CHAPTER 3  Topography Effects in Deposition and Etching

Fundamental physical mechanisms in deposition and etching generate both desired and undesired topographic features. The goal of this chapter is to provide a basic foundation for understanding and modeling their effects on topography profile time-evolution. A common framework for modeling etching and deposition is given along with the terminology used to describe various physical phenomena and effects. Sweeping the profile with a domain of influence for a point source can be used to model the time-advance. Alternatively facets in a representation of a surface can be advanced using a vector sum of advancement rates normal to the facet. In many cases the processes themselves produce planar facets and analytical solutions are given for several simple cases. Several phenomena in ion milling including lateral shifts and corner faceting are described. A more rigorous methodology for analyzing the generation an annihilation of slow-advancing and fast-advancing facets is described using results developed by F.C. Frank and C.H. Sequin for crystal etching based on slowness surfaces. Examples of simulation of several basic deposition and etching processes conclude the chapter.

3.1 Four Aspects Common to Etching and Deposition

Deposition and etching are nearly opposites and there is a wide diversity of processing equipment used to perform them. Yet from the topography profile time-evolution point of view they have a lot in common. The starting point for both is the nature of flux which arrives from the source on the wafer. A second commonality is how the self-shadowing of the existing profile affects the visibility of the source and how the re-emission from the profile or radiosity affects other points on the profile. Once the arriving species are known locally at each point on the profile then the physical and chemical reactions on the profile surface must be described. Finally the deformation of the current profile must be followed
for a time step including continuous local and the occasional global topological changes which are take place.

Figure 4.1 schematically shows geometries of typical process tools used for etching and deposition species. In the parallel plate system on the left a plasma exists between the system electrodes. The wafer with a simple rectangular trench is indicated. To begin to characterize the process a mathematical surface can be drawn just above the wafer and the angular distribution or equivalent sources of the various species crossing this surface can be recorded. In etching there may be one or more positively charged species which bombard the wafer with a nearly vertical Gaussian distribution of incidence angles due to collisions in the sheath. There may also be an accompanying set of neutrals with a broad angular spectrum. The same geometry might be used for sputter deposition in which case a broad angular distribution of small particles of target material from the upper electrode would be incident. The system on the right is a typical geometry for a planetary evaporator. In this system the wafer is moved about on a spherical dome or planet which rotates about a tilted axis to present many orientations of the wafer to the flux from the evaporation source. The equivalent source for the evaporated material in this case is a near delta function in angle which changes in its angular location and even intensity during processing as the wafer is moved about. In the case of evaporation determining the equivalent sources is very geometrical. In parallel plate sputtering collisions in the plasma produce a broad almost hemispherical distribution of incident angles. For dry etching the characteristics of the plasma and even the loading of the plasma by consumption and generation of species on the wafer may need to be included.

A second common aspect is that the topography profile on the wafer affects the visibility of local points on the profile. As shown in Figure 4.2 certain parts of the profile may cast shadows on other parts of the profile and thus reduce the visibility to various flux.
components. In deposition this plays a very important role in filling contacts with metal because as the aspect ratio of the contact increases it becomes very difficult to get enough metal on either the bottom or the sidewalls due to shadowing. More complex point to point interactions along the topography profile can also be important. In deposition a material may not stick where it first lands (re-emission) and instead plays a small game of billiards before coming to rest (re-deposition). In plasma etching or more properly reactive ion etching it is the directed flux of species which passes through the mask opening, enhances the etch rate where it impinges and extrudes the pattern in directional etching. The selectivity of the etch rate of the substrate relative to the mask is a consideration. High energy bombardment has associated mechanical etching effects which are less selective than chemical etching and a lower selectivity results. On the other hand sidewalls which are shadowed may accumulate protective polymers which in turn result in vertical sidewalls. In reactive-on etching energetic ion reflection from sidewalls can occur and even re-emission of etch by-products may redeposit other parts of the profile. These source shadowing and intra-profile interactions are basically similar to visibility and radiosity effects in graphical modeling.

A third common aspect is that mechanical and chemical reaction at the surface determine the local advancement rate and are one of the most interesting aspects of deposition and etching. Several examples are as shown in Figure 4.3. In deposition, columnar grain growth is possible and the column angle tilts with the angle of incidence according to the billiard players rule. In addition, the density of the material can be affected by bombardment in a peening action. In depositing oxides with organic molecules there is evidence for molecules of a particular shape that a Y upward or Y downward orientation in an initial layer can affect the step coverage. Surface mobility can introduce diffusion of species along the surface in both deposition and etching. Quartz heating lamps are in fact
used to improve step coverage with aluminum. In plasma etching the ion bombardment can both accelerate reactions and remove by-products. It is the polymer which forms in the shadowed regions which protect even from energetic neutrals and leads to vertical etch profiles. In etching the ability of the chemistry of the etch gas to form volatile by-products with the material to be etched which is of key importance and appropriate mixtures are used to reduce the etching of the masking material and etch stop material and enhance the etching of the material to be removed.

The final common stage of deposition and etching is the **time-advance of the surface profile** as is illustrated in Figure 4.4. The local fluxes and etch reactions provide sufficient information on how the surface is to deform for a short time step. The time-evolution of the profile requires many time increments which allow the change of the profile shape to influence its future shape through shadowing etc. As the surface evolves there may be major topological changes. For example, outgrowths of material from sides of a trench might collide and close off a void. Or etch fronts from two trenches might move laterally, collide and from a tunnel or an air bridge. There are also minor topological changes such as shadowed regions in deposition lagging behind and forming cracks. Or multiple deposition or etching fronts emanating like a fan from one point and creating breadloaf or faceting effects.

The list of physical effects which are known to have an influence on the time-evolution of topography profiles in deposition and etching is quite extensive. They will be considered again in Chapter 4 and can be found in textbooks such as Sze, Wolf and Tauber, Manos and Flamm, etc. and conference literature from IEDM, VMIC, etc. Some of the more interesting recent observations are the effect of the sticking coefficient [rzz.mcvittie.vmic]
3.2 Modeling Profile Time-Evolution

The most basic and correct model of the incremental profile time-evolution for line-edge profiles and 3D topography is that of using a domain of influence for a point source and making a sweep over the initial topography as shown in Figure 4.5. As in the Huygen’s equivalent source modeled used in electromagnetics, every point on the initial profile is considered to generate a domain of influence. The locus of the boundary of the region swept out by the domain of influence is the new topographical surface. This model works for both deposition and etching. The domain of influence in etching an deposition is more complex than the simple sphere of influence in Huygen’s model. The shape in ion milling and crystal etching is dependent on the material etch rate versus angle. Additional simultaneous isotropic and directional etching as well as shadowing may need to be considered. Once the shape of the domain of influence is known for a time step the profile time-evolution during processing can be simulated by repeatedly over the topography for the duration of the process. Several simulators have been developed which directly emulate this process by starting with what is essentially a bitmap of the initial geometry and bitmap operator for the domain of influence. The operator is then applied about each point on the surface to toggle the content of the bit locations in the geometry bitmap [rzz.xxx.japan, rzz.TUV.erlang].

More theoretical approaches are helpful in gaining physical insight in to the profile shapes which evolve and can also be used to determine the shape of the domain of influence from a point source. An alternative viewpoint is to consider the profile to be made up of a set of planar facets which advance in space with time to create the moving profile as was introduced by Frank in describing crystal etching [rzz.frank. 1958, rzz.frank.1972]. Frank showed that if the etch rate depended only on orientation, then each facet moved along a straight trajectory. The trajectory is not always perpendicular to the facet but is instead the

and molecule shape [rzz.VMIC94] in LPCVD TEOS, grain growth in deposition [rzz.VMIC94.shay], vacancy diffusion in removing voids in aluminum [rzz.VMIC94.shay], and charging effects [rzz.sawing].
facet moves in a direction normal to the reciprocal of the rate function in a polar plot. In cases where the etch rate depends on angle this results in collisions between facets or shock fronts. When the facets diverge new fans of facets must be created between the initial facets. The initial profile shape along with the angular dependent etch rate can thus give rise to new topographical features. The vertices where the facets meet can also be tracked in time including the generation of faces by projecting the vertex figure onto the slowness function in a method developed by C.H. Sequin [rzz.sequin.sa 1992] which will be presented in Section 3.6.

To simplify the presentation in this chapter the simpler 2D view will be used. In 2D the profile is sometimes said to be made of line segments and intersections may also be called nodes. Initially deposition with a spherical domain of influence is assumed as shown in Figure 4.6. Eight facets can be seen to be expanding radially outward in the domain of influence for a time step $\Delta t = t_2 - t_1$. Each point on the profile at time $t_1$ can be viewed as releasing a set of these planar fronts which can produce the profile at time $t_2$. Note that where the surface has curvature it is very important to consider planar facets which completely fill a cone of the possible outward angles allowed. Thus the top right convex outward corner point causes a fan of facets to be generated which create a rounded section of the profile at time $t_2$. Facets from points along the planar facets at time $t_1$ behave in a similar manner and the locus of their domains of influence reproduce the planar facets and make them appear to advance uniformly with time. At the concave outward corner the planar fronts from the horizontal and vertical facets intersect each other in a line which is the location of a new corner point with time. These collisions where overlapping fronts occur (and some information about the initial profile is lost) are said to be shocks. Note that the shocks and fans play a very important role in determining the topography changes during processing.

**FIGURE 3.5** Profile time-evolution as modeled by sweeping the point influence function over all possible point sources on an initial profile at time $t_1$ to generate the profile at time $t_2$ [rzz.Stras.tuv].
For isotropic etching the profile moves from the surface into the material as shown in Figure 4.7. Again, each of the facets moves in the direction perpendicular to its normal. The

Figure missing: Similar to 3.7 and shows that the location of the shocks and fans is interchanged.

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convex outward corner now produces a shock and the concave outward corner now pro-
duces a fan.

Directional deposition and etching is also an interesting special case in which the visible
part of the entire wafer surface moves toward or away from the source. Thus it is a simple
matter to take every point on the profile and translate it according to a flux vector. To be
consistent with the facet motion view above it is also possible to consider the directional
process to be a uniform vector translation of every facet regardless of its orientation. Some
computer simulation programs are also written on the basis of translating each facet in a
profile only in a direction normal to the facet by the projection of the motion vector nor-
tal to the facet.

To model processes such as ion milling and chemical etching etch rates which orientation
dependent must be considered. As an example consider a typical ion milling rate versus
angle curve shown in Figure 4.8. A maximum etch rate of about double the etch rate at
normal incidence occurs when the flux is at $\theta_{\text{MAX}}$ or about $55^\circ$ from the normal. Note that
$\theta_{\text{MAX}}$ is both the angle that the outward surface normal make with the direction back
toward the source and the angle between the inward normal and the downward direction
of the flux. This increase in the etch rate with angle may in part be due to the forward
momentum of the incident particle which tend to be more effective in vibrating substrate
atoms near the surface when the incident beam is tilted. The increase in etch rate with
angle up to $55^\circ$ will make tapered sidewalls etch much more rapidly than horizontal sur-
faces. At corners multiple tangent surface planes exist. Of these the one with the fastest
etch rate usually dominates $R(\theta_{\text{MAX}})$ and the corner tends to facet at the angle $\theta_{\text{MAX}}$.

It is instructive to look at a polar plot of the etch rate and its inverse the slowness surface.
Examples for ion milling and anisotropic crystal etching are shown in Figure 4.9. In a
polar plot the etch rate for ion milling takes on a butterfly shape with a simple single max-
imum. The inverse reciprocal of this function is the slowness function in 2D or slowness

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**FIGURE 3.8** Etch rate versus angle for Ion Milling, the movement of the facets making up the domain of influence and the profile faceting which results.
surface in 3D. The slowness function has a local maximum at normal incidence, goes through a simple minimum at $\theta_{\text{MAX}}$ and then goes to infinity at grazing incidence. For anisotropic crystal etching of single crystal silicon in KOH the etch rate versus angle changes by a factor of 100 over a few degrees. The densely packed \{111\} planes at an angle of

\[\theta_{111} = \arccos\left(1/\sqrt{3}\right) = 54.7^\circ\] \hspace{2cm} \text{EQ 3.2 -1}

etch extremely slowly compared to the fastest etching \{320\} and \{110\} planes at (78\degree C) or (40\degree C) temperatures [rzz.satoJIEE].

\[\theta_{320} = \arccos\left(1/\sqrt{13}\right) = 73.9^\circ\] \hspace{2cm} \text{EQ 3.2 -2}

\[\theta_{110} = \arccos\left(1/\sqrt{2}\right) = 45^\circ\] \hspace{2cm} \text{EQ 3.2 -3}

Data for the ion milling etch rate versus angle for typical materials used in IC processing are shown in Figure 4.10. Gold is very unusual in that it etches even faster than photore sist. Even more distinguishing is the fact that its ion milling rate is maximum at normal incidence which means that it does not facet. The other materials tend to facet and have $\theta_{\text{MAX}}$ between 40\degree to 60\degree and peak rates from 1.5 to 2 times the rate at normal incidence. The variation among ion milling rates for different materials is extremely low compared to
the variation in their plasma and wet etching rates. The later also show a strong dependence on the gas and liquid chemistries but ion milling is similar for most gases.

### 3.3 Segment Motion and Vector Addition of Rates

Given an existing description of a profile as a set of facets it is possible to track the surface time-evolution by advancing each of the existing facets. This is a consistent approach provided that the facets are extended in length to form a closed surface. This also assumes that effects of fans being generated at convex corners and collisions at concave corners will be treated separately an additional operation such as surface regularization. In 2D this facet or segment motion works well because for connected segments always have a well defined collision vertex and for advances on the order of 15% of the vertices of the two ends of a segment do cross each other. An example is shown in Figure 4.11 of a segment motion algorithm including faceting, shadowing and a option for a slowing at concave corners in case clearing of debris is an issue. This approach requires careful generalization in 3D because an initial vertex on the surface has multiple facets which intersect in lines instead of planes and even advancing each facet according to Frank’s method results in multiple possible locations for the initial vertex [rzz.scheckler.IEEE].

In general the isotropic, directional and angular dependent advancement mechanisms may all be present simultaneously. When multiple process effects are to be taken into account the vector sum of their rates on each facet can be added and the location of the new facet computed. The isotropic contribution is generally attributed to the neutral plasma species and results in a component in direction $\hat{n}$ normal to the surface and inward.
The directional component is attributed to the directed flux of species impinging on the surface and is in the vector direction of the flux.

More generally the local etch rate can be a function of the direction of the flux relative to the surface normal. This is the case in ion milling and this effect is included through a third component normal to the surface with angular dependent rate \( R_p(\theta) \) where \( \theta = \cos(\mathbf{\hat{n}} \cdot \mathbf{\hat{t}}) \) which depends on the angle of the flux with the normal is also included.

The composite etch rate is the vector sum of the three components or

\[
\mathbf{R}_{TOTAL} = \mathbf{R}_{ISO} \mathbf{\hat{n}} + \mathbf{R}_{DIR} (\mathbf{\hat{n}} \cdot \mathbf{\hat{t}}) \mathbf{\hat{n}} + \mathbf{R}_p (\mathbf{\hat{n}} \cdot \mathbf{\hat{t}}) \mathbf{\hat{n}}
\]  

The algorithms used for profile advance must also keep track and modify the advancement as underlying nonplanar device features become uncovered as shown in Figure 4.12 for the case of opening a source/drain contact by etching. Here materials I through V are the silicon substrate, thermal oxide, polysilicon, deposited oxide and photoresist. The starting...
profile is nonplanar and the algorithm must be convenient to initialize. In general the underlying topography is nonplanar and the algorithm must detect when the interface between two materials is reached. At that interface the advancement rates and even physical mechanisms producing the advancement may change. For example, when the etching reaches the substrate the high selectivity of oxide to silicon would require the advancement of any vertex reaching the interface to be immediately slowed. Dissimilarities in advancement characteristics of the materials at the interface may produce profile altering effects such as can be seen in the undercutting beneath the resist mask edge. Concerns in process development often require geometrical properties to be extracted such as angles on etched faces or the minimum thickness of a protective material (e.g. distance between the current profile and the polysilicon gate III).

3.4 Analytical Solutions for Simple Cases

The profile shape which evolves is a function of the characteristics of the process advancing it as well as the initial profile of the topography. Several cases of deposition under different process conditions are shown in Figure 4.13 for illustration. A small amount of isotropic deposition simply amounts to sweeping the surface with either a spherical (3D) or a cylindrical (2D) domain of influence. Directional deposition, differs in that every visible point simple translates in the growth direction. This of course produces unusual effects at shadow boundaries. When the thickness deposited becomes a significant fraction of the feature size major topological changes may occur through collisions of unconnected sections of the surface. For example with isotropic deposition in a vertical trench the two sides will grow outward and collide. This may serve a useful purpose of filling a trench or
contact hole when the thickness deposited $d$ exceeds half the width of the trench or contact $w$. The dip formed which remains on top has a height $h_{DIP}$ given by

$$h_{DIP} = d \left(1 - \sqrt{1 - \left(\frac{w}{2d}\right)^2}\right) \quad \text{EQ 3.4-1}$$

It is interesting to consider etching the surface back to the initial surface height in the planar areas in what is known as the blanket deposition and etchback method of filling contacts. If the etch back were done with directional etching a simple vertical translation would occur and the dip would be unchanged. If this were done with isotropic etching the minimum in the dip would spawn a fan or etch cylinder which would turn the sharp point of the dip into a rounded bowl. However, the trench would remain filled (except for the bowl). An important observation is that an isotropic deposition cannot be undone by an isotropic etch.

In wet etching of phosphorous doped oxide and in dry etching of trenches the processing is often found to generate planar facets at repeatable angles as indicated in Figure 4.14r,. The phosphorous doping turns about 200 nm of oxide to glass which reflows at a low temperature and helps to planarize oxide etch steps. In wet etching with HF it etches about three times faster than the undoped oxide underneath. As the HF proceeds in through openings in a resist mask it races laterally through the PSG continually exposing more and more undoped oxide to HF etching. This lateral movement at the etch rate of the PSG or $R_{FAST}$ creates a series of time-delayed equivalent sources which proceed to etch the undoped oxide at a rate $R_{SLOW}$. The angle $\theta_{\text{FRONT}}$ which the etch front makes with the horizontal interface is
For this etching application the PSG etches about three times faster than the undoped oxide producing an angle of 17°. This is a considerable reduction in the nearly 90° sidewall angle but it comes at the cost of the underetching being three times more sensitive to the endpoint.

In dry etching it is the difference between the mask and unmasked etch rates of the underlying material which contributes the facet. In the unmasked region the profile marches downward at the sum of the isotropic and directional rates. At the shadow boundary this spawns a time delayed series of equivalent sources whose domain of influence reaches under the mask edge. The angle $\theta_{\text{FRONT}}$ is given by

$$\sin \theta_{\text{FRONT}} = \frac{R_{\text{SLOW}}}{R_{\text{FAST}}}$$

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$$\sin \theta_{\text{FRONT}} = \frac{R_{\text{SLOW}}}{R_{\text{FAST}}} = \frac{R_{\text{UNDOPED}}}{R_{\text{PSG}}}$$

EQ 3.4 - 2

Notice that a portion of a circular cylinder is generated at the top of the layer by a fan of facets from the lower corner of the mask. The tapered sidewall is a tangent plane to this cylinder. For this reason $\theta_{\text{FRONT}}$ is given by asin rather than acos of the rate ratio.

It is also possible to work backwards from the profile at the end of a process and identify potential problems. This as has been useful in diagnosing rapid lifting of the masking resist from the oxide interface in wet etching [rzz.arn.kodak]. The interpretation of the profile signature is most easily understood by first considering types of profile features created by a moving source with nonuniform velocity as illustrated in Figure 4.15. The region from $x_0$ to $x_1$ is opened to etching at rate $R_0$ at time $t_0$ and produces the horizontal facet directly below it. The region from $x_1$ to $x_2$ is opened at a uniform rate $R_1$. This produces planar facet $s_1$ to $s_2$ at an angle $\alpha = \frac{\sin(R_1/R_0)}{\sin(R_1/R_0)}$ which must be connected by a circular contour $s_1$ to $s_1$ to the previous horizontal facet. Note that all of this circular section is produced by etching starting from point $x_1$. Opening the region $x_2$ to $x_3$ at time $t_2$ when the moving source arrives at $x_2$ again produces a horizontal facet $s_2$ to $s_3$. It is inter-
estimating to note that the information between points $x_2$ and $x_3$ is lost as the two associated planar facets advance into each other with time. The effect of changing from a slow moving source rate $R_1$ to a fast one $R_2$ and back again is shown from $x_3$ to $x_6$. The facet shapes and loss of information are again very similar. The final contour shown corresponds to the time $t_6$ when the source is at $x_6$. Contours similar to this one with tell tale slope changes and plateaus are indicative of resist adhesion problems.

The bombardment during etching generally leads to erosion or facetting of the top corner of the masking layer. This lateral effect can be a drawback and lead to unusual profiles in the substrate when the mask material etches faster than the substrate material as shown in Figure 4.16. The etch rate versus angle curves assumed are given in Figure 4.17 and are AM2 for the mask and AS for the substrate. For the equal time steps shown the advance of the horizontal regions is given by the etch rates at normal incidence. However, the top corner of the mask immediately begins to facet at an angle $\theta_{MAX}$ of 50° and advance normal to that facet at the maximum etch rate $R_p(\theta_{MAX})$. The thickness of the mask at the line-edge erodes at an even faster rate $R_{DOWN}$ which is approximately given by the intersection of angular facet with the mask edge.

$$R_{DOWN} = \frac{R_p(\theta_{MAX})}{\cos(\theta_{MAX})}$$  \hspace{1cm} \text{EQ 3.4-3}

In a typical case where the maximum rate is twice the rate at normal incidence at $\theta_{MAX}$ of 55°, the vertical masking thickness at the mask edge erodes 3.5 times faster than in the large flat areas. Alternatively the mask might be thought of being only 29% as effective as it should be due to this lateral effect.

No lateral encroachment of the substrate profile across the mask edge occurs until the mask edge is completely eroded away. However, once the corner facet files off the mask edge completely to the substrate it proceeds to recede laterally at a rate given by
Topography Effects in Deposition and Etching

**FIGURE 3.16** Effect of mask erosion on substrate profiles in ion milling [rzz.am.mim].

**FIGURE 3.17** Hypothetical etch rate versus angle curves used to illustrate the effect of ion milling mask erosion on substrate profiles.

\[ R_{\text{LATERAL}} = \left( \frac{R_{\text{MAX}}(\theta_{\text{MAX}})}{\sin(\theta_{\text{MAX}})} \right) \]  

**EQ 3.4-4**
For the parameters above this rate is 2.44 times the etch rate at normal incidence. As the mask recedes in this uniform manner it creates a time delayed release of equivalent sources. These sources in turn create a planar facet whose angle \( \theta_{\text{RECEDE}} \) with respect to the horizontal is

\[
\theta_{\text{RECEDE}} = \arcsin \left( \frac{R_{\text{LOWER}}(\theta_{\text{RECEDE}})}{R_{\text{LATERAL}}} \right)
\]

EQ 3.4 -5

Notice that \( R_{\text{LOWER}} \) depends on \( \theta_{\text{RECEDE}} \) which make the exact value a little difficult to predict. For the example here it is about 23°. These facets would extend out to the mask edge were it not for additional faceting of the corner formed there. The faceting occurring there is due to the etch rate versus angle of the substrate material and occurs at \( \theta_{\text{MAX}} \) for the substrate.

The cases considered in this section have been sufficiently simple that either cylindrical or planar facets were formed. Some complex initial profiles might be treated by combining these simple results. However, care should be taken as there my be more sophisticated mathematical and physical issues which must be considered. For example, in deposition and etching constraints may need to be added at concave and convex corners to make the profile motion satisfy conservation of material and to have advancement rates independent of surface roughness. Care is also needed at concave upward corners when angular dependent etch rates occur such as in crystal etching.

3.5 Basic Facet Analysis and Physical Phenomena

To understand the faceting of the initial profile the advancement of two neighboring facets will be considered as shown in Figure 4.18. Of key interest is the direction and rate of

\[ \text{FIGURE 3.18} \quad \text{Geometry for analyzing the advancement of the intersection between two adjacent facets.} \]
advance of the vertex where they intersect. The two facets have downward normals which make angles $\theta_1$ and $\theta_2$ with respect to the vertically downward direction. They advance a distance which is the product of the planar etch rate for their orientation $R_p(\theta)$ and the time step $\delta t$ as $R_p(\theta_1)\delta t$ and $R_p(\theta_2)\delta t$ respectively. The vertex where they intersect travels at an angle $\theta_v$ and rate $R_v(\theta_v)$ a distance $R_v(\theta_v)\delta t$. The angle of path of the vertex with respect to the normal to the two facets is $\alpha_1$ and $\alpha_2$ which are $\theta_v - \theta_1$ and $\theta_v - \theta_2$ respectively. Projecting the distance of travel of the vertex onto the distances advanced by the facets gives two equations.

$$R_v\delta t \cos(\theta_v - \theta_1) = R_p(\theta_1)\delta t \quad \text{EQ 3.5 -1}$$

$$R_v\delta t \cos(\theta_v - \theta_2) = R_p(\theta_2)\delta t \quad \text{EQ 3.5 -2}$$

Since the cos is an even function $\theta_v - \theta_2$ can be replaced by $\theta_2 - \theta_v$ so that both arguments are positive when $\theta_1 < \theta_v < \theta_2$. Taking the ratio to eliminate $R_v(\theta_v)$ gives

$$\frac{\cos(\theta_2 - \theta_v)}{\cos(\theta_v - \theta_1)} = \frac{R_p(\theta_2)}{R_p(\theta_1)} \quad \text{EQ 3.5 -3}$$

Once $\theta_v$ is known the associated rate $R_v(\theta_v)$ can be found from EQ 3.5 -1 or EQ 3.5 -2 and is of course larger than either $R_p(\theta_1)$ or $R_p(\theta_2)$.

The previous equation EQ 3.5 -3 makes a number of interesting predictions about the physical nature of the motion of the vertex. If rate $R_p$ is not a function of the facet angle $\theta$ then the right hand side is unity, forcing $\theta_2 - \theta_v = \theta_v - \theta_1$ or $\theta_v = (\theta_2 + \theta_1)/2$ which means that the vertex moves along the bisecting angle. Now consider $R_p$ to increase with angle $\theta$. This makes the right hand side of EQ 3.5 -3 > 0. It follows that $\theta_2 - \theta_v < \theta_v - \theta_1$ or $\theta_v > (\theta_2 + \theta_1)/2$. This means that the faster moving facet will encroach into the region of the slower moving facet and likely expand in size. Two other interesting observations of this type of analysis were pointed out by Stewart et al. [rzz.stewart.1969]. The first is that in etching the crest of a ridge will move laterally toward the side for which the etch rate is the lowest. (And also that a valley will move laterally toward the side with the fastest etch rate. The second is that vertices or nodes on a representation of a curved step will migrate away from the region where the etch rate is the largest as it expands to form the dominant facet. This phenomena is shown in Figure 4.19. To explore further how the domain of influence depends on the shape of the etch rate function the direction of travel of a facet at angle $\theta$ with etch rate function $R(\theta)$ will now be derived. A source point can be thought of releasing a continuous set of facets at all angles. Any two facets may collide in a shock or diverge requiring fans of additional etch fronts to be added in-between. In the limit of the angle between a pair being small enough their intersection vertex will propagate in the direction of motion of the facet. This limiting case can be determined from EQ 3.3 -3 by taking the special case of $\theta_1 = \theta$ and $\theta_2 = \theta + \delta \theta$ and letting $\delta \theta$ go to zero. Substituting, using a trigonometric identity, and expanding $R_p$ in a Taylor series gives
This equation indicates that a facet at angle $\theta$ moves laterally with a rate component proportional to the slope of the etch rate function with angle $\delta$ as well as normal to the surface at the usual etch rate $R(\theta)$. We are on the verge of discovering Frank's observation that the facet moves in a direction normal to the reciprocal of the rate function in a polar plot.

### 3.6 Rigorous Analysis of Vertex Motion via the Slowness Surface

Earlier it was simply assumed that a corner which could contain a facet with a fast etch rate would simply facet at that angle. Actually there are many possibilities such as generating multiple facets and even slow-advancing facets. A rigorous technique for analyzing such cases was developed by F.C. Frank for crystal etching [rzz.frank.52.58]. A complete methodology for analyzing vertex motion including generation and annihilation as been given recently by C.H. Sequin [rzz.sequin.sa]. A prototype simulation program based on this methodology has been developed by W. Foote [rzz.foote.ms]. The methodology paper...
by C.H. Sequin includes very clear geometrical presentations which are restate here using several of the original figures. These presentations were developed for the more difficult case of crystal etching where the minimum to maximum etch rate ratios can change by over 100 in several degrees. The approach is certainly applicable to process like ion milling although the generation and annihilation of faces is much more tame.

Consider the concave and convex cases of advancing facets shown in Figure 4.20. The arrows show that the vertex might be considered to advance in three modes: as the rate and direction of face \( a \), face \( b \) or as the vertex itself with rate vectors \( r_a \), \( r_b \) and \( r_c \) respectively. Consider a vector between \( r_a \) and \( r_c \) which is \( r_{ac} \) (not shown). This vector is perpendicular to \( r_a \), \( r_{ac} \), \( r_c \) and forms a right triangle. Since it is a right triangle \( r_a^2 + r_{ac}^2 = r_c^2 \) it follows that the point \( r_a \) lies on a circle \( c_{ab} \) whose diameter is \( r_c \). Similarly for the point \( r_b \) also lies on a circle \( c_{ab} \) whose diameter is \( r_c \). A reference circle centered at the origin is now defined with radius \( c_u \) (since the radius can be arbitrarily scaled it is simply referred to as the unit circle). If the original circle \( c_{ab} \) is inverted in the reference circle a straight line \( L_{ab} \) is generated. This line forms the chord between two slowness vectors \( S_a \) and \( S_b \) which have resulted from the inversion of the two etch rate vectors \( r_a \) and \( r_b \). The corresponding slowness vector \( S_{ab} \) of the vertex motion is the inverse of vector \( r_c \). Because of the symmetrical position of the later in the circle \( c_{ab} \), \( S_{ab} \) is also perpendicular to the chordal line \( L_{ab} \). This is basically Frank’s observation that the facet moves in a direction normal to the reciprocal of the rate function in a polar plot.

Depending on shape of the etch rate versus angle curve the situation can get more complicated: faces can not only disappear, but new faces with orientations not previously seen can emerge along edges or at corners. This includes the generation of slow-advancing as well as fast-advancing facets. Specific etch rate and slowness curves for ion milling and anisotropic crystal etching were considered previously in Figure 4.9. An analysis for a
general zigzag slowness curve is shown in Figure 4.21 using a convex hull to identify all the possible faces which are generated [rzz.sequin.sa]. First consider the convex corner. A detailed plot of the slowness factor from $S_a$ to $S_b$ is shown. Anytime the slowness factor lies further from the corner than the cord facets will be generated. To find the actual facets a convex hull (a convex polygon which contains the slowness function) which connects the maxima of the slowness curve from $S_a$ to $S_b$ is constructed. Here the convex hull is made up of new points $S_c$ and $S_d$ as well as $S_a$ and $S_b$. Since this curve has three segments or new chords there will be three vertices and they will move in the directions corresponding to the perpendiculars to these chords. This generates two new facets whose orientation and advancement rate can be determined from that of the vertices. For a convex corner a convex hull through the minima of the slowness factor will determine the number of vertices, their direction and advancement rate, and hence the new facets.

The analysis for three-dimensional corners is more difficult because they can be of several different types. There are not just convex and concave corners to be distinguished but there are also saddle corners. At a polyhedral corner more than two planar facets meet. Bevel faces along edges can be generated as well as facets at corners. Nevertheless the analysis that has to be done is conceptually the same as in the planar two-dimensional case. A convex hull must be found over the slowness surface within the solid angle of the normals formed by the face normals around the vertex of interest. In all cases, the analysis is facilitated by looking at the vertex figure projected onto the slowness surface. A number of interesting three-dimensional cases are discussed by C.H. Sequin [rzz.sequin.sa].

The domain of influence for a point source can now be determined by tracing the paths of possible vertices according to the convex hull. Alternatively facets at various angles could be moved. The facet at the angle of the maximum etch rate will move perpendicular to itself, rapidly sweep away material and create a facet at the angle of the maximum etch rate. Facets at other angles (according to Frank’s theory) will move in directions which make them tend to diverge away from the fast direction. By tracking each of the possible facet angles which could be generated by a corner formed by facets on an initial profile it is possible to determine the exact etch shape of the domain of influence. Obtaining a closed form solutions even for a general etch rate function is a difficult task.
In ion milling it is an interesting question as to what the boundary condition should be at the apex of a V-shaped trench particularly when the trench angle is acute. Three factors are likely to reduce the etch rate of the apex of concave corner as indicated by the ‘concave limit’ in the segment motion algorithm of Figure 4.11. First, the apex presents a normal and hence slow-advancing facet to the incident beam such as that seen in the convex hull case above. There are also two reasons that the etch rates measured on large flat areas may not be applicable to acute concave corners. First, it seems likely that the mechanical sputtering mechanism would be inhibited somewhat by the fact that as the impact energy rumbles forward it no longer finds atoms near the surface and even when it does the take-off solid angle of the atom at the vertex is restricted. Second, redeposition is ever present and material etched from the sides of the V-shape might accumulate at the apex.

These issues were investigated by first creating V-shaped trenches with 54.7° sidewalls by wet etching and then ion milling them at a wafer tilt angle of 27.5° [rzz.arn.mim]. The results in Figure 4.22 show faceting on the left corner as expected (the 20 min profile needs to be flipped left to right). Surprisingly, the trench bottom retains the initial V-shape. It appears that none of the tree factors (slow-etching facets, restricted take-off angles, and redeposition) have contributed to slowing the movement of the apex. It appears that a simple advance of the two facets making up the concave corner should be used in simulating ion milling.
3.7 Deposition

Deposition systems may be designed to produce good step coverage in the cases of sputtering and planetary systems or poor step coverage in special tooling for lift-off techniques. A discussion of the tooling geometry and factors which affect the distribution of arriving species and their tendency to stick is beyond the scope of this monograph. Classic examples can be found in texts such as Yeager, Sze and Wolf and Tauber. Key issues are the geometry, apparent source size, collisions in transit from the source to the wafer, and the impingement and sticking rate of both contaminants and the material being deposited. The later are a strong function of the pressure in the system with very low pressures (and long mean free paths) needed to for direct geometrical deposition with little contamination.

Sputtering systems are operated at only moderately low vacuum conditions such that the sputtered material under goes several collisions in transit from the sputter target to the wafer. These multiple collisions result in the material flux at the wafer arriving from widely differing angles over almost the full $2\pi$ sr half space. This broad set of angles is very effective at covering sidewalls and the coating thickness perpendicular to the sidewall even for vertical profiles is 50% of the deposited film thickness. High aspect ratio trenches and contact holes, however, still pose a problem in that double shadowing sets in where portions of the initial profile such as the bottom and vertical walls near the bottom are shadowed by both the left and right side of the feature. This of course worse for contact holes where the visibility of the bottom of the trench to the incident flux is almost completely occluded by the top rim. An example of the severity of the double shadowing effect for a trench is shown in Figure 4.23. Here the step coverage for trenches with both

![Figure 3.23](image)
vertical and tapered walls are shown. The design curves show the resistance of the layer of material crossing the trench compared to that for a flat surface as a function of trench width and sidewall angle. Once a 1:1 aspect ratio is reached the resistance rises very rapidly. And sidewalls steeper than 60° also result in a significantly increased resistance.

An alternative to sputtering is planetary deposition. This is done at low pressure so that the stream of material appears to come directly from the source. To achieve the broad angular distribution which is good for step coverage the wafer itself is moved to present many different angles of arrival. Typically the wafer is mounted on a planetary spherical dome which rotates. The planetary axis is tipped almost 60° degrees with respect to the system axis and the material streams upward from a source located on the system axis. The geometry shown in Figure 4.24 may be helpful to visualize the system. The profile shown in

![Geometry](image)

**FIGURE 3.24** Geometry for a planetary evaporator system and the resulting asymmetrical step coverage for lines tangential to the edge of the spherical dome. In the system model proposed by Blech [rzz.blech] and modified here the wafer is mounted at a radius \( r \) and angle \( \beta \) on a rotating shaft which is of length \( p \) and makes an angle \( \gamma \) with the system axis a distance \( s \) up the system axis from the source (after [rzz.blech]).

Figure 4.24 from this system is clearly asymmetrical as was pointed out by Blech et al. in their initial simulation work [rzz.blech]. The asymmetry arises because lines at the largest radius \( r \) which are horizontal when the rotating planet puts them in a down position receive flux at nearly 40° from vertical. These same lines while at the furthest distance from the source see flux at less than 10° from vertical.

A very useful process called lift-off was developed by exploiting poor step coverage of evaporated metal on a patterned sacrificial resist layer with undercut profiles [rzz.hatzakis]. It is helpful to make the initial profile in what will be a sacrificial layer undercut (bottom wider than the top) and limit the deposition to be nearly vertical. In this case the
completely shadowed regions of the profile will occur and will result in cracks completely through the deposited layer. If the initial sacrificial layer is now removed by for example wet etching, the deposited material will only remain in the patterned openings in the initial sacrificial layer. A simulation of metal lift-off in a modified planetary evaporator is shown in Figure 4.25. This aluminum profile was subsequently covered by deposition of SiO₂.

![Simulated metal lift-off profile showing that complete shadowing has created cracks which extend all the way through the material to the substrate](image)

Note that the left side of the aluminum has a vertical foot due to the aluminum arriving at other than vertical angles and piling up on the sidewall of the resist profile. This results in shadowing during sputtering of the SiO₂ and results in cracks in the insulator. Since the material at these cracks has not been deposited with the usual bombardment of particles it tends to be less dense and have a significantly higher etch rate which often leads to inadvertent etching. A wet etchant such as HF can work laterally into the masked area in these weak spots and create what are some times called ‘rat holes.’

Rigorous process simulators such as SAMPLE can be used to emulate the time-evolution of the topography during deposition processes. The example input files in Figure 4.26 and Figure 4.27 give an indication of the various models and physical parameters which must be specified for sputtering and planetary evaporation. The input information content is typical of that for any simulator and consists of a description of the deposition tool (geometry and throw rate), simulation window with the initial profile (turning points), simulation accuracy (level of approximation) and finally the processing conditions (deposition time and number of contours to display). More detailed information on the commands can be found in the SAMPLE User Guide which as well as the SAMPLE source code is available from the ILP Software Office [rzz.ILP.address].
3.8 Etching

In dry etching the plasma source and extraction of species must be modeled. The reader is referred to texts which cover these characteristics in detail such as those by xxx.IBM, Monus and Flamm, Lieberman, etc. The key concepts are that the plasma generates both charged and activated neutrals. The neutrals diffuse to the surface and generally lead to isotropic etching as for example can occur with fluorine. The plasma charges up to is the highest positive potential due to the electrons having low enough mass to respond to the high frequency RF fields. The ions which are less mobile can be extracted across the boundary sheath layer when the wafer is at a lower voltage than the sheath. The pressure affects the number of collisions in the sheath and the directionality on arrival of the ions is typically proportional to the ratio of the square root of power to the pressure. Due to the large number of charged and uncharged species generated by collisions in a plasma it is a very difficult task to make a detailed model of the chemistry. Global gas mixture effects are also important such as the use of additive H to control the C/H ratio and limit the tendency to polymer coat the wafer surface.

A typical profile from reactive ion etching is shown in Figure 4.28. Here the aluminum oxide was initially patterned by wet etching. The underlying silicon dioxide was then etched with a very directional reactive etching process and once through this layer the silicon substrate also began to etched. The silicon dioxide has a nearly vertical albeit tapered sidewall due to the highly directive nature of the etching. The silicon substrate for which the etching is only moderately directional shows the tapered planar facet and circular cylinder region describe earlier in Figure 4.14.
Rigorous process simulators such as SAMPLE can be used to emulate the time-evolution of the topography during etching processes. The example input file in Figure 4.29 gives an indication of the various models and physical parameters which must be specified for reactive ion etching. The input information content is typical of that for any simulator and consists of a description of the effects of the etching tool on each layer (isotropic and directional etch rates), simulation window with the initial profile (etch profile), simulation accuracy (level of approximation) and finally the processing conditions (etching time and number of contours to display). More detailed information on the commands can be found in the SAMPLE User Guide which as well as the SAMPLE source code is available from the ILP Software Office [rzz.ILP.address]
Topography Effects in Deposition and Etching

Sweeping the profile with the domain of influence for a source point can be used to model the time-advance and this creates fans and shocks.

A vector sum of rate components normal to the facet surface is often used to model process with multiple physical mechanisms such as dry etching where isotropic, directional, and angular dependent ion milling occur.

Analytical solutions can be found for simple case of simple geometries and uniformly moving equivalent sources.

When the advancement rate normal to the surface is a function of the angle of the surface, fast-advancing and even slow-advancing planes can be generated such as is present in corner faceting in ion milling.

A rigorous methodology for following facets/vertices and their generation can be based on the properties of the slowness surface which is the reciprocal of the etch rate surface.

Deposition modeling is primarily a matter of determining the angular distribution of arriving material and its shadowing by the topography.

In etching each material has its own etching characteristics and boundaries between materials must be considered and often give rise to faceting.

3.10 References
FIGURE 3.29

Typical set of input parameters and simulated line-edge profiles for reactive ion etching from SAMPLE [rzz.sample.ug].