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# Surface Evolution During Semiconductor Processing

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We discuss our approach to using the Riemann problem to compute surface profile evolution during the simulation of deposition, etch and reflow processes. Each pair of segments which represents the surface is processed sequentially. For cases in which both segments are the same material, the Riemann problem is solved. For cases in which the two segments are different materials, two Riemann problems are solved. The material boundary is treated as the right segment for the left material and as the left segment for the right material. The critical equations for the analyses are the characteristics of the Riemann problem and the 'jump conditions' which represent continuity of the surface. Examples are presented to demonstrate selected situations. One limitation of the approach is that the velocity of the surface is not known as a function of the surface angle. Rather, it is known for the angles of the left and right segments. The rate as a function of angle must be assumed for the explicit integration procedure used. Numerical implementation is briefly discussed.

## 1. INTRODUCTION

Simulations of the time evolution of topography during deposition, etch, reflow and planarization processes used in the fabrication of integrated circuits is becoming increasingly important for the development of advanced device structures. To this end, there has been considerable effort devoted to developing topography evolution algorithms for completely three dimensional (3d) surface evolution, which is appropriate for simulating the fabrication of most device structures. On the other hand, two dimensional (2d) structures have been and will continue to be used to develop the transport and reaction kinetic submodels which demonstrate process understanding and which should be used in 3d simulations. Thus, moving algorithms for 2d surface evolution must be refined to the point that computed surface profiles compare quantitatively with experimental results, if the correct transport and reaction submodels are used. This allows accurate assessment of proposed transport and reaction models as well as the estimation of their parameters.

In this paper, we discuss an approach to moving 2d surfaces which has proven itself to be reliable over the last few years as part of EVOLVE [1-3], a low pressure transport and reaction (deposition and etch) process simulator, as well as high pressure deposition [4] and reflow [5] codes. The same approach has been presented previously for single material substrates and for multiple material substrates, under the assumption that the rate of surface evolution was a function of the local surface angle [6-9]. The moving algorithms used consist of; 1) conservation law based calculation of growth vectors based upon normal velocities input by a calling program (EVOLVE for example), 2) algorithms which decide how far to move the surface, based on the growth vectors established in 1 and 3) algorithms to actually move and refine the surface. In this paper, we focus on the first set of algorithms.

## 2. SURFACE EVOLUTION

Several groups have related topography evolution to the Riemann problem for surfaces which are represented by line segments [6-9]. In two-dimensional rectangular coordinates, an evolving surface can be defined as:

$$\phi(x(s,t),y(s,t),t) = 0 \qquad (2.1)$$

where, t is the process time, s is a parameter along the surface ($0 \le s \le 1$), and x and y are the coordinates of the surface at s,t. The material is to the right of the surface. After some manipulation, the surface evolution equation is

$$\phi_t + c\sqrt{\phi_x^2 + \phi_y^2} = 0 \qquad (2.2)$$

where subscripts t, x and y indicate partial derivatives and c is the normal velocity of the surface at s,t. As presented, the velocity is into the material if c is positive; i.e., etching is occurring or the velocity is inward during reflow. A local coordinate system can be defined such that the y axis points in the direction of the normal to the local surface pointing into the vacuum. We also consider the local velocity to be a function only of the slope at s along the surface at some time t. This assumption is appropriate for some processes [6,8,9]; however, in general, the local velocity is a function of the entire surface; e.g., because of shadowing and re-emission during low pressure transport and reaction. The assumption that the local velocity is only a function of slope at a given s,t is done here for mathematical convenience. Since y is a single valued function of x and t in this coordinate system, we can arrive at a conservation form of Equation 2.2 in terms of the slope $p=y_x$

$$p_t + f_x(p) = 0 \qquad (2.3)$$

where

$$f(p) = c(p)\sqrt{1+p^2} \qquad (2.4)$$

is the 'flux function' of the conservation law. Equation 2.3 can also be written as

$$p_t + f'(p)p_x = p_t + \lambda p_x = 0 \qquad (2.5)$$

Since p is a function of x and t, Equation 2.5 indicates that in the characteristic direction $f'(p)=\lambda$, the values p, f(p) and $\lambda$ are constant. Introducing the angle measured relative to the x axis,

$$\theta = \tan^{-1}(p) \qquad -\pi/2 < \theta < \pi/2 \qquad (2.6)$$

we have,

$$f(p) = c(p)\sqrt{1+p^2} = \frac{c(\theta)}{\cos(\theta)} \qquad (2.7)$$

and

$$\lambda = \left(\frac{dx}{dt}\right)_c = f'(p) = c'(\theta)\cos(\theta) + c(\theta)\sin(\theta) \qquad (2.8)$$

Because y is a function of x and t, we may write the characteristic equation for y as

$$\gamma = \left(\frac{dy}{dt}\right)_c = pf'(p) - f = c'(\theta)\sin(\theta) - c(\theta)\cos(\theta) \qquad (2.9)$$

and p is constant.

## 3. THE RIEMANN PROBLEM

Consider two consecutive line segments which approximate the local surface, for which the normal velocities of evolution have been specified. For the moment, we assume that the materials to the right of the two segments are the same. Considering the node which joins the segments as the origin of the local coordinate system introduced above, the slope of the left segment is equal in magnitude to the slope of the right segment, but has the opposite sign. In the following, superscript – is used for values to the left of the node at t, and superscript + is used for quantities to the right. In general, the flux function f(p) is not known for the values of p between $p^-$ and $p^+$. In order to proceed, it is assumed the rate is a linear function of the slopes (angles) between the rates on the left and right segments; i.e., linear interpolation is used. The different rates are due to different flux conditions on the two segments, but either both segments are being deposited on or both segments are being etched for the case where both segments are on the same material. Thus, there will be a single rarefaction wave or a single shock wave emanating from the origin. The solution to this Riemann problem is used to compute

the time evolution of the surface which is represented at some time t by the two segments.

Formally, the motion of the node (origin) as a function of time (X(t),Y(t)) can be arrived at by considering the evolution of the left and right sides and the maintenance of continuity. Equations 2.8 and 2.9 give

$$\frac{dX}{dt} = \frac{f^- - f^+}{p^- - p^+} = \frac{c^- \cos(\theta^+) - c^+ \cos(\theta^-)}{\sin(\theta^- - \theta^+)} \tag{3.1}$$

$$\frac{dY}{dt} = \frac{p^+ f^- - p^- f^+}{p^- - p^+} = \frac{c^- \sin(\theta^+) - c^+ \sin(\theta^-)}{\sin(\theta^- - \theta^+)} \tag{3.2}$$

In the following, Equations 3.1 and 3.2 are referred to as 'jump conditions'. If the x characteristics on the left are 'slower' in the x,t plane than the characteristics on the right, then a rarefaction wave emanates from the origin. In that case, the solution is

$$p = p^- \quad x/t \le \lambda^- \tag{3.3}$$

$$\lambda = x/t \quad \lambda^- \le x/t \le \lambda^+ \tag{3.4}$$

$$p = p^+ \quad x/t \ge \lambda^+ \tag{3.5}$$

where Equation 3.4 is used to interpolate between the characteristics on the left and those on the right; i.e., it is used to 'attach' the left wave to the right wave. The new surface is represented by the endpoints of growth vectors which emanate from the left segment, the origin, and the right segment. The characteristic equations are used for the left and right sides and the growth vectors for intermediate angles are obtained by introducing a number of angles between $\theta^-$ and $\theta^+$, and using either the characteristic equations or the 'jump conditions' for each angle. If $\theta^-$ and $\theta^+$ are equal or almost equal, then the characteristic equations are used. In the case considered in this paper, a simple form of the 'entropy condition' suffices; a shock is formed if the characteristics on the left are faster than the characteristics on the right. In that case, the jump conditions are used to compute the growth vector.

## 4. TWO MATERIALS

If the two surface segments considered are different materials, then different deposition or etch reactions may occur, and the evolution rates will in general be different even in an otherwise uniform environment. The two materials are treated as two separate single material Riemann problems, with the right segment of the left material and left segment of the right material having zero normal velocities. As a result of continuity, the jump conditions and the speeds at the material boundary, using 1 to refer to the left material and r to refer to the right material, are

$$\frac{dX^l}{dt} = \frac{f^l}{p^l - p^{bl}} = \frac{c^l \cos(\theta^{bl})}{\sin(\theta^l - \theta^{bl})} \tag{4.1}$$

$$\frac{dY^l}{dt} = \tan(\theta^{bl}) \frac{dX^l}{dt} \tag{4.2}$$

$$c^l = \sqrt{1 + \tan^2(\theta^{bl})} \frac{dX^l}{dt} \tag{4.3}$$

for the left material, and

$$\frac{dX^r}{dt} = \frac{-f^r}{p^{br} - p^r} = \frac{-c^r \cos(\theta^{br})}{\sin(\theta^{br} - \theta^r)} \tag{4.4}$$

$$\frac{dY^r}{dt} = \tan(\theta^{br}) \frac{dX^r}{dt} \tag{4.5}$$

$$c^r = \sqrt{1 + \tan^2(\theta^{br})} \frac{dX^r}{dt} \tag{4.6}$$

for the right material. Equations 4.1 and 4.4 are essentially those presented by Ross for the evolution of material boundaries [6]. Because the normal velocities of the boundary are zero, there is no reason to include superscripts + and – in these equations; they are implied. Superscripts bl and br refer to the boundary in the left and right Riemann problems; i.e., they will have different angles in the two problems, because the coordinate systems are different.

In the case of etching on both sides of the material boundary, the angle of the material boundary is known. If the angle of the left material at the boundary was known, then the flux function would specify the normal velocity as well as the velocity of the left side along the boundary. Similarly for the right side. The angles of the segments at the boundary need to be determined. If the characteristics on both sides of the material boundary go into the boundary, then the speed computed using Equation 4.3 and the original segment angle is compared with the speed computed

using Equation 4.6 and the original right segment angle. The boundary speed selected is

$$c^b = \max(c^l, c^r) \tag{4.7}$$

The solution on the fast side is constructed using the original segment angle for that side. The angle of the other segment is determined by solving either Equation 4.1 or 4.4 using the correct (higher) value of $c^b$ to compute dX/dt. In the absence of a known dependence of the flux function f(p) on p, one is assumed. For the purposes of this paper, we assume that the flux function is isotropic; i.e., the normal velocity does not depend on the angle of the segment. If one or both of the sets of characteristics diverge from the material boundary, the speed(s) along the boundary are computed using the isotropic assumption. The remainder of the solution procedure is the same as outlined above.

In the case of deposition on both sides of the boundary, the direction of the new material boundary and the angles of the segments on either side of that boundary need to be determined as part of the solution. A value for the angle of the material boundary is guessed, and the two Riemann problems are used to compute the speeds of the left and right sides along the boundary. A solution is found when the two speeds are the same. During this search for $\theta^b$, if the left or the right side is a rarefaction wave, then the isotropic assumption is used to attach the wave to the boundary. In the isotropic assumption, this means that the angle on that side, at the boundary, is perpendicular to the boundary. If a shock wave is indicated on either side, then the angle on that side is the original angle of the segment.

If there is deposition on one material and etching on the other material, then the one which controls the interface is determined as part of the solution. If etching is fastest along the boundary, again using the isotropic assumption if a rarefaction wave is indicated, then the material boundary is the subsurface interface. In that case, the angle of the boundary is known, and the angle of the depositing side is computed using the jump condition for that side with the speed along the boundary as computed for the etching side. If deposition controls the material boundary evolution, a new boundary is formed. Its angle is unknown, as in the case of deposition on both materials. After guessing the material boundary angle, and using the isotropic evolution assumption to attach waves to the boundary if necessary, the boundary angle can be computed along with the angles of the left and right materials.

## 5. EXAMPLES

Examples 1 through 10 shown in figure 1 are examples of the application of the solution method outlined in the previous two sections for deposition and etch processes. Reflow processes are not considered separately. In these figures, the growth vectors for the left and right segment endpoints are retained in order to aide visualization. Actually, each node is processed sequentially; i.e., the original right segment of one Riemann problem (node) is used as the left segment for the next Riemann problem (node). Examples 1 and 2 show deposition on a single material. In the first case a rarefaction wave is formed, and a shock wave is formed in the second case. Example 3 shows a rarefaction wave during etching, while Example 4 shows a shock wave formed during etching. Examples 5 through 10 show deposition and/or etching on two materials. Example 5 shows a situation for which deposition of material on the left segment is larger than on the right segment. A rarefaction wave is computed for the left side, while a shock forms on the right side. Example 6 shows a situation for which shocks form on both sides. Example 7 shows a situation in which both materials are being etched, with the material on the right having the higher rate. A rarefaction wave forms on the right side and it controls the evolution of the material boundary. The angle of the left segment at the boundary is computed using the boundary velocity determined by the etch rate on the right segment, as described in the previous section. Thus, the amount of etching which occurs as the left material is exposed is taken into account. Example 8 shows a situation for which the left material is being etched and determines the boundary velocity. In this case, a shock wave forms for the left Riemann problem. Example 9 shows deposition on the left side and etch-

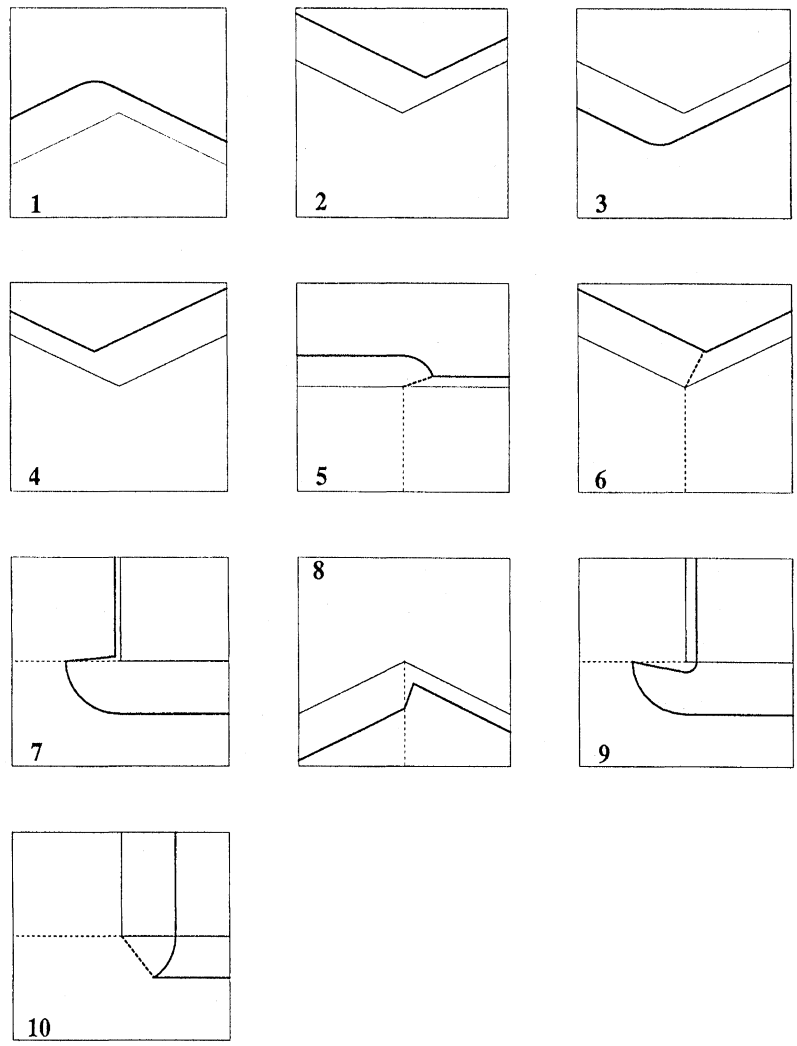


FIGURE 1 Examples to demonstrate the surface evolution for pairs of segments which represent the local surface, as described in Section 5. The thin lines are the original segments, the thick lines are the final surfaces, the thin dashed lines are the original material boundaries and the thick dashed lines are the generated material boundaries

ing on the right, with the etch rate controlling the boundary. Example 10 shows a situation for which deposition on the left controls the evolution of the material boundary.

## 6. NUMERICAL IMPLEMENTATION

The evolution of each node (pair of segments) is determined, with nodes inserted as needed using a user specified value of a nominal angular increment, as described above. The endpoints of the surface are moved in the direction of the appropriate segment normals, just as for the outside endpoints of the segment pairs shown in the examples. After this process, one has the original surface and a number of 'growth vectors' which essentially represent a trial surface at a nominal time step. If growth vectors cross each other, the time step is adjusted to be the minimum time reflected by these intersections. If an etch vector

along a subsurface material boundary goes beyond the first node inside the material, and if the material boundary angle changes at that subsurface node, then the time step is decreased to prevent this from occurring. A minimum time step is also used in order to make simulation times reasonable in some situations. If the minimum time step is larger than the limiting times as determined above, loops may form. The procedures for handling these loops, feature closure during depositions, breakthrough into a subsurface material during etching, or undercutting of material during etching are beyond the scope of this paper.

## 7. CONCLUSIONS

We have described the Riemann problems used to compute the growth vectors at each node along the surface at some time during the process. Although it has proven useful in EVOLVE and related codes, there are clear limitations. Because we use an explicit time integration to determine the growth vectors, we are forced to assume a dependence of the velocity on the surface angle over the range of angles in a given Riemann problem (pair of segments). Other assumptions regarding the angular dependences of the rate described here have been used, as well as directional etch and deposition, and will be discussed in future publications.

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