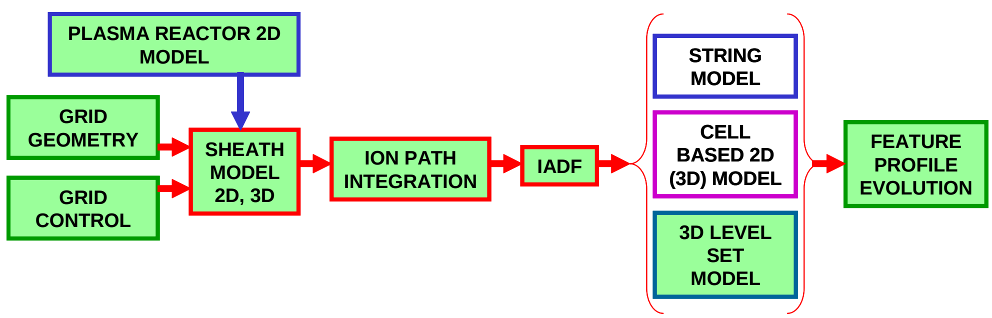
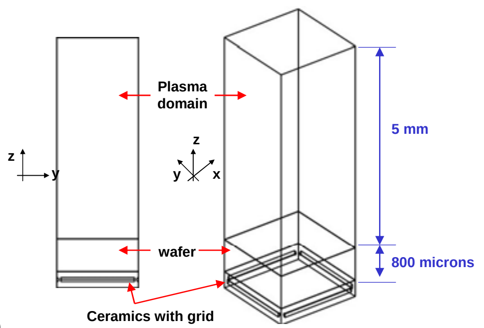


Figure 5: Block scheme of the model to investigate the IADF impact on the surface features.

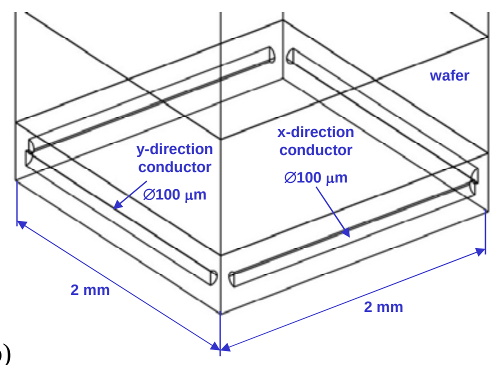
3. Model description

3.1 Sheath model

It is apparent from a block scheme (Figure 5) that feasibility study of the task described in Sec. 2 could be executed under single platform – Multiphysics COMSOL (this is illustrated by blocks in green color). Scope of this paper is focused on the sheath model and IADF determination (see red-frame blocks in Figure 5). We used Electrostatics from AC/DC module to compute and investigate the electric field within a sheath domain. Considering only one-dimensional grid gave option to start with 2D model, However, the actual grid (Figure 2) is planar structure in plane {x,y} and it is quite reasonable, and actually necessary, to build sheath model in 3D to explore the real impact of ions on the surface. In the case of rectangular grid (Figure 2) we used simple geometry for sheath model within a single cell of the grid with 3 domains CERAMICS, WAFER and PLASMA (see Figure 6). Ceramic coating with integrated grid is made of alumina (relative permittivity ε_r=10), and silicon wafer (ε_r=10) is interfacing with plasma domain (ε_r=1). Larger 3D models with multiple cells were computationally more expensive.



a)



b)

Figure 6: Model in 3D geometry: (a) Basic cell for sheath model; (b) detail of ceramic coating with integrated grid.

We used Lieberman's formulation[7] for collisionless DC sheath. Definition of the parameters and variables in model is obvious from Figure 7. The assumptions are: Maxwellian electrons at temperature T_e, cold ions (T_i=0) in bulk region and quasi-neutrality of the plasma in bulk (n_e=n_i=n) and presheath (n_{es}=n_{is}=n_s) region. Boltzmann relation for electrons in sheath defines $n_e(x)$ as it follows

$$n_e(x) = n_{es}\, exp\left(\frac{\Phi(x)}{T_e}\right) \qquad (1)$$

Sheath edge is considered at potential Φ=0. From ion energy conservation it follows that ion density within a sheath is described by relation

$$n_i(x) = n_{is}\left(1 - \frac{2e\Phi(x)}{m_i u_s^2}\right)^{-1/2} \qquad (2)$$

The nonlinear equation governing the sheath potential and ion and electron densities is obtained by rewriting Poisson's equation after substitution of relations (1) and (2) in form

$$\frac{d^2\Phi}{dx^2} = \frac{en_s}{\varepsilon_0}\left[exp\left(\frac{\Phi(x)}{T_e}\right) - \left(1 - \frac{2e\Phi(x)}{m_i u_s^2}\right)^{-1/2}\right] \qquad (3)$$

Above, the electron temperature is considered in electronvolt units.

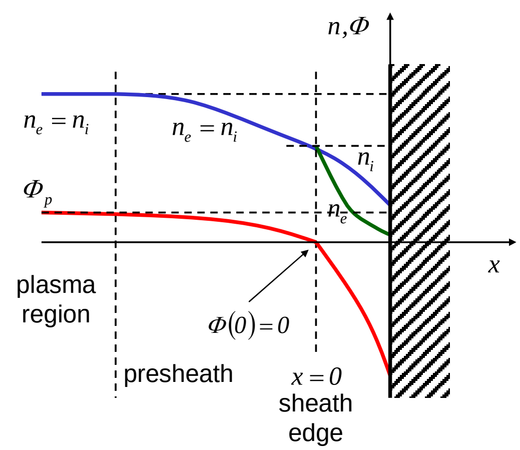


Figure 7: Parameter definition, behavior of the charged particles density and potential in plasma contact with a wall.

Procedure described in paragraph above is easily implemented by GUI in Physics formulation in Comsol. We kept Poisson equation in default form, that is in 3D space potential Φ(x,y,z) it is coupled with variables n_e(x,y,z) and n_i(x,y,z) in form

$$-\nabla \cdot \varepsilon_r \varepsilon_0 \nabla \Phi = \rho = -e(n_i - n_e) \qquad (4)$$

however, when defining subdomain expressions for plasma region we set conditions given in Table 1.

Table 1:

Name	Expression
ni	if(2*q0*V/(Mi*us^2)>1,ns,ns*(1-q0*V/(Mi*us^2))^(-0.5))
ne	if(V>0,ns,ns*exp(V/Te))

Described conditions are governing numerical solution of Poisson’s equation under assumption done at the beginning of this section.

Symmetrical surface boundary conditions (BC) are set at the vertical sidewalls of each subdomain from Figure 6, the top surface boundary is set to relative plasma potential V_{plasma}=20 V (in terms used in this model), and bottom surface boundary is set to electric potential equal to negative DC selfbias (V_{DC}). Interior boundaries are represented by continuity BC. Surface boundary of the grid conductors are set to electric potential per specification for given biasing in simulation.

3.2 Coupling to reactor model

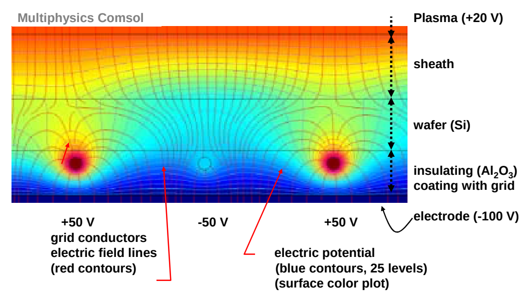
It is possible to obtain input variables for sheath model from suitable plasma model coupled with sheath model. In this particular study – an investigation the impact of grid potential on the IADF - we used preset data known from previous plasma simulation and/or experiment. However, it is straightforward to complement our earlier work[11,12] on plasma fluid model under Multiphysics Comsol (v.3.x) platform by described sheath model. Of course, the outputs from other plasma fluid models or kinetic models can be used as source as well. For instance, recent release of Plasma Module[13] will serve well to couple with described sheath model.

3.3 Coupling to processes on the surface – extrapolation of IADF impact

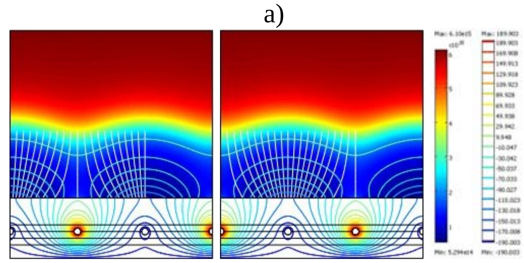
Using computed IADF, the interaction with processed surface for particular technology is involved into model to extrapolate the IADF impact. Etch or deposition process is characterized by feature profile evolution (FPE) simulator. As it is shown in Figure 5, we may consider approach that is complying with a need of immediate availability, for example, code for computing FPE by “string” model.[14] More sophisticated coupling would be option to interface sheath model with “cell-based” FPE simulator[15] which will be available in later phase of this development. However, neither of them are “comsol-friendly environment”. To keep same platform it is necessary to develop PDE-based model in 3D space by using fast marching “level set“ method[16] for FPE simulator under Multiphysics Comsol. Then, it is apparent from a block scheme that feasibility study of above described task could be executed under single platform.

4. Results and Discussion

Currently, work is going from model development phase into feasibility study phase. In this section we will expose several sets of simulation, however more consistently analysis will be done in future work. Main scope of this contribution was to develop a suitable computational sheath model for IADF that can be used evaluation under various geometry and biasing conditions to validate novel device for specific applications.



a)



phase: 0 phase: π

b)

Figure 8: Simulation by 2D model (a) showing electric potential and field in sheath under biased grid, and (b) illustrating ion path at phase 0 (LEFT) and π (RIGHT). Grid potential was ±50V and electrode DC bias -200 V.

Initially, we developed sheath model in 2D geometry. In first moment, it is noticeable in Fig. 8, that application of the grid potential has an impact on the sheath width. Electric field streamlines are focused into location with more negative grid potential (Figure 8-a). Due to this the ions are focused into “negative” grid locations (spots). Actually, we can interpret the total ion flux towards the wafer is split into multiple individual ion flux beams. Thus, grid gives an opportunity to control and modify individual beams. Ion path in Figure 8-b illustrates focusing of single beam into different spots in dependence on the phase of applied bias. Obviously 2D sheath model setup was valid only for one-dimensional grid. Afterwards, we found out that electrical fields will be influenced by the two-dimensional grid. Such focusing effect was also noticeable in 3D sheath model (Figure 9).

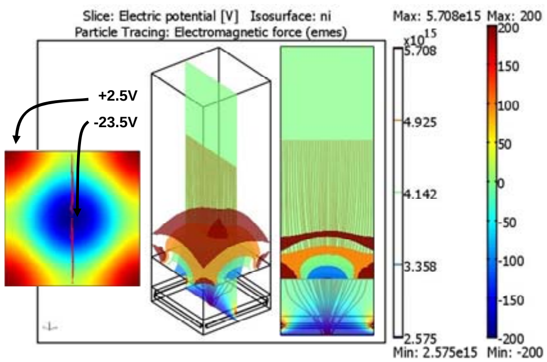
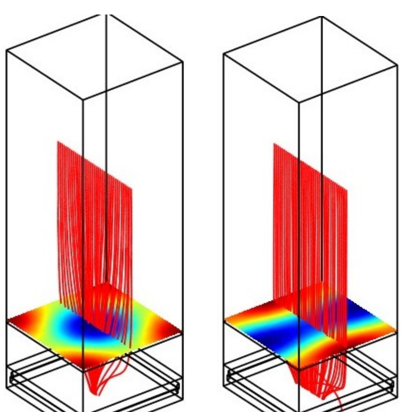


Figure 9: Simulation by 3D model showing electric potential (slice plots in YZ plane) and isosurface plots of the ion density ($n_0=10^{16}$ m^{-3}). On left side is top view on electric potential just above the wafer surface. Particle tracking feature shows focusing behaviour for ions. The grid potential was ±200V and electrode DC bias -200 V.



a) b)

Figure 10: Simulation by 3D model showing argon ions path under varios grid bias conditions. The grid potential was +200V both in x and y-direction, (b) -200 V applied in y-direction. The electrode DC bias was -200 V.

Increased speed of the computation and post-processing were achieved by multiplying individual cells in the model and setting various boundary conditions or parameters settings but keeping them as independent cells (see, Figure 10). Parallel visualization of the results enhanced post-processing significantly.

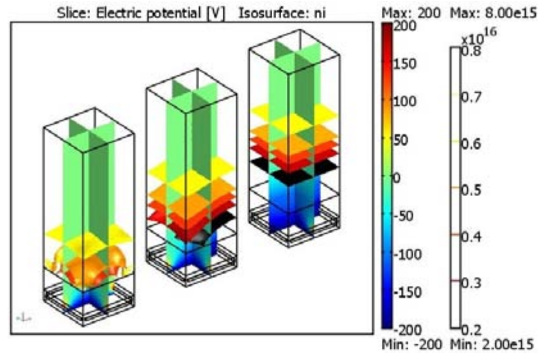


Figure 10: Simulation by 3D model showing electric potential (slice plots in XZ and YZ planes) and isosurface plots of the ion density for various plasma bulk density. The grid potential was ±200V and electrode DC bias -200 V.

5. Conclusions

It is noticeable, that described task is quite extensive and here we are giving only snapshot from proposed approach and model formulation. Sheath model was developed under COMSOL Multiphysics environment. Outputs from reactor scale plasma model under same platform can be used to input data for IADF investigation. The 2D sheath model utilizes Poisson solver from AC/DC module and was extended into transient 3D model. The transient bias at diverse grid geometry was tested investigated. Computed feature profiles will illustrate the feasibility of the proposed technique. Briefly, perspective on PDE-based FPE model in 3D by using fast marching “level set“ method is discussed to support a multiscale model feasibility under single platform.

6. References

1. Jonathan K. Kwan and Jeremy C. Sit, *Nanotechnology* **21** (2010) 295301 (6pp).
2. K. Ostrikov and S. Xu, Plasma-Aided Nanofabrication. Wiley VCH Verlag GmbH & Co. KGaA, Weinheim (2007).
3. J.F.AuBuchon, L-H. Chen, and S. Jin, *Jour. Phys. Chem*. **B109**, 6044 (2005).
4. I. Levchenko, K. Ostrikov, M. Keidar and S. Xu, *Appl. Phys. Lett.* **89**, 033109 (2006)
5. E. Tam, I. Levchenko and K. Ostrikov, *J. Appl. Phys. Lett.* **100**, 036104 (2006)
6. M. Yan, H.T. Zhang, E.D. Widjaja, and R.P.H. Chang, *J. Appl. Phys.* **94**, 5240 (2003).
7. M. A. Lieberman, A.J. Lichtenberg, Principles of plasma discharges and materials processing, John Wiley & Sons, New York (1994); ibid 154.
8. J. R. Woodworth, M. E. Riley, and P.A Miller, Ion distribution functions in inductively coupled radio frequency discharges in argon-chlorine mixtures, *J. Vac. Sci. Technol.* **A 15**(6), 1997, 3015-3023.
9. L. Raja, Analytical model for ion angular distribution functions at rf biased surfaces with collisionless plasma sheaths, *J. Appl. Phys.* **Vol. 92**, No. 1, 2002, 7032-7040.
10. J. Brcka, Control of Ion Angular Distribution Function at Wafer Surface, *US Pat. Appl.* No. 20080242065 (2008).
11. J. Brcka, Stochastic Approach in Approximation of the Transient Plasma Sheath Behavior in FEM. Comsol Conference, Boston, MA (2008).
12. J. Brcka and Song-Yun Kang, Multiphysics Coupling Simulation of Silicon Nitride CVD Using an RLSA Source, *Plasma Processes and Polymers*, DOI: 10.1002/ppap.200931903
13. Multiphysics Comsol v.4.0
14. J. Brcka et al., Simulation of vertical profiles in technology of ICs, *J. El. Eng.* **2**, 33-41 (1992).
15. P. Moroz, URP.00101, GEC, Saratoga, NY, (2009)
16. J.A. Sethian, Level set methods and fast marching methods: Evolving interfaces in computational geometry, fluid mechanics, computer vision, and material science, Cambridge University Press, (1999).