Chapter 15

THERMALLY INDUCED BPSG FILM VISCOUS FLOW ON STEPPED IC DEVICE STRUCTURES

BPSG films are now routinely used as a Pre-Metal Dielectric (PMD) (another term used is Inter Layer Dielectric, ILD) between the polysilicon or silicide gate and the first level of device metallization (see Figure 1.2). Once deposited, a BPSG film underwent thermal treatment at elevated temperatures that allowed implementation in IC device technology the major glass film property – its ability to soften and to flow. The main advantage of BPSG is the ability to flow at significantly lower temperatures in comparison with previously used PSG films.

As shown in Chapter 11, the effective decrease of the viscosity of PSG glass is due to introducing several percent of boron oxide into the glass in addition to the phosphorus oxide. The decreasing of PMD flow temperature was a general direction in IC technology. It was necessary for decreasing the thermal budget of VLSI and ULSI circuits.

In integrated circuit technology, the BPSG film capability to soften can be realized at both isothermal furnace anneal (FA) and rapid thermal anneal (RTA). Although the flow properties of BPSG thin films in device manufacture have been addressed by many authors, most of them treated the subject in a qualitative manner. Cross-sectional scanning electron microscope (SEM) images of processed specimens form the core of these reports. The author’s research into the thermal flow of BPSG thin films started in the mid-1980s. Unlike other research, the author’s group proceeded from well-known viscous properties of bulk glasses and found their quantitative correlations with thin film glass flow on stepped IC device surfaces.

Chapter 15 is a consolidation of long-term quantitative studies of BPSG film flow issues and solutions. It focuses on the detailed analysis of the main practical aspects of BPSG film flow studies. As a result of these studies, an approach for quantitative characterization of BPSG film flow was developed. In addition, the acceptance of developed approaches for films flow analysis in quaternary glass systems, such as GeO$_2$-SiO$_2$ glass enriched with B$_2$O$_3$ and P$_2$O$_5$ is shown.
15.2. A Brief Historical Review of Flow-Able PMD in IC Technology

An analysis of published data as well as the results of BPSG film implementation allowed selection of three basic directions of the flowable film application in VLSI and ULSI technology.

Historically, the first implementation of BPSG film capability to flow at enhanced post-deposition temperatures was the so-called film “planarization” of device steps (see Figure 1.1(c,d,e,f)). The term “planarization” meant the smoothing of an insulator surface in order to prevent the breaking and short-circuiting of conducting paths that will run on the surface. The glass film anneal was used in a few hours time delay after film deposition. Different gas ambient compositions, such as oxygen, nitrogen, argon and steam, were used. This application was linked mainly to the advent of high-speed integrated multilevel device technology with short transistor channels and shallow p-n junctions. The place of PMD in the device structure is very important, because it affects a quality of a metallization layer sputtered above. For instance, non-conformal PMD film on device steps and strictly vertical side-walls of etched in PMD contact holes enhance non-conformality of metal sputtering (as shown in Figure 3.1(a,c)). In such a case, the metal thickness on a side wall is not sufficient for proper metal line conductivity. Moreover, metal bridging issues are also known for these structures because of the shortening of neighbor metal lines after etch. Thus, in order to make metallization reliable, device topography needs to be smoothening (as shown in Figure 1.1(d,f) and Figure 3.1(b,d)).

Film flow allowed the smoothening of high device steps covered with BPSG film. Numerically, it corresponded to a decrease of the initial angle \( \alpha_0 \) (step coverage angle on device step after film deposition) to final low value \( \alpha_f \) after anneal at a certain temperature \( T_a \) for a certain anneal time \( t_a \) (see Figure 3.2(a,b)). The main advantage of BPSG films is about 200 – 300 °C difference (depending on the additive concentration level) between flow temperatures as compared to PSG films with the same quality of planarization. The main results of the planarization properties of BPSG, which were studied mainly qualitatively, are presented in Table 3.1.

Later, the second BPSG film anneal, frequently called “reflow”, was introduced in IC device technology in order to smooth sharp edges and taper contact holes. This second anneal was performed after lithography and plasma etch procedures forming openings in BPSG film – contact holes. This second anneal allowed decreasing of the side wall angle in contact holes from \( \Theta_0 \) to \( \Theta_r \), as shown in Figure 1.1(e,f) and Figure 3.3(a,b,c,d). In such a case, an inert gas ambient was used in order to prevent the oxidation of the silicon surface in these holes. Some data regarding this issue can also be found in Table 3.1.

According to many researchers, it was established that practical BPSG films should contain no more than 8 – 10 wt % boron and phosphorus totally combined and that the furnace-annealing (FA) temperature should be above 900 °C. Almost complete planarization is possible under the stated conditions. However, defects were found to arise in the glass at certain concentrations of boron and phosphorus at relatively high annealing temperatures. The defects were traced to the intense interaction of the two additives with the moisture that penetrates into the glass from the air (see Chapter 13). Thus, the use of BPSG in ICs requires the careful optimization of the film composition. Some particular quantitative
investigations other than ours were presented in Table 3.1. However, there were no detailed papers and, therefore, no deep understanding on the impact of the underlying device geometry, BPSG film parameters and anneal processes on the effectiveness of BPSG film flow and device planarization.

The thermal-flow planarization of BPSG thin films was proven to be suitable for IC device technology of minimum feature sizes down to 0.35μm. Below this level, chemical mechanical polishing technology emerged as a viable alternative. Nevertheless, glass-flow techniques have found another application in ULSI circuits of feature sizes down to 0.15 – 0.18 μm. Among the technology challenges, the drive of the ULSI technology node towards the 100 nm and below resulted in the decrease of device gap spacing in conjunction with the increase of aspect ratios at transistor level. Small gaps with below 0.1 μm spacing and aspect ratios (AR) higher than 10 become a feature of sub-100 nm IC technology and these numbers are improving further [341]. The decrease of gap spacing goes along with a change of gap shape and re-entrant gap profile is a common shape in ULSI devices. These peculiarities with CVD film deposition features enhance the issue of a void-free PMD gap-fill, which is known as a “voiding” phenomenon and reflects a certain empty space between device elements (see Figure 3.4(a-d)). Thus, providing a void-free BPSG film gap-fill with film flow, e.g. elimination of key-holes formed during film deposition, became a new issue of BPSG films implementation in the mid 1990s.

Figure 3.1. Cross-sectional schemes of stepped device structure with a polysilicon strip (it models a conventional poly gate region of a MOSFET) covered with BPSG film and plasma-etched pre-sputtered metal (a,b) and schemes of vias in BPSG films filled with sputtered metal (c,d). Left side – without BPSG film flow, right side – after BPSG film planarization using thermal flow.
Table 3.1. Summary of accumulated flow-related quantitative results for glass films used in IC technology (in a chronological order)

<table>
<thead>
<tr>
<th>Ref</th>
<th>BPSG object (thermal treatment conditions)</th>
<th>Results, equations or correlation obtained</th>
</tr>
</thead>
<tbody>
<tr>
<td>[52]</td>
<td>CVD films (FA)</td>
<td>After FA of BPSG films, contact hole side wall slope was found to be about 2 times more effective with boron as compared to phosphorus.</td>
</tr>
<tr>
<td>[54]</td>
<td>Bulk glass</td>
<td>Introduced glass transition temperature ( T_g ), that was found to correlate with glass flow temperature ( T_f ) as follows: ( T_f = T_g + 288^\circ C ).</td>
</tr>
<tr>
<td>[339]</td>
<td>CVD films (FA)</td>
<td>At contact hole reflow, slope was found to be higher than 90° if a geometric ratio of BPSG film element thickness to this element length exceeded ~0.393.</td>
</tr>
<tr>
<td>[82]</td>
<td>CVD films (FA)</td>
<td>Proposed an empirical equation ( A = 51.5 - 1.4[P] - 9.5[B] ) for film planarization on device steps. A possibility to use a non-destructive surface profilometer technique for film flow analysis on device step was shown.</td>
</tr>
<tr>
<td>[86]</td>
<td>CVD films (FA/RTA)</td>
<td>An equation ( \cot A \sim t^{1/n} ) for film planarization was proposed, where ( A ) is an angles of device step with glass film. Empirical values of “( n )” were defined to be ~2.1 ± 0.5 for RTA and ~2.4 ± 0.8 for FA.</td>
</tr>
<tr>
<td>[340]</td>
<td>CVD films (FA)</td>
<td>A modeling of BPSG and PSG films viscosity was done using EVOLVE-FLOW simulator, values for viscosity and surface tension were analyzed.</td>
</tr>
<tr>
<td>[175]</td>
<td>CVD films (RTA)</td>
<td>Defined activation energy of void elimination in small device gaps using BPSG films with about 5 wt. % each additive at RTA (~3 eV).</td>
</tr>
<tr>
<td>[178]</td>
<td>CVD films (FA)</td>
<td>Both boron and phosphorus affect BPSG (Method 1) planarization capability equally once used in equal oxides weight % ( B_2O_3 ) and ( P_2O_5 ) concentrations in the glass film.</td>
</tr>
</tbody>
</table>

![Figure 3.2. Cross-sectional schemes of SEM images: (a) in Figure 1.1(c), (b) in Figure 1.1(d) which show BPSG step angle definitions \( A_0 \) and \( A_f \), accordingly.](image)

Generally, BPSG films were successfully employed for the filling of voids that may arise in BPSG film during deposition (see an example in Figure 3.4 (a)). However, there are some
issues there. Thermal-flow planarization was commonly performed by relatively high-temperature FA, which was a comparatively long process, sufficient for proper film softening and flow. In contrast, for sub-0.18 µm ULSI circuits, it was generally accepted that the thermal annealing after the formation of transistors should be carried out at temperatures below about 750 °C for FA and about 850 °C for RTA. To ensure void filling at such low temperatures, one had to increase the boron and phosphorus concentrations in the glass above a certain “commonly accepted” values. However, this measure enhanced defect formation processes in BPSG films. Thus, an optimized BPSG film flow became a major issue along with the gradual shrinking of device design rules as well as a need to decrease the thermal budget of ULSI devices.

Figure 3.3. Cross-sectional (a,b) SEM images of vias in as-deposited (a) and thermally flowed (b) BPSG films [339]. Figures (c,d) are cross-sectional schemes of SEM images (a,b) and show BPSG step angle definitions Θ₀ and Θᵱ. Figures (e,f) show a cross-sectional scheme of a spherical glass element formed in case of non-optimized height to length ratio of the glass element before the film anneal [339]. Reproduced by permission of ECS – The Electrochemical Society.
Figure 3.4. Cross-sectional holes between device elements for as-deposited (a) and rounded voids in thermally flowed (b) BPSG films (highlighted by block arrows). Figures (c,d) are cross-sectional schemes of respective SEM images. Image (a) was presented at 4th Intern. Dielectric for ULSI Multilevel Interconnection Conf. (DUMIC), 1998 [208], image (b) was presented at 8th Intern. Symp. on IC Technology, Systems and Application (ISIC-99), 1999) [231].

The author and his co-workers based their studies [90,93,105] from a well-known relation between the viscosity ($\mu$) and the absolute temperature $T$ of bulk glass (3.1):

$$\mu = \mu_0 \times \exp\left(\frac{U}{RT}\right),$$

(3.1)

where $U$ is activation energy for viscous flow. To apply this knowledge to IC technology, the following logic was assumed. A step of an as-deposited glass film on IC device structure exists in a thermodynamically non-equilibrium state. When heated causing glass flow, the step evolves to equilibrium and eventually disappears if heating is long enough (a planar surface is thus obtained). Strictly speaking, planarization occurs under the action of both surface tension and gravity forces. However, the latter is negligible for actual step heights in ICs (they are less than 1 $\mu$m). On the other hand, practical thermal-flow processes were usually performed at moderate temperatures and for limited lengths of time, with the result that perfect (to completely flat surface) planarization is rarely feasible. A deep understanding of the planarization mechanism was therefore necessary for the optimization of the flow process.

This framework allowed the quantitative analysis of the thermal-flow planarization of stepped BPSG surfaces and summarization of relevant data from the literature. It was
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Proposed that the basic properties of BPSG films prepared by different deposition methods were similar and they could be generalized for the comprehensive characterization of BPSG material for multilevel ULSI circuit technology. Using this proposal, the approaches for quantitative characterization of BPSG planarization and optimized additive concentration range in BPSG films were developed.

It was proposed that the change of angle $A_0$ on device step should follow the temperature dependence for glass viscosity (see Eq. 3.1). In such a proposal, similar dependence for angle was proposed to be as follows (3.2):

$$\cot A_f = \cot A_0 \times \exp(E_a \times B_T)$$

(3.2)

where $A_0$ and $A_f$ are initial step coverage (as-deposited) and post-flowed angles of device step with glass film, and $B_T$ is a temperature-related member. For example, we carried out an electron-microscopy study of the angle $A_f$ as a function of the boron and phosphorus concentrations, the annealing temperature, and the angle $A_0$ in the case of 30-min FA. A set of empirical formulas was proposed for the flow of BPSG over a step of dimensions typical of actual chips. This model configuration will be considered below.

The proposed formulas were later confirmed by experiments on BPSG films produced by two modern CVD methods. One of them was plasma-enhanced chemical vapor deposition (PECVD) involving organic ethers in the presence of oxygen, i.e. Method 8. The other was based on the oxidation of the above-mentioned ethers with an ozone-oxygen mixture, i.e. Method 5. As a further step, the model was modified to include the dependence on annealing time. We thus arrived at a multi-factorial, quantitative picture of BPSG flow under FA. Afterwards the approach was generalized to rapid thermal annealing (RTA). Despite a much smaller amount of relevant experimental data, an empirical formula was derived for this regime as well. Later, studies of BPSG film gap-fill using FA and RTA technique were performed and an approach for quantitative BPSG film gap-fill evaluation was developed.

15.3. A METHODOLOGY FOR ANALYSIS OF BPSG FILM PARAMETERS ON STEPPED DEVICE SURFACES

Our early studies on the thermal flow of BPSG films dealt with device structures with a minimum feature size of about 2 $\mu$m. In that case the post-etch angle between a sidewall and the substrate surface was far less than 90° and gaps between device components were fairly wide. These facts allowed us to essentially assume that the initial flow angle $A_0$ is 85° at most. Thermal flow was examined from cross-sectional SEM images of test structures fabricated on silicon single crystals by CVD, photolithography, and plasma etching. A test structure was an array of polycrystalline-silicon lines (strips) with fixed width and spacing, as shown in Figure 3.5(a). This structure with a number of lines was covered with BPSG film, as shown by schematic cross-section in Figure 3.5(b), followed by its anneal if necessary.

The glass thickness $d_{BPSG}$ and the dimensions of the array were chosen in accord with practical chips: the strip spacing $x_{poly}$ was set to 1 − 3 $\mu$m, $d_{poly}$ was 0.3 − 0.5 $\mu$m for practical chips, and the ratio of $d_{BPSG}$ to the strip thickness $d_{poly}$ was taken as 1.5 − 2. The latter was
important, otherwise the speed of BPSG flow on device step could be artificially decreased. The individual concentrations of boron and phosphorus were 3 – 6 wt %. Some wafers with specimens, spaced a fixed distance apart, were subjected to FA in a horizontal-tube or a vertical-tube quartz diffusion furnace using argon, nitrogen, or oxygen; the process lasted 12 – 60 min at atmospheric pressure and a temperature of 850 – 990 °C. RTA was performed in nitrogen at 700 – 900 °C, the flat-temperature period being 20 – 90 sec. With the latter type of annealing, the author employed a Centura-RTP system (Applied Materials, Inc.) and apparatuses from AG and Associates.

For cross-sectional SEM imaging, the specimens were broken across the poly lines (for this reason, the line array was usually a few millimeters long and wide). The same approach was also followed in the examination of contact vias in a glass film. In this case a test structure was an array of trenches or contact vias made by dry etching of a BPSG film. The vias were of different dimensions and were distributed over a large area (to facilitate breaking).

After breaking a specimen, a sample of area 1 cm$^2$ was split off at a site of interest and attached to a stainless-steel holder. The surface to be examined was etched for a few seconds in hydrofluoric acid with a buffer (to show the interfaces), rinsed in deionized water, and dried. Finally, a thin layer of a conductive material, such as platinum, was deposited to prevent charge buildup during SEM examination.

![Figure 3.5. Optical microscopy top view on polysilicon strips (a) and a model of stepped BPSG surface used for SEM analysis (b).](image-url)
The flow of BPSG films was characterized by the angles $A_0$ and $A_f$ (Figure 3.2) on the basis of micrographs, the angles being measured with a protractor. The same SEM procedure was used for contact hole analysis to measure angles of $\Theta_0$ and $\Theta_f$, as shown in Figure 3.3. However, in such a case the openings were etched in BPSG film followed by anneal to make a desirable side wall slope. Perspective and cross-sectional images were analyzed. As the research progressed, we changed from one type of SEM to another. In the latest phase, we employed XL 30 FEG microscopes (Philips, Germany) with a magnification of up to $10^6$ times.

The time variation of $A_f$ was also studied nondestructively, using the B5000 NanoScope III model of large tapping mode atomic-force microscope (AFM) from Digital Instruments. Conceptually, it was possible to rapidly derive the profile of a stepped surface from a computer-generated AFM image of the surface, so that it was not necessary to fabricate special test structures in the evaluation of a glass-flow technology. Note that this approach was proposed by Williams et al. [82] as early as in 1987 (see images in Figure 3.6(a-e)), but the sensitivity of the method was insufficient. In our studies, AFM data were found to agree with SEM ones within about 5 % for angles < 80°, see Figure 3.7(a-c) [225].

![Figure 3.6. Surface profilometer trace over polycide runner: a) before BPSG deposition; b) after BPSG deposition, and after 900 °C anneal for 1.9 wt % [B] – 4.7 wt % [P](c); 3.1 wt % [B] – 5.8 wt % [P] (d); 4.1 wt % [B] – 5.5 wt % [P] (e) [82]. Reproduced by permission of ECS – The Electrochemical Society.](image-url)
The quality of gap-fill with flowed BPSG films was normally evaluated using similar device structures with lines, placed at different spacing one from another. After film deposition or film anneal at desired conditions, void appearance in device gaps could be observed (as shown in Figure 3.4(a)). Voids were dark rounded areas in photos from SEM and their shape and size could differ significantly. It is important to note that voids existence was not an artifact due to cross-section etch for SEM sample preparation. Their appearance was confirmed by the SEM analysis of non-etched and etched samples. However, in order to measure void size, the SEM picture must be very contrasted and this can be achieved only with proper sample etch.

15.4. QUANTITATIVE CHARACTERIZATION OF PRIMARY FACTORS AFFECTING BPSG FILM FLOW

BPSG film flow under FA conditions in dry gas. Figure 3.8(a) gives examples of $A_0$-$T_a$ relations for the FA of BPSG films. More than 60 specimens were examined, differing in deposition technique, composition, and annealing conditions. As already noted, we assumed that $A_0< 85^\circ$, which is the case with devices of a minimum feature size over 1 µm.
It was found that the graphs can be conveniently transformed into straight lines by recalculating them into a so-called Arrhenius plot, namely into the $1/T_a \cdot \log \cot A_f$ graph, where $T_a$ is stated in Kelvins, as shown in Figure 3.8(b). A number of straight lines refer to the same deposition technique met at a point whose coordinates correspond to $A_0$ and the temperature $T_{bf}$ at which thermal flow begins. Indeed, $T_{bf}$ depended on the composition of the glass, but it was difficult to calculate this dependence. It was therefore assumed that $T_{bf}$ (beginning flow) was $700 \pm 20$ °C for the glasses considered.

In Figure 3.8(b), the gradients (tangents) of the lines were proportional to the $E_a$ term of Eq.(3.2) and, therefore, depend on the concentrations of boron and phosphorus. Let us change to the concentrations of $B_2O_3$ and $P_2O_5$ stated as weight percent of elements (the respective conversion factors from [B] and [P] concentrations are about 3.2 and 2.3). The dependence of the gradient on the total additive oxides content was represented by a simple curve (as in Figure 3.8(c)). This characteristic was found to generally agree with data derived from experimental micrographs for similar surface configurations, available from the literature. (The behavior of closed circles in Figure 3.8(c) will be discussed below).

![Figure 3.8](image_url)

Figure 3.8. Thermal-flow BPSG film planarization by 30-min FA. Figures (a) and (b) depict the annealing-temperature dependence of the final flow angle. Figure (c) represents the activation term of Eq. (3.3) vs. the total concentration of additive oxides for annealing in dry gas. In each figure, data points and lines refer to measurements and calculations, respectively [223].
It is important to note that the concentration dependence of $E_a$ was found to indicate that the viscous flow of BPSG over a step was equally sensitive to the concentrations of $B_2O_3$ and $P_2O_5$. By contrast, it was widely held that the effect of $B_2O_3$ is more than 2 times stronger than that of $P_2O_5$. However, changing from $B_2O_3$ and $P_2O_5$ to B and P concentrations, we can see that boron was only 1.5 times more effective than phosphorus in affecting BPSG flow. It is also important to note that there was a rapid decrease in $E_a$ for total concentrations of $B_2O_3$ and $P_2O_5$ below 12 wt %, signifying that the viscous-flow capability of the glass was impaired. In Figure 3.8(c), the straight segment of the curve extended to the straight line:

$$\text{lg } E_a = \text{lg } E_{a(0)} + \chi(3.2[B] + 2.3[P]), \quad (3.3)$$

where a coefficient of proportionality $\chi = 0.05$. From here on a chemical formula or the symbol of a chemical element in brackets denotes the concentration of the compound or the element in weight percent. The last equation can be re-drawn to be equivalent to:

$$\text{lg } E_a = \text{lg } E_{a(0)} + \chi([B_2O_3] + [P_2O_5]) \quad (3.4)$$

In both cases of additive representation, the intercept on the vertical axis gives $E_{a(0)} = 562$. Eventually, the flowing properties of BPSG films at isothermal furnace conditions were described by the following empirical equation (3.5):

$$A_f(t_a=\text{const}) = \arctan \left\{ \tan A_0 \times 10^{-562(T_a-973)/973/T_a \times 10^{0.045(3.2[B]+2.3[P])}} \right\}, \quad (3.5)$$

where $T_a$ is the annealing temperature in degrees Celsius. Equation (3.5) was written for a fixed annealing time (in our experiments, annealing was performed in dry gas for 30 min).

The constraints (3.6) were found to determine the range of use of Eq. (3.5) and the range of linearity for the concentration dependence of log $E_a$: 

$$5.2 < 1.4[B] + [P] < 13$$
$$0.35 < [B]/[P] < 5.55$$
$$A_0 < 85'$$
$$d_{\text{BPSG}}/d_{\text{poly}} > 1.6$$
$$t_a = 30 \text{ min } \quad \text{(isothermal anneal)}$$
$$\text{Anneal ambient } N_2, \ O_2, \ \text{Ar} \quad (3.6)$$

Note that constraints (3.6) were derived from experimental data for limited concentration intervals, so that Eq.(3.5) appeared to be applicable to higher additive concentrations as well. Curves calculated by Eq.(3.5), such as those shown in Figure 3.8(a) (full curves), generally
agree with experimental data points. The exception was higher temperature conditions, but this case was less important in practical terms.

The above approach enables one to simulate the variation of the angle $A$ subject to step (surface) parameters, the properties of the glass, and annealing conditions. For example, we calculated by Eq.(3.5) the concentrations of B and P for which $A$ will evolve from $A_0 = 85$ degrees to $A_f^{FA} = 6$ degrees during annealing in dry nitrogen at a given temperature. Figure 3.9 shows the results, expressed as so-called flow isotherms for the desired angle of glass planarization, together with SEM data for 850 °C annealing temperature. Notice that there is a good agreement between the calculation and the experiment.

**BPSG film flow under RTA conditions in dry gas.** For the RTA of BPSG in dry gas, we regarded the annealing time $t_a$ as not being a principal difference to the thermal flow processes. This assumption was suggested by the results of Mercier [86], which are included in the Table 3.1. Looking at the $\cot A_f$ vs. $t_a^{1/n}$ relation for FA or RTA, one notices that the two regimes have close enough values of $1/n$. Accordingly, we followed the same line of reasoning as with FA (see section above), checking the results against a limited amount of experimental data available for RTA [223]. For $t_a = 40$ sec, we proposed that:

$$A_f^{RTA}(t_a=\text{const}) = \arctan \left\{ \tan A_0 \times 10^{-143(T_a-998)/998} \times 10^{0.050(3.2[B]+2.3[P])} \right\}, \quad (3.7)$$

with the same notation as in Eq.(3.5). Figure 3.10(a) shows calculated and measured variations of $A_f$ with $t_a$. A deviation from the experimental data was again observed only for higher temperature conditions. Figure 3.10(b) represents the calculated concentrations of B and P for which $A$ will evolve from $A_0 = 50$ ° to $A_f^{RTA} = 30$ ° during annealing at a given temperature. Thus, Eq.(3.7) can serve as a preliminary model of flow under RTA. Its parameters should be refined based on future experimental results.

![Figure 3.9](image-url)

Figure 3.9. The calculated (lines) and measured (open circles) concentrations of [B] and [P] for which the flow angle $A$ will evolve from $A_0 = 85$ degrees to $A_f = 6$ degrees during 30-min FA at a given temperatures [192,223].
Figure 3.10. Thermal-flow planarization by 40-sec RTA [223]. Figure (a) shows measured (data points) and calculated (curves) values of the final flow angle as functions of annealing temperature. Figure (b) represents the calculated concentrations of [B] and [P] for which the flow angle \( A \) will evolve from \( A_0 = 50 \) degrees to \( A_f = 30 \) degrees during the annealing at a given temperature.

**Annealing-time dependence.** There are different ways to describe the dependence of \( A_f \) on the annealing time \( t_a \) for FA and RTA. For example, one might represent experimental data in the \( t_a \)-cot \( A_f \) or the \( t_a^{1/n} \)-cot \( A_f \) plane (see Table 3.1). Following the latter approach, we transformed the general equation introduced by Mercier [86] for \( A_f \) as a function of \( t_a \) to a more convenient form:

\[
A_f(t_a) = \arctan \left\{ \tan A_{f(t=\text{const})} \left( \frac{t_{\text{const}}}{t_a} \right)^\lambda \right\},
\]

(3.8)

where \( A_{f(t=\text{const})} \) is the value of \( A_f \) for the annealing time of interest \( t_a \), \( A_{f(t=\text{const})} \) is an experimental value of \( A_f \) for a known annealing time, and \( \lambda \) is a coefficient and it is either 0.42 \pm 0.10 for FA or 0.47 \pm 0.16 for RTA.

**Comparative analysis of primary factors affecting the film flow.** The thermal flow of BPSG films is mainly governed by the initial step coverage angle \( A_0 \), the respective concentrations [B] and [P] of boron and phosphorus, the annealing temperature \( T_a \), and the annealing time \( t_a \). Equations (3.5) and (3.7), used in conjunction with Eq. (3.8), facilitate the evaluation of how \( A_f \) changes with these parameters. These complex equations for \( A_f \) for FA and RTA conditions at any anneal time are shown below (with the same notation as in Eqs. (3.5), (3.7) and (3.8):

\[
A_f^{FA}(t_a) = \arctan \left\{ \tan A_0 \times 10^{-562(T_a-973)/973/T_a \times 10^{0.506(3.2[B]-2.3[P])}} \right\} \times \left( \frac{t_{\text{const}}}{t_a} \right)^{0.42\pm0.10}
\]

(3.9)
We investigated the dependence in the case of FA, with the parameters varied about the baseline values $A_0 = 75$ degrees, $[B] = 4.5$ wt %, $[P] = 4.5$ wt %, $T_a = 850$ °C, $t_a = 30$ min. The change in $A_f$ was calculated as a function of the fractional deviation of each parameter from its baseline value. A straight line was fitted to the data points for each parameter, as presented in Figure 3.11.

The gradients of the lines in Figure 3.11 were found to be $-27$, $+16$, $-7$, $-5$, and $-1$ for $T_a$, $A_0$, $[B]$, $[P]$, and $t_a$, respectively. It can be seen that:

1. the annealing temperature $T_a$ and the initial step coverage angle $A_0$ revealed the strongest influence on BPSG flow;
2. the two major factors revealed an opposite influence on $A_f$.

The latter strongly confirms that the thin film BPSG deposition method strongly affects film planarization properties. For instance, PECVD BPSG films were very non-conformal and, therefore, $A_0$ is higher than 90 degrees. In contrast, step coverage with SACVD BPSG films were always significantly better, about 60 degrees. This simple comparison of typical step coverage values predicts the fact that PECVD BPSG film planarization is always worse. Therefore, PECVD BPSG film needs a higher temperature in order to obtain similar film planarization efficiency as compared to SACVD films. Moreover, the conclusion (2) is of crucial importance to sub-0.25 μm ULSI circuits, for which problems in gap filling combine with constraints on annealing temperature and time.
Contact-via reflow. Little was known about the mechanism of the evolution of sidewall angles in contact vias under reflow, due to the complexities of preparing test specimens. Our SEM analysis led us to the fundamental conclusion that the sidewall angle $\Theta_f$ will change in a way similar to that for the angle $A_f$ of a stepped glass surface (see Figs.3.2(a,b)) for the given glass composition, deposition technique, and annealing conditions. Specifically, for the glasses of the same composition, we drew an empirical relation (3.11):

$$ (\Theta_0 - \Theta_f) \approx 0.5(A_0 - A_f) $$

Equation (3.11) is supposed to be applicable to both BPSG and phosphosilicate glass (PSG) and different annealing conditions, including annealing in dry or wet gas (Figure 3.12). The coefficient 0.5 may reflect the fact that the glass in a via flows in a single direction, whereas the glass on a surface flows in two opposite directions. Thus, the reflow of contact vias might be investigated by analogy with the thermal-flow planarization of stepped glass surfaces.

15.5. SECONDARY FACTORS AFFECTING BPSG FLOW

Equations (3.5) and (3.7) were derived under constraints (3.6). However, our experiments and data from the literature indicated the existence of other factors that may, in some situations, also affect the flow of glass under annealing, thus reducing the accuracy of calculations. This section briefly analyzes three such cases in order to encourage the reader to carefully examine all relevant factors while studying glass flow.

Method of the film deposition. Returning to Figure 3.8(c), consider the closed circles, which slightly yet consistently deviate from the straight line representing a number of deposition methods. The reason for this behavior may be the retardation of thermal flow caused by the effect of clustering in the form of pure $P_2O_5$ of a certain proportion of the phosphorus that is present. $P_2O_5$ is meant to be linked to the $\equiv Si – O –$ groups forming. This practically means that just a part of the phosphorus linked to silicon ($\equiv Si – O – PO =$) is involved in the flow process and the rest of the $P_2O_5$ clusters would evaporate from the film and transform into $\equiv Si – O – PO =$ groups at the elevated temperature taking a part in the glass flow process. Note that the CVD of the BPSG films involved tetraethylorthosilicate (TEOS), esters of boric acid and orthophosphoric acid, and an ozone-oxygen mixture. This is probably the most common production method of BPSG deposition in ULSI manufacturing.

Effect of a $SiO_2$ cap layer. A thin (from tens to hundreds angstroms) $SiO_2$ cap layer was frequently used to increase the stability of the BPSG film and to reduce its surface-defect density by protecting, to a degree, the film from atmospheric water. The first time that this simple solution was proposed was by Nauka et al [109]. Such a layer was produced in the same CVD process once the BPSG film was fabricated and the additive compound flows were switched off. Experiments showed that a $SiO_2$ cap layer could inhibit or enhance the thermal flow of the film.
Thermally Induced BPSG Film Viscous Flow on Stepped IC Device Structures

Figure 3.12. Contact-via thermal reflow: correlation between the final sidewall angle of a contact via and the final flow angle of a stepped glass surface for given glass composition and annealing conditions. Data description: (1) PSG, 6 wt %, RTA 1050 °C, steam-oxygen ambient; (2) PSG, 6 wt %, RTA 1100 °C, steam-oxygen ambient; (3) PSG, 6 wt %, RTA 1150 °C, oxygen ambient; (4) PSG, 8 wt %, RTA 1000 °C, steam-oxygen ambient; (5) PSG, 8 wt %, RTA 1050 °C, steam-oxygen ambient; (6) PSG, 6 wt %, RTA 1100 °C, steam-oxygen ambient; (7) PSG, 6 wt %, RTA 1150 °C, oxygen ambient; (8) BPSG, 4 wt % [B] – 4 wt % [P], FA, 850 °C, argon ambient. Data on PSG are derived from cross-sectional images published by Shah et al [342], data on BPSG were obtained by the author.

The former effect was discovered and explored by Bar-Ilan et al. in BPSG films produced by PECVD from esters-oxygen mixtures [143]. It was concluded that the thickness of a cap layer should not exceed 50 Å (Figure 3.13); otherwise, the layer will seriously suppress and hinder thermal-flow planarization.

The latter effect was discovered and examined by Lu et al. [212]. The BPSG films were fabricated by the TEOS-ozone based CVD Method 5 using mixtures of organic ethers at atmospheric or a subatmospheric pressure. Unlike PECVD, as-deposited films showed much higher porosity and were more liable to form defects on the BPSG film surface (see Chapter 10 and Chapter 13 in Part 2 of the monograph). A cap layer thicker than 50 Å was therefore required.

The relationship was addressed between the minimum cap-layer thickness and the total concentration of boron and phosphorus in the glass. It was approximated by a straight line, which gave a minimum cap-layer thickness of over 200 Å for B and P concentrations of 5 wt % each. As noted in the preceding paragraph, this thickness should prevent the BPSG film from being planarized. Investigation of the thermal-flow planarization of BPSG films with different compositions for cap-layer thickness ranging from 0 to 900 Å established that planarization can even be “enhanced” by a cap layer with a thickness in excess of about 300 Å (Figure 3.13). This unexpected and dramatic effect was thoroughly analyzed and traced to the elastic properties of porous silicon dioxide produced by TEOS-ozone interaction. Additionally, such a thick cap layer should impede the escape of boron and phosphorus from the BPSG layer under annealing, thus enhancing the flow [212].
Effect of ambient during BPSG film anneal. The method above could be extended to the case of wet-gas annealing. Regrettably, this area was poorly explored by experimenters. According to Tauber [7], the same standard of planarization can be achieved by wet-gas annealing at temperatures lower by about 50 °C.

Effect of glass element geometry – via reflow. It was shown by Levy et al [339] that the shape of glass element affects the glass film flow. Particularly, if the height to width ratio of etched element with vertical side walls more than 0.393, after film anneal and flow, the side wall angle can significantly exceed 90 degrees.

This means after contact via the reflow process the size of via can be less that after etch. The reason of this effect is the surface tension of the melting glass causes the rounding of the glass element or even droplet formation from the initially “vertical” glass element (see schemes and photos in Figure 3.3(e,f)).
Modern ULSI devices tend to have rectangular step profiles due to the ongoing decrease in feature size and the advent of dry etching. As a result, in most of the current cases $A_0$ greatly exceeds 90 degrees even when the BPSG film demonstrates perfectly conformal step coverage. In practice, deposition technologies tend to provide modest conformity. This is especially true for PECVD, despite its widespread use. As a result, this method is not suitable for most types of PMD. However, PECVD may be a preferable option, if not the only proper one, with multicomponent glasses because the complex kinetics of the reactions involved makes it difficult to maintain a desired composition of films. It follows from the above that a novel approach is required to the characterization of the flow of BPSG over submicrometer steps. This approach should be universal in the sense that it should work for BPSG thin films with any practical additive concentrations and with an arbitrary $A_0$.

The author for the first time introduced a dimensionless flow parameter called “glass flow capability” [244]. It was defined as $(A_0 - A_f)/A_0$ or $1 - A_f/A_0$ (detail background and description can be found in cited paper). Glass flow capability varies over the range $[0, 1]$ and it is at a maximum when the glass surface becomes perfectly planar under annealing: $A_f = 0$. The minimum glass flow capability implies the absence of planarization: $A_f = A_0$.

The value of $A_f$ can be determined by measurement on the step surfaces. Alternatively, it can be calculated by Eq.(3.9) and Eq.(3.10), provided that the parameters meet the constraints of (3.6). It is wise to find out how flow effectiveness, $1 - A_f/A_0$, varies with annealing temperature or additive concentrations, by analogy with Figure 3.8; note that these relationships can be examined for any $A_0$. Figure 3.14(a) shows examples of the temperature dependence for the additive concentrations of Figure 3.8(a). Figure 3.14(b) depicts the concentration dependence of the gradient $k_f$ of straight lines fitted to experimental data points. The concentration characteristics are similar to those for the activation term $E_a$ in Figure 3.8(c). In Figure 3.14(a), the intercepts of the lines on the $T_a$ axis give values of $T_{bf}$. These essentially depend on the additive concentrations, as illustrated by Figure 3.14(c). Also notice that $T_{bf}$ is indeed 700 ± 20 °C for the concentrations of interest [267,268]. For the additive concentrations considered and any $A_0$ (the process is 30-min FA in dry gas), Figure 3.14 suggests the equation:

$$1 - A_f/A_0 = 2.61 \times 10^{-4} ([B_2O_3] + [P_2O_5]) \times [T_a - 754 + 3.21([B_2O_3] + [P_2O_5])]$$

(3.12)

Here the definitions are the same as above in Eq.(3.5) and Eq.(3.7).

### 15.6. BPSG GLASS FLOW CHARACTERIZATION BY FLOW EFFECTIVENESS ON THE DEVICE STEPS

Sub-quarter micron ULSI circuits tend to be fabricated by RTA, which minimizes the overall thermal effect on the devices. On the other hand, RTA is inferior to FA in flow effectiveness and hence in the quality of planarization. There have been efforts to improve the
RTA flow of BPSG included raising the total additive concentration above 8 wt % or annealing at elevated humidity and, possibly, elevated pressure. However, most of the approaches were unsuccessful in the context of ULSI due to unacceptable defect density at higher additive levels or the oxidation of layers beneath the glass due to the wet environment. The qualitative character of experimental data published so far indicates that research was urgently required into the quantitative characterization of glass flow under arbitrary annealing conditions. Assuming that the laws of glass flow are independent of the annealing method, the author presumed [244,267,268] that the above equations provide a framework for comparing the patterns of flow in different annealing regimes. This strategy allowed one to reduce the amount of experimental work embracing different process conditions.

Studies were initiated by gathering and analyzing published experimental data in order to compare FA and RTA conditions with respect to similar BPSG films (deposition method and composition). The results are summarized in Table 3.2. Another flow parameter was introduced, termed “thermal budget”, which was defined as the product of annealing temperature in Kelvin degrees and annealing time in minutes: \((T_a + 273) \times t_a\). The data were analyzed in terms of the ratio:

\[
\frac{(T_a + 273) \times t_a}_{FA} \div \frac{(T_a + 273) \times t_a}_{RTA} = m
\]  

\[\text{(3.13)}\]

![Figure 3.14](image-url)

**Figure 3.14.** Example of calculated dependence of glass flow capability on annealing temperature or additive level [268].
Table 3.2. Comparison of FA and RTA planarization for BPSG thin films [268]

<table>
<thead>
<tr>
<th>[B]-[P] (wt %)</th>
<th>(A_0) (degrees)</th>
<th>(A_f) (degrees)</th>
<th>FA (T_a) (\circ C)</th>
<th>(t_a) (min)</th>
<th>RTA (T_a) (\circ C)</th>
<th>(t_a) (min)</th>
<th>(m)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-4</td>
<td>92</td>
<td>65</td>
<td>875</td>
<td>30</td>
<td>1075</td>
<td>0.33</td>
<td>77</td>
<td>[72]</td>
</tr>
<tr>
<td>4-4</td>
<td>82</td>
<td>65</td>
<td>825</td>
<td>30</td>
<td>1025</td>
<td>0.33</td>
<td>77</td>
<td>[72]</td>
</tr>
<tr>
<td>3-6</td>
<td>52</td>
<td>11</td>
<td>907</td>
<td>30</td>
<td>1070</td>
<td>0.33</td>
<td>79</td>
<td>[72]</td>
</tr>
<tr>
<td>3-6</td>
<td>52</td>
<td>11</td>
<td>907</td>
<td>30</td>
<td>1040</td>
<td>0.66</td>
<td>41</td>
<td>[177]</td>
</tr>
<tr>
<td>5-5</td>
<td>50</td>
<td>3</td>
<td>907</td>
<td>30</td>
<td>1100</td>
<td>0.33</td>
<td>78</td>
<td>[177]</td>
</tr>
<tr>
<td>5-5</td>
<td>50</td>
<td>3</td>
<td>907</td>
<td>30</td>
<td>1050</td>
<td>0.66</td>
<td>41</td>
<td>[177]</td>
</tr>
</tbody>
</table>

The BPSG films considered were deposited under the same conditions, were equal in boron and phosphorus content, and showed the same change in \(A_f\) under FA and RTA. The values of \(m\) calculated from the published reports were found to strongly indicate a correlation between the characteristics of the two annealing regimes (see Table 3.2). At the same time, the author was not clear why the maximum and the minimum value of \(m\) differed by a factor almost as large as 2.

As a further step, the variation in \(1-A_f/A_0\) was calculated with the thermal budget for the known glass composition and process conditions, using Eq.(3.9) and Eq.(3.10) for simplicity. Figure 3.15 presents example graphs for different annealing temperatures and fixed values of [B], [P], and \(A_0\), with annealing assumed to be in dry gas. The annealing time is 15 – 60 min for FA and 20 – 120 sec for RTA. Notice the distinction in the glass flow capability between FA and RTA.

The relationship between glass flow capability and thermal budget provided an understanding of the spread in \(m\). We observed that the glass films differed in \(A_0\). As pointed out above, \(A_0\) as well as \(T_a\) exert the strongest influence on BPSG flow, their respective variations having opposite effects on \(A_f\). Figure 3.16(a) illustrates the vital importance of \(A_0\) to glass flow capability. With this factor taken into account, we achieved good agreement between the calculation and the experiment for both FA and RTA on the basis of the tabulated experimental data (despite their scarcity), as demonstrated in Figure 3.16(b). This result supports our approach to the modeling of BPSG flow under arbitrary annealing conditions in ULSI manufacturing.

15.8. Calculating Optimum Flow Temperatures

We have seen that annealing conditions should be set so as to minimize the adverse thermal effect on the devices. More specifically, the thermal budget applied to the PMD should be at a minimum yet sufficient for adequate planarization (or gap filling).

It was generally accepted that the flow temperature \(T_f\) of thin films can be identified for an arbitrary glass composition by determining the glass-transition temperature \(T_g\) of bulk specimens and using the empirical relation \(T_f = T_g + 288 \pm 16 \circ C\), as proposed by Nassau et al [54]. However, the authors failed to give specific values of flow parameters. Furthermore, the reported values of \(T_g\) and, hence, the corresponding values of \(T_f\), were inapplicable to RTA.
Thus, the problem of identifying an optimum annealing temperature remained unsolved for a long period of time.

Figure 3.15. Calculated glass flow capability vs. anneal thermal budget in dry gas for 5 wt % [B], 5 wt % [P], and $A_0 = 85$ degrees [268].

Figure 3.16. Calculated glass flow capability: (a) dependence on initial step-coverage angle and (b) comparison with experimental values (see table). Figure (a) refers to BPSG films with 4 wt % [B] and 4 wt % [P], which were subjected to FA processes with almost equal thermal budget [268].
It was believed that the optimum annealing temperature (i.e. acceptable maximized temperature) $T_{a(max)}$ is related to a maximum glass flow capability for either type of annealing. Further, $T_{a(max)}$ as a function of concentration appears to be the most informative characteristic. The optimum annealing temperature can be determined from the annealing-temperature dependence of the rate of change of glass flow capability with respect to thermal budget:

$$d(1-A_f/A_0)/d(T_a \times t_a)$$

(3.14)

Figures 3.17(a) and 3.17(b) give examples of the dependence for FA and RTA, respectively. They are calculated from Eq.(3.9) and Eq.(3.10) for various boron and phosphorus combinations.

![Graphs](image)

Figure 3.17. Calculated $d(1-A_f/A_0)/d(T_a \times t_a)$ vs. annealing temperature for the (a) FA and (b) RTA of BPSG films differing in composition and (c) experimental graphs of post-annealing step-coverage angle vs. FA annealing temperature for different glass compositions [268]. BPSG film compositions are presented in wt % [B] and wt % [P].
The comparison of calculated curves in Figure 3.17(a,b) with experimental ones obtained for the same additive concentrations and plotted in the $T_a$-$A_f$ graph, as shown in Figure 3.8(a), revealed that the peaks of the former approximately correspond to the points of inflection on the latter. It appears reasonable to propose that the corresponding values of $T_a$ are related to optimum annealing temperatures. Figure 3.18 shows values of $T_{a(max)}$ calculated in this way versus $[B_2O_3] + [P_2O_5]$. The sum of the oxide concentrations is used because the flow of BPSG is equally sensitive to the oxides, as noticed above; this fact greatly simplifies the calculation. In addition, for wet gas anneal ambient these curves are believed to be shifted downward by about 50 °C.

15.9. GLASS FLOW CAPABILITY OF GeO$_2$-SiO$_2$ GLASS FILMS

The tendency toward lower annealing temperatures for sub-0.18 μm ULSI stimulated research into silicate glasses that could replace BPSG as a PMD. For example, GeO$_2$-SiO$_2$ glasses and multicomponent glasses that contained Si, Ge, B, P, As, Pb were evaluated as candidates [54,120,239,240]. Until recently, practical importance has only been placed on Ge-contained glasses.

The flow of Ge-contained silicate glass thin films over wafer topography has been poorly explored. Experimental results tend to be presented in qualitative form, as micrographs. Nevertheless, we believe that the flow effectiveness $1 - A_f/A_0$ could be instrumental in interpreting the published data and quantifying the flow.

The author applies his approach below to the analysis of data presented by Simpson et al [239,240]. The flow of GeO$_2$-SiO$_2$ glasses was studied over a wide range of composition, including the case of $B_2O_3$ and $P_2O_5$ additives. The glass films were produced by PECVD from hydrides. Annealing was performed in argon, steam, or forming gas. The authors were able to reduce the step-coverage angle $A_0$ from over 100 degrees to $A_f = 0$ degrees. Regrettably, planarization was characterized in general terms, on a three-point qualitative scale. We analyzed the results only for 1 hour FA in argon because the authors explored this case in greater detail.

The flow effectiveness was estimated by measuring $A_0$ and $A_f$ on the SEM micrographs. Figures 3.18(a,b) show flow effectiveness versus annealing temperature and $k_f$ versus GeO$_2$ concentration in mole percent, respectively. It is seen that the flow starts at about 45 mol % GeO$_2$ and the $k_f$ characteristic becomes nonlinear at about 80 mol % GeO$_2$. Figures 3.19(a,b) allow one to derive formulas similar to Eq.(3.12). These indicate that flow effectiveness over 0.5 can be obtained at annealing temperatures below 850 °C if the GeO$_2$ concentration is raised above 60 wt %. Note that the corresponding value of $k_f$ is about 0.005 (see Figure 3.19(b)). The same value was observed in BPSG film with a total additive content $[B_2O_3] + [P_2O_5]$ equal to 25 wt % (see Figure 3.14(b)). This was the most common level of additives in BPSG films; it correlated with fairly low defect densities. However, we think that the corresponding level of GeO$_2$ was excessive for GeO$_2$-SiO$_2$ glass, as evidenced by crystallization [239].

If GeO$_2$-SiO$_2$ glass contains $B_2O_3$ and $P_2O_5$, it showed a higher flow effectiveness and a sharply reduced $T_{bf}$. Figure 3.19(c) illustrates this effect by means of $(1 - A_f/A_0)$ vs. $T_a$ characteristics for GeO$_2$-SiO$_2$ (the ratio of mol % SiO$_2$ to mol % GeO$_2$ is about 1/4) and for
two combinations of the $\text{B}_2\text{O}_3$ and $\text{P}_2\text{O}_5$ levels, together with estimated values of $k_f$ and $T_{bf}$. Notice that the boron- and phosphorus-contained glasses exhibit an almost 200 °C decrease in $T_{bf}$ as compared with the GeO$_2$-SiO$_2$ glass. Furthermore, boron- and phosphorus additives significantly raise $k_f$. Indeed, a more detailed comparison will be possible with a larger amount of experimental data on a wider variety of glass compositions.

15.10. EVALUATION OF BPSG GAP-FILL PROCESS

In ULSI manufacture, glass films deposited on stepped surfaces often contain voids located in gaps between adjacent features. This is unacceptable. The shape of voids depends on the deposition technique, keyhole voids being the most common example. Other frequently encountered void types were depicted in Chapter 4. With further advances in miniaturization, voids may approach the size of the gaps themselves.

After deposition, a BPSG film is subjected to thermal annealing in order to take a planar form and make the material fill the gaps (Figure 3.4). Figure 3.20 depicts the effect of annealing on voiding for two BPSG annealing processes commonly used in ULSI manufacture: long high-temperature isothermal annealing (FA) completely eliminating the voids, and pulse annealing (RTA) that remained with some small voids. It can be seen that the thermal annealing of BPSG film must be performed at a fairly high temperature and during a fairly long period. Otherwise, keyhole voids become spherical ones (see Figure 3.4(b)) instead of disappearing, which is also unacceptable.

![Figure 3.18](image-url)  
Figure 3.18. Calculated optimum annealing temperature and BPSG film gap-fill capability for almost vertical gaps vs. total additive concentration for FA and RTA. The data are obtained by measurement (open marks) or computation (closed marks) [268].
Figure 3.19. Using glass flow capability in the evaluation of thermal-flow planarization for GeO$_2$-SiO$_2$ glass films with $\theta > 90$ degrees: (a) glass flow capability vs. annealing temperature subject to GeO$_2$ concentration, (b) $k_f$ vs. GeO$_2$ concentration, and (c) glass flow capability vs. annealing temperature for GeO$_2$-SiO$_2$ glasses with and without additives. The experimental data treated by Vasilev in [268] were taken from Simpson et al. [239]. Details for graph (c):

1. 20 mol % SiO$_2$, 80 mol % GeO$_2$; $k_f = 0.009$, $T_{bf} = 737$ °C;
2. 14 mol % SiO$_2$, 73 mol % GeO$_2$, 12 mol % P$_2$O$_5$, 1 mol % B$_2$O$_3$; $k_f = 0.020$, $T_{bf} = 546$ °C;
3. 16 mol % SiO$_2$, 77 mol % GeO$_2$, 6 mol % P$_2$O$_5$, 0 mol % B$_2$O$_3$; $k_f = 0.011$, $T_{bf} = 604$ °C.

The author proposed a new, less laborious and expensive approach to the evaluation of deposition--planarization processes in terms of gap-fill capability [244,257]. His approach was based on the relationship, in graphic form, between the flow effectiveness and the parameters of gaps that can be adequately filled by glass flow. Based on background analysis above, he concluded that flow characteristics of flow-able glass on the device step were strongly affected by three major parameters:

- the shape of the structure incoming to the flow-able film deposition;
- the shape of growing on this structure film (or CVD features);
- the glass flow capability.
Taking the information above as a starting point for developing an approach of quantitative evaluation of CVD film gap-fill capability, the following simple proposal was done: gap-fill improvement at thermal treatment of flow-able film and the characteristics of structure, which is covered with this flow-able film, can be linked, as shown schematically in Figure 3.21(a). In this drawing the “x” axis was proposed to represent a certain complex parameter accumulating a set of parameters, like glass properties (boron and phosphorus concentrations) and anneal conditions ($T_a$, $t_a$, anneal ambient, etc.). It reflects a capability of flow-able film to flow. The author named this parameter “Glass Flow Capability” (GFC). Axis “y” represents a certain complex structure parameter, which was defined in Chapter 4 as a ratio of AR to the gap size G, or a ratio of structure height (H) to gap size in power two ($G^2$), e.g. $H/G^2$, and named as “Structure Complexity” (SC). The SC is supposed to include a set of parameters, such as gap characteristics, aspect ratio, etc. It is clear from general considerations that the SC of ULSI structures is enhanced along with a decrease of IC device technology nodes.

Following the proposed logic, the tighter structures should have a higher $H/G^2$ value. In fact, the decrease of device technology nodes rules means that gaps become a few times smaller, but the thickness of structures (e.g. gap height) become about a twice thinner. For instance, for selected gap height ~0.2 μm of a “vertical” structure with gap values of $G_v$=0.1 μm and $G_v$=0.05 μm, the structure complexity can be calculated to be $SC_{0.1}$=20 and $SC_{0.05}$=80, respectively.

The GFC parameter is characterized by the dimensionless value $(1 - A_t/A_0)$, defined above. It varies from zero to unity; it is higher for a material with a better flow capability. This flow parameter can be evaluated by SEM analysis or calculated using Eq.(3.9) and Eq.(3.10). The former requires no knowledge of the composition of the material and flow conditions as long as $A_t$ has been found. The latter strategy is applicable to BPSG only and requires that $A_0$ and anneal conditions be specified.
Figure 3.21. Graphic representation of deposition-planarization processes in terms of deposition gap-fill capability (vertical axis) and glass flow capability (horizontal axis). Figures (a) and (b) are an elementary and a sophisticated form of comparative process evaluation, respectively. In Figure (b), the numerals designate (1) plasma deposition processes, (2) low-pressure and atmospheric pressure processes, and (3) High-Density-Plasma CVD processes and the cross-sectional schemes reflect the conventional shape of gap: tapered, vertical or re-entrant.

The scheme in Figure 3.21(a) can help us to do a simple qualitative analysis. Obviously, an enhancement of glass flow capability will lead to the possibility of better gap-fill even for very complicated structures. This means that we can achieve gap-fill for very high values of SC. Theoretically, at extremely high thermal anneal conditions, where GFC can be defined to be infinity, any device gaps can be filled with very liquid glass, producing void-free structures even with extremely low gaps. Following the logic, the zero GFC value on the graph, which reflects “zero” glass flow capability, corresponds to the SC of as-deposited CVD films. At the same time, if GFC is getting worse due to the changes of any factor responsible for film flow parameter (either glass composition, of thermal anneal conditions), an improvement of gap-fill with flow-able glass film becomes less possible. Eventually, a curve in Figure 3.21(a) should reflect a certain boundary between voiding conditions and a void-free area. Thus, any coordinates above the drawn line should reflect void existence in structures, and at the same time, any coordinates below the drawn curve should give us void-free structures after proper film flow. It is clear that an improvement of GFC achieved with wet anneal ambient, or high-pressure anneal, will lead to the shift of a particular point from the void area towards the void-free area. At the same time, a decrease of structure complexity will also lead to the void-free gap-fill.

All considerations above assume a structure with vertical side-wall slope. However, additional structure definitions, such as “vertical”, “tapered” and “re-entrant” are also needed despite the fact that they cannot be defined quantitatively in most cases. Taking into account our classification of structures made in Chapter 4, and simple general considerations as well, the graph in Figure 3.21(a) can be re-drawn in order to analyze the gap shapes, as well as CVD process effects on glass flow gap-fill capability. These graphs are presented in Figure 3.21(b). It is clear that the structure complexity, which is able to be filled with flow-able glass film will follow the sequence: $\text{SC}_{\text{re-entrant}} < \text{SC}_{\text{vertical}} < \text{SC}_{\text{tapered}}$. In fact, significantly tighter structures can be filled with flow-able films if structure tapering is used. This figure also reflects that as-deposited film gap-fill is supposed to be much better for “tapered” structures as-compared to the “vertical” or “re-entrant” structures, which is shown as much higher
structure complexity value of “tapered” structures at GFC=0. From the deposition process point of view, an improvement of growing film conformality should give us an improvement of as-deposited gap-fill, e.g. smaller key-holes. Obviously, the trend of smaller key-hole formation during film deposition will follow showed above sequence: LPCVD≥APCVD>PECVD. Eventually, the better as-deposited film gap-fill will lead to the better post-flowed gap-fill. For instance, use of fluorinated subatmospheric pressure BPSG films with better as-deposited step coverage as compared to non-fluorinated one, helped improve as-deposited gap-fill and, therefore, post-anneal gap-fill [243]. Therefore, a best HDP CVD BPSG method will allow achievement of the best gap-fill at relatively low thermal budget conditions.

Based on the general analysis performed, it was concluded that the whole vision of gap-fill issue presented in Figure 3.21(a,b) linked qualitatively very well with the device structure types, CVD process features, film features and anneal characteristics, revealing no logical discrepancies. It allows the use of this logic as a basis for further quantitative characterization of the gap-fill issue with flow-able glass films.

An analysis of three selected groups of structures with different shapes of gaps was performed by the author in [244]. He used summarized experimental results of our gap-fill studies for “re-entrant”, “vertical”, and “tapered” structure types and data from some other references. Most of the data presented were found to be for TEOS-ozone-based BPSG films, deposited either at APCVD, or at SACVD conditions. The author also put on these graphs a few additional data points defined as “critical”, which were found to correspond to the exact void-free gap-fill achieved or reported in the literature. This can be seen in Figure 3.22 for the “vertical” structure type.

There was a very high spread of data especially for the “tapered” gap shape. This confirms that the definition for tapered structures was not clear and it was very difficult to compare one structure to another. At the same time, the expected trend of voiding at not sufficient enough film flow was obvious. Comparing all of the experimental graphs, the author concluded that it was very difficult to find a functional correlation of structure complexity and glass flow capability. That was due to the wide spread of data obtained for different types of structures. Nevertheless, it was believed that the summarized data presented confirm the idea of the approach.

To date, there has not been sufficient published experimental data for BPSG films flow, showing numerically what conditions are sufficient for proper gap-fill. In section 15.8, the author introduced the optimum annealing temperature (i.e. acceptable maximized temperature) $T_{a(max)}$, which is related to a maximum flow effectiveness for either type of annealing. Assuming that this temperature is also optimized for gap-fill purposes, one can plot experimental data points, as shown in Figure 3.18 for both FA and RTA conditions. These data points reflect reported good gap-fill data achieved at dry inert ambient and for mostly slightly tapered structures. It can be seen that for FA the correlation can be evaluated to be good. At the same time, for RTA conditions experimental data points are placed at significantly lower anneal temperatures as compared to the calculations. This comparison indicates that anneal temperature for proper gap-fill can be chosen slightly lower as compared to calculated maximums. The author found that temperatures corresponded to the ~0.8 from obtained maximums can meet the experimental data point for both RTA and furnace anneal as well. In this case, almost all published data points are placed above calculated curves reflecting certain void-free areas above these curves.
Figure 3.22. Summarized experimental and published gap-fill data for “vertical” gap shapes recalculated into the basic complex parameters: structure complexity $H/G^2$ and glass flow capability $(1-A_f/A_0)$ [244].

Another important feature of the approach presented is a possibility of simple calibration of gap-fill data with film planarization after anneal. Scanning microscope analysis for gap-fill can be performed together with a measurement of flow angle $A_t$ on the single step. In this case, knowing the value $A_0$ as well, an experimental value of glass flow capability can be easily calculated. Flow angles can be measured using the atomic-force microscope technique [225] (see Figure 3.7). We believe, this kind of experimental calibration for gap-fill together with calculation using the presented approach can be effectively used in the case of more complex glass film use, such as GeO$_2$ contained BPSG films.

**CONCLUSION**

In this chapter, a detailed overview of a 30-year experimental investigation into the thermal flow of BPSG thin films on stepped device surfaces is presented. The viscous flow over a stepped surface under FA or RTA was examined by SEM for different BPSG compositions. A few numerical equations were considered for the calculation of changes in flow angle during thermal-flow planarization, subject to the primary factors affecting glass flow: annealing temperature, initial flow angle, the boron and phosphorus concentrations of the glass, and annealing time. The impact of each factor was quantified and the factors were compared numerically. Consideration was also given to secondary factors which may have a significant influence on the process in some situations. The empirical formulas proposed can be directly employed in VLSI and ULSI device technology and manufacturing, reducing the amount of costly measurement.

Two important parameters were considered for the characterization of the flow of BPSG over ULSI steps in details: glass flow capability and thermal budget. They are related to annealing temperature, annealing time, topographical parameters, and glass additive concentrations. The approach to using these parameters reduces the cost of measurement,
facilitates the interpretation of data, works for both FA and RTA, and is applicable to ULSI gap filling as well as glass planarization. It also enables the optimization of the annealing temperature for thin films of multicomponent glasses, such as GeO$_2$-SiO$_2$ glass contained B$_2$O$_3$ and P$_2$O$_5$. 