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Computer Physics Communications 174 (2006) 127–132
Computer Physics Communications
www.elsevier.com/locate/cpc

Sparse field level set method for non-convex Hamiltonians in 3D plasma etching profile simulations

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Received 5 May 2005; received in revised form 28 July 2005; accepted 17 September 2005

Available online 27 October 2005

Abstract

Level set method [S. Osher, J. Sethian, J. Comput. Phys. 79 (1988) 12] is a highly robust and accurate computational technique for tracking moving interfaces in various application domains. It originates from the idea to view the moving front as a particular level set of a higher dimensional function, so the topological merging and breaking, sharp gradients and cusps can form naturally, and the effects of curvature can be easily incorporated. The resulting equations, describing interface surface evolution, are of Hamilton–Jacobi type and they are solved using techniques developed for hyperbolic equations. In this paper we describe an extension of the sparse field method for solving level set equations in the case of non-convex Hamiltonians, which are common in the simulations of the profile surface evolution during plasma etching and deposition processes. Sparse field method itself, developed by Whitaker [R. Whitaker, Internat. J. Comput. Vision 29 (3) (1998) 203] and broadly used in image processing community, is an alternative to the usual combination of narrow band and fast marching procedures for the computationally effective solving of level set equations. The developed procedure is applied to the simulations of 3D feature profile surface evolution during plasma etching process, that include the effects of ion enhanced chemical etching and physical sputtering, which are the primary causes of the Hamiltonian non-convexity.

PACS: 85.40.-e; 81.65.-b; 52.75.R

Keywords: Plasma etching; Etching profile; Level set method; Sparse field method; 3D simulations; Non-convex Hamiltonians

1. Introduction

In various fields of science and engineering often arise phenomena in which different materials (or phases) can coexist without mixing. A surface bounding two materials is called an interface, a phase boundary, or front depending upon situation. In some processes a boundary is moving by external driving forces and its velocity does not depend on its geometrical properties. Since the evolution of a boundary is unknown and it should be determined as a part of solutions, the problems including such a boundary are called in general a free boundary problems. The motion of a phase boundary between ice and water is a typical example, and it has been well studied (the Stefan problem).

Another important class of problems are those where the evolution of an interface does not depend on the physical situation outside the boundary, but only on its geometry. There are several examples of such a behavior in material sciences and they are sometimes called the interface controlled problems. Examples are not limited only to material sciences. Some of those comes from geometry, crystal growth problems and image processing.

Level set method, introduced by Osher and Sethian [1], is a powerful technique for analyzing and computing moving fronts in a variety of different settings. Some references to earlier works with similar ideas, as well as deeper analytical results concerning foundations of this method can be found in [3]. The level sets are used in image processing, computer vision, computational fluid dynamics, material science, and many other fields. Detailed exposition of the theoretical and numerical aspects of the method, and applications to different areas can be

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0010-4655/$ – see front matter
doi:10.1016/j.cpc.2005.09.010

found in books [4] and [5], and recent review articles [6–8]. Ref. [9] is a popular and lucid introduction to the subject.

The profile surface evolution in plasma etching, deposition and lithography development is a significant challenge for implementation of numerical methods in front tracking. The level set methods for evolving interfaces are specially designed for profiles which can develop sharp corners, change of topology and undergo orders of magnitude changes in speed. They are based on Hamilton–Jacobi type equation for the level set function using techniques developed for solving hyperbolic partial differential equations. During last several years several variants of the level set methods have been developed with application to micro fabrication problems. In this paper we describe shortly the level set method as well as sparse field method for solving the level set equations. The sparse-field method itself, developed by Whitaker [2], and broadly used in image processing community, is an alternative to the usual combination of narrow band and fast marching procedures for the computationally effective solving of the level set equations [4,5]. After that, we analyze the case of non-convex Hamiltonians in more details. This type of problem is of special interest in studying the evolution of the profile surface during the etching process, especially if we treat it as an interface controlled problem.

Our primary goal is to develop an accurate, stable and efficient 3D code for tracking of the etching profile evolution that includes different physical effects such as anisotropy, visibility conditions and material-dependent propagation rates, yet being computationally effective to run on desktop PCs. This work is one of the preparation steps for accomplishing it.

2. Level set method

The basic idea behind the level set method is to represent the surface in question at a certain time t as the zero level set (with respect to the space variables) of a certain function $\phi(t,\mathbf{x})$, the so-called level set function. The initial surface is given by $\{\mathbf{x} \mid \phi(0,\mathbf{x}) = 0\}$. The evolution of the surface in time is caused by forces or fluxes of particles reaching the surface in the case of the etching process. The velocity of the point on the surface, normal to the surface, will be denoted by $V(t,\mathbf{x})$, and is called velocity function. For the points on the surface this function is determined by physical models of the ongoing processes. In the case of etching it is determined by the fluxes of incident particles and the subsequent surface reactions. The velocity function generally depends on time and space variables and we assume that it is defined on the whole simulation domain. At a later time $t > 0$, the surface is as well the zero level set of the function $\phi(t,\mathbf{x})$, namely it can be defined as a set of points $\{\mathbf{x} \in \mathbb{R}^n \mid \phi(t,\mathbf{x}) = 0\}$. This leads to the level set equation

$$\frac{\partial \phi}{\partial t} + V(t,\mathbf{x})|\nabla \phi| = 0 \tag{1}$$

in the unknown function $\phi(t,\mathbf{x})$, where $\phi(0,\mathbf{x}) = 0$ determines the initial surface. In reality the physical models determine the velocity function only at the zero level set, so it must be extrapolated suitably at the grid points not adjacent to the zero level set.

Having solved this equation the zero level set of the solution is the sought surface at all later times. Actually, this equation relates the time change to the gradient via the velocity function. This equation can be rewritten in Hamilton–Jacobi form

$$\frac{\partial \phi}{\partial t} + H\big(\nabla \phi(t,\mathbf{x})\big) = 0, \tag{2}$$

where Hamiltonian H is given by $H = V(t,\mathbf{x})|\nabla \phi(t,\mathbf{x})|$ (in this context the term "Hamiltonian" denotes a Hamiltonian function, not an operator). A detailed exposition about the Hamilton–Jacobi equation, the existence and uniqueness of its solution (especially about its viscosity solutions), can be found in [10]. We say that such a Hamiltonian is convex (in $\mathbb{R}^n$) if the following condition is fulfilled:

$$\frac{\partial^2 H}{\partial \phi_{x_i} \partial \phi_{x_j}} \geqslant 0, \tag{3}$$

where ϕ_{x_i} is a partial derivative of $\phi(t,\mathbf{x})$ with respect of x_i. If the surface velocity $V(t,\mathbf{x})$ does not depend on the level set function $\phi(t,\mathbf{x})$ itself, this condition is usually satisfied. In that case, we can say that the problem is of free boundary type.

In the numerical implementation the level set function is represented by its values on the grid nodes, and the current surface must be extracted from this grid. In order to apply the level set method a suitable initial function $\phi(0,\mathbf{x})$ has to be defined first. A natural choice for initialization is to adopt the signed distance function of a point from the given surface. This function is the common distance function multiplied by -1 or $+1$ depending on which side of the surface the point is. As already stated, the values of the velocity function are determined by the physical models. In the actual numerical implementation Eq. (1) is represented by the upwind finite difference schemes that requires the values of the function at the all considered grid points. Let denote a discrete approximation of $\phi(t,\mathbf{x})$ at the nth discrete time step with ϕ^n_{ijk}. Then the first-order upwind finite difference scheme updating level set function (see Refs. [1,4] for the details) is given by

$$\phi^{n+1}_{ijk} = \phi^n_{ijk} - \triangle t\big[\max(V_{ijk},0)\nabla^+ + \min(V_{ijk},0)\nabla^-\big], \tag{4}$$

where operators ∇^+ and ∇^- are defined as

$$\begin{aligned}
\nabla^+ = \big[&\max(D^{-x}_{ijk}\phi,0)^2 + \min(D^{+x}_{ijk}\phi,0)^2 \\
&+ \max(D^{-y}_{ijk}\phi,0)^2 + \min(D^{+y}_{ijk}\phi,0)^2 \\
&+ \max(D^{-z}_{ijk}\phi,0)^2 + \min(D^{+z}_{ijk}\phi,0)\big]^{1/2}, \\
\nabla^- = \big[&\max(D^{+x}_{ijk}\phi,0)^2 + \min(D^{-x}_{ijk}\phi,0)^2 \\
&+ \max(D^{+y}_{ijk}\phi,0)^2 + \min(D^{-y}_{ijk}\phi,0)^2 \\
&+ \max(D^{+z}_{ijk}\phi,0)^2 + \min(D^{-z}_{ijk}\phi,0)\big]^{1/2}.
\end{aligned} \tag{5}$$

D^{+x}_{ijk} and D^{-x}_{ijk} are usual forward and backward differences:

$$\begin{aligned}
D^{+x}_{ijk} &= \frac{\phi^n_{i+1,jk} - \phi^n_{ijk}}{\triangle x}, \\
D^{-x}_{ijk} &= \frac{\phi^n_{ijk} - \phi^n_{i-1,jk}}{\triangle x}.
\end{aligned} \tag{6}$$

The time step $\triangle t$ is limited by the usual CFL stability condition. The initial discrete level set function ϕ^0_{ijk} should be calculated in accordance with the initial interface shape (defined by $\phi(0,\mathbf{x})=0$). The boundary conditions are such that the derivatives towards the outside calculational domain are zero (Neumann boundary conditions).

3. Sparse field method for non-convex Hamiltonians

Several approaches for solving the level set equations exist which increase the accuracy and decrease the computational effort. They are all based on using some sort of adaptive schemes. The most important is the narrow band level set method [4,5], widely used in the etching process modeling tools (for a detailed review see [13]), and recently developed the sparse-filed method [2,11,12], implemented in ITK medical image processing library [14], as well as in the general purpose image and surface processing library VISPACK [15]. Adaptive methods use the fact that actual calculations should not be performed for points far away from the zero level set, since these points do not have any influence on the result. This is the starting assumption in the narrow band methods—the width of the narrow band is predefined and should be as small as possible. In the actual implementations it is necessary to choose a new narrow band whenever the front hits the boundary of the current narrow band. Another problem is to find a balance between the width of the narrow band and the frequency of reinitializations. This technique provides a substantial speed up; in three dimensions the computational effort is reduced from $O(N^3)$ to $O(N^2)$ compared to fixed grids on fixed simulation domains (N is a number of the grid points along one coordinate axis).

The sparse-field method uses an approximation of the distance function that makes it feasible to recompute the neighborhood of the zero level set at each time step. In that way, it takes the narrow band strategy to the extreme. It computes the updates on a band of the grid points that is only one point wide. The width of the neighborhood is such that the derivatives for the next time step can be calculated. This approach has several advantages. The algorithm does precisely the number of calculation needed to compute the next position of the zero level set surface. The number of points being computed is so small that it is feasible to use a linked-list to keep a track of them, so that at each iteration only those points whose values control the position of the zero level set surface are visited. As a result, the number of computations increases with the size of the surface, rather than with the resolution of the grid. In fact, the algorithm is analogous to a locomotive engine that lays down tracks before it and picks up them up behind. As a result, considerable improvements in computational efficiency without accuracy penalties comparing to the original narrow-band methodology can be obtained. The detailed analysis of the computational efficiency of the sparse field method is presented in Ref. [2]. It is shown that, depending on the size of the problem, the computational speedup can be up to two orders of magnitude, comparing to the narrow band calculations. For more exact numbers see Table 1 and Fig. 6 in [2].

The upwind difference scheme (4) cannot be used in the case of non-convex Hamiltonians. The simplest scheme that can be applied in these cases is the Lax–Friedrichs, one which relies on the central difference approximation to the numerical flux function, and preserves monotonicity through a second-order linear smoothing term:

$$\begin{aligned}\phi^{n+1}_{ijk} = \phi^n_{ijk} &- \triangle t\Bigg[H\left(\frac{D^{-x}_{ijk}+D^{+x}_{ijk}}{2}, \frac{D^{-y}_{ijk}+D^{+y}_{ijk}}{2}, \frac{D^{-z}_{ijk}+D^{+z}_{ijk}}{2}\right)\\ &- \frac{1}{2}\alpha_x(D^{+x}_{ijk}-D^{-x}_{ijk}) - \frac{1}{2}\alpha_y(D^{+y}_{ijk}-D^{-y}_{ijk})\\ &- \frac{1}{2}\alpha_z(D^{+z}_{ijk}-D^{-z}_{ijk})\Bigg],\end{aligned} \tag{7}$$

where $\alpha_x(\alpha_y,\alpha_z)$ is a bound on the partial derivative of the Hamiltonian with respect to the first(second, third) argument:

$$\alpha_x = \max\left|\frac{\partial H}{\partial \phi_x}\right|, \qquad \alpha_y = \max\left|\frac{\partial H}{\partial \phi_y}\right|, \qquad \alpha_z = \max\left|\frac{\partial H}{\partial \phi_z}\right|. \tag{8}$$

The terms on the second row of the above equation are the smoothing terms. They are similar to the second derivatives in each variable. In general, these terms need not be calculated exactly. Overestimated values will produce non-realistic smoothing of the sharp corners in the implicit surfaces. Too little smoothing usually leads to numerical instabilities in calculations. Various methods for determining acceptable values of the smoothing terms are given in [16]. The detailed description of the application of Lax–Friedrichs scheme in the "traditional" narrow-band level set simulation of the etching process can be found in frequently cited Refs. [17–19].

The non-convex Hamiltonians are characteristic for plasma etching and deposition simulations. During these processes the etching (deposition) rate, that defines the surface velocity function $V(t,\mathbf{x})$, depends on the geometric characteristics of the profile surface itself, or more precisely, on the angle of the incidence of the incoming particles. In the cases under study here we shall consider an etching beam coming down in the vertical direction. These conditions are characteristic for ion milling technology, but angular dependence of the etching rates appears, more or less, in all etching processes.

Let θ be the angle between the surface normal (at the particular surface point) and the direction of the incoming particles, and let all the particles have the same direction. The relation defining surface velocity (etching rate) can be given as

$$V = V_0(1 + B\sin^2\theta)\cos\theta. \tag{9}$$

This type of the etching processes can be characterized as the interface controlled problems. In the rest of the paper we shall deal primarily with this type of the problems. The angle θ is connected to the level set function itself with a simple relation

$$\theta = -\frac{\phi_z}{|\nabla\phi|}, \tag{10}$$

so the Hamiltonian takes the form

$$H = V_0\phi_z\left[1 + B\left(1 - \frac{\phi_z^2}{|\nabla\phi|^2}\right)\right]. \tag{11}$$

It can be easily shown that this Hamiltonian is non-convex for $B > 0$. The parameters in Lax–Friedrichs scheme (7) are then

$$\alpha_x = \max\left|\frac{2V_0B\phi_x\phi_z^3}{|\nabla\phi|^4}\right|, \qquad \alpha_y = \max\left|\frac{2V_0B\phi_y\phi_z^3}{|\nabla\phi|^4}\right|,$$
$$\alpha_z = \max\left|V_0\left\{\frac{B(\phi_x^2+\phi_y^2)}{|\nabla\phi|^2}\left(\frac{2\phi_z^2}{|\nabla\phi|^2} - 1\right) - 1\right\}\right|. \tag{12}$$

In the actual implementation these maxima are calculated by sweeping the linked lists containing the active layer (zero level set) and its neighboring layers on both sides. The number of cells visited in that way is proportional to the area of the profile surface, so the procedure is numerically effective. Because of the nature of the sparse field method there is no reasons to consider more sophisticated procedures (e.g., Local Lax–Friedrichs [16]) for finding these maxima. Instead, we implemented the possibility to reduce the values of these parameters by simple scaling:

$$\alpha_x' = R_x \times \alpha_x; \qquad \alpha_y' = R_y \times \alpha_y; \qquad \alpha_z' = R_z \times \alpha_z. \tag{13}$$

By some experimenting with these reduction parameters we were able to reduce the amount of smoothing of the Lax–Friedrichs scheme, while preserving the stability of the numerical procedure.

In the case of the ion enhanced chemical etching the dependence of the surface velocity on the incident angle is simpler [20]: $V = V_0\cos\theta$, so the same Eq. (12) with $B = 0$ can be used for determining the Lax–Friedrichs parameters. The pure chemical etching velocity, or more precisely the etching yield, does not depend on the incident angles. This case can be safely treated by the upwind scheme (5), and using the Lax–Friedrichs scheme would lead to unnecessary rounding of the profile surface.

So, we have completed the set of the relations being necessary for implementing the sparse field method in the case of non-convex Hamiltonians. Some results obtained in this way will be shown in the next section.

4. Results

The details about the code design and implemented algorithms will be published elsewhere. Our implementation is based on ITK library [14]. The classes describing the level set function and the level set filter are reimplemented according to the procedures for treating non-convex Hamiltonians described in the previous section. Here we will present some results of calculations illustrating our approach to dealing with non-convex Hamiltonians in the etching profile simulations. We did not try to relate the etching rate (velocity function $V(t,x)$) with the realistic etching conditions (particle fluxes and surface processes). Instead, we used simple analytical expressions (9) describing the typical model etching rates, following the interface controlled problem description from the previous paragraph. Numerical value of the V_0 is taken to be 5 nm/s.

All calculations are performed on $128 \times 128 \times 384$ rectangular grid. In Fig. 1 the initial profile surface is shown. It is a rectangle deep with dimensions of $0.1 \times 0.1 \times 0.05$ μm. Above the profile surface is the trench region. The particles involved in the etching process come from the top, while the non-etched material is bellow.

The actual shape of the initial surface can be described using simple geometrical abstractions. In the beginning of the calculations this description is transformed into the initial level set function using the fast marching method [4]. The evolution of the etching profile surface with time is shown in the following figures. The results obtained for constant velocity function $V = V_0$ (purely isotropic etching case) using Lax–Friedrichs and upwind schemes, are shown in Figs. 2 and 3, respectively. It is supposed that only the bottom surface could be etched; i.e. that the top and the vertical surfaces belong to photo-resistive layer. The behavior of the etching profile is as expected. Fig. 2 shows that the numerical dissipation contained in the Lax–Friedrichs scheme produces too much rounding of the resulting surfaces. It is obvious that it is much better in that case to use the upwind scheme (Fig. 3).

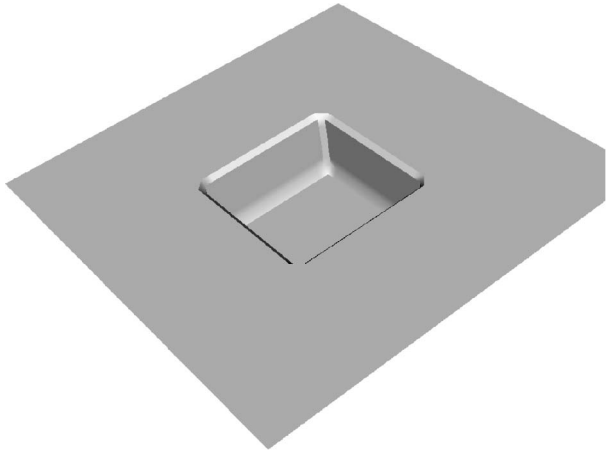

Fig. 1. The initial profile surface.

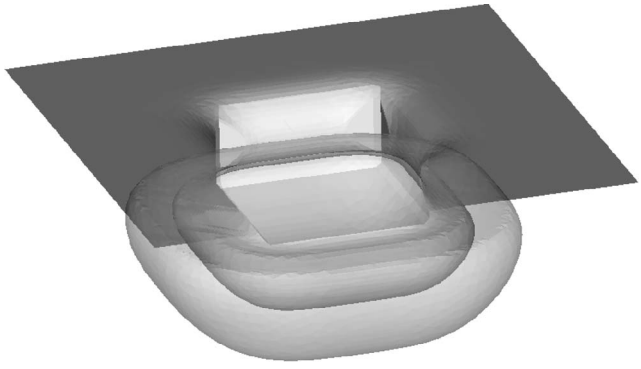

Fig. 2. The Lax–Friedrichs scheme ($R_x = 1$, $R_y = 1$, $R_z = 1$): The etching profiles for $V = V_0$ at $t = 0$, $t = 9$ s and $t = 15$ s.

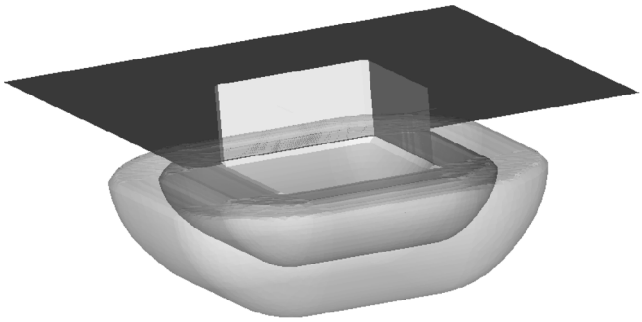

Fig. 3. The upwind scheme: The etching profiles for $V = V_0$ at $t = 0$, $t = 9$ s and $t = 15$ s.

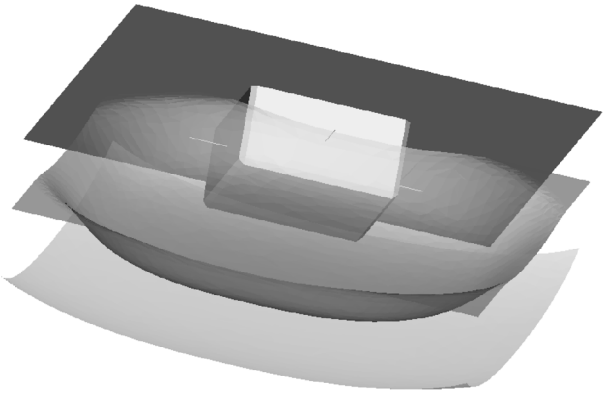

Fig. 4. The Lax–Friedrichs scheme ($R_x = 1$, $R_y = 1$, $R_z = 1$): The etching profiles for $V = V_0(1 + 4\sin^2\theta)\cos\theta$ at $t = 0$, $t = 9$ s and $t = 15$ s.

In Fig. 4 the more interesting results of the angular dependent etching rate simulation are presented. Velocity function in the form $V = V_0(1 + 4\sin^2\theta)\cos\theta$ is usually used for the ion milling processes. In this case it is supposed that the whole profile surface can be etched. The faceting of the sharp corners is reproduced correctly.

The high aspect ratio (depth/width) etching is a common situation in semiconductor technologies. In the following figures the evolution of the etching profile, when etching rate is proportional to $\cos(\theta)$, is presented. This is the simplest form of angular dependence, but it describes the ion enhanced chemical etching process correctly [20]. In this case we expect that the horizontal surfaces move downward, while the vertical ones stay still. Figs. 5–7 show the results for various values of the smoothing in the Lax–Friedrichs scheme, according to the relations (13). These figures show that it is possible to find optimal amount of smoothing ($R_z = 0.3$ in Fig. 6) that gives minimal rounding of sharp corners, while preserving the numerical stability of the calculations. Actually, this is one of the most delicate problems in the etching profile simulations. It is obvious from Fig. 7 that too drastic reduction of the smoothing ($R_z = 0.1$) violates the numerical stability, and the vertical edges become noticeably rough.

5. Conclusions

In this paper we have presented an extension of the sparse field method for solving the level set equations in the case of non-convex Hamiltonians, suitable for the application in the 3D simulations of the profile surface evolution during the plasma etching and deposition processes. The obtained results show that it is possible to use the Lax–Friedrichs scheme in conjunction with the sparse field method, and to preserve sharp interfaces and corners by optimizing the amount of smoothing in it. This is of special importance in the simulations of the etching processes in which spatially localized effects appear, like notching and microtrenching. The calculations are performed using various model interface velocity functions $V(t, x)$. The same methodology can be used in simulations in which this function is determined more precisely, by calculating particle fluxes reaching the profile surface during the etching process using the Monte Carlo method. Such a calculations are in due course now, and we hope that it will be reported soon.

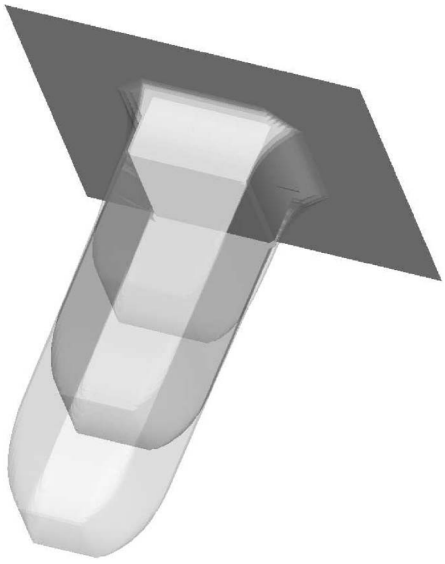

Fig. 5. The Lax–Friedrichs scheme ($R_x = 1$, $R_y = 1$, $R_z = 1$): The etching profiles for $V = V_0\cos\theta$ at $t = 0$, $t = 20$ s, $t = 40$ s and $t = 60$ s.

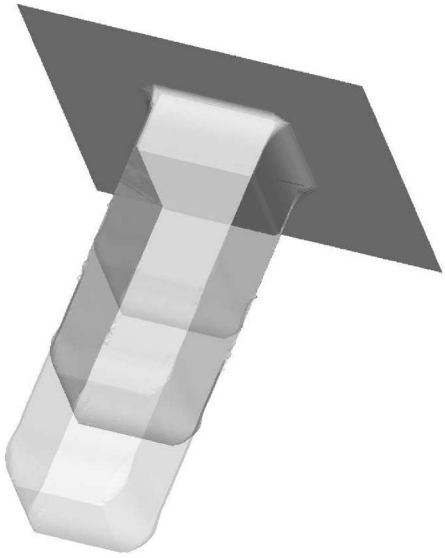

Fig. 6. The Lax–Friedrichs scheme ($R_x = 1$, $R_y = 1$, $R_z = 0.3$): The etching profiles for $V = V_0\cos\theta$ at $t = 0$, $t = 20$ s, $t = 40$ s and $t = 60$ s.

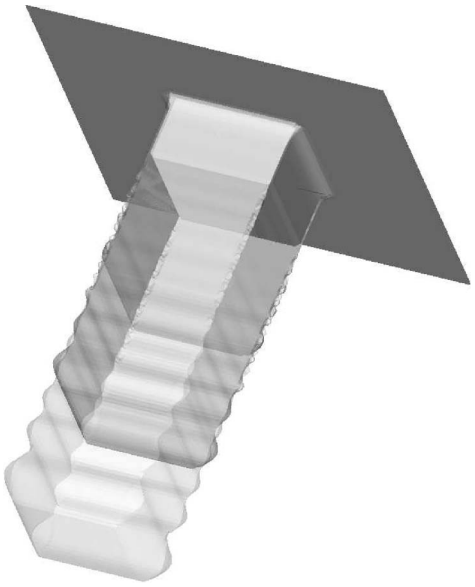

Fig. 7. The Lax–Friedrichs scheme ($R_x = 1$, $R_y = 1$, $R_z = 0.1$): The etching profiles for $V = V_0 \cos\theta$ at $t = 0$, $t = 20$ s, $t = 40$ s and $t = 60$ s.

Acknowledgement

This work was supported by the Lam Research Corporation and Tera-level Nano Devices Project, 21c Frontier R&D Program of Korea Ministry of Science and Technology.

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