

Silicon Processing

for the VLSI Era
Volume 1 – Process Technology

S. Wolf and R.N. Tauber

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SILICON PROCESSING FOR THE VLSI ERA

VOLUME 1:

PROCESS TECHNOLOGY

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SILICON EPITAXIAL FILM GROWTH

The epitaxial growth process is a means of depositing a thin layer (0.5 to 20 μm) of single crystal material upon the surface of a single crystal substrate. If the film is the same material as the substrate the process is called *homoepitaxy*, but is often referred to as *epitaxy* or simply *epi*. Silicon deposition on a silicon substrate is the most important technological use of homoepitaxy, and is the primary subject of this chapter. If, on the other hand, the deposit is made on a substrate that is chemically different, the process is termed *heteroepitaxy*. This process has found application in the deposition of *silicon on sapphire* (Al_2O_3) which is termed *SOS*. The term *epitaxy* is derived from two Greek words meaning "arranged upon".

Epitaxial growth can be achieved from the vapor phase (VPE), liquid phase (LPE), or solid phase (SPE). For silicon processing, VPE has met with the widest acceptance, since excellent control of the impurity concentration and crystalline perfection can be achieved. Liquid phase deposition has found its widest use in producing epitaxial layers of III-V compounds (e.g. GaAs, InP). Solid phase epitaxy is observed in the crystalline regrowth of ion implanted amorphous layers, as described in the *Annealing Amorphous Layer Damage* section of Chap. 9.

The major impetus for developing silicon epitaxy was to improve the performance of bipolar transistors and later bipolar integrated circuits. By growing a lightly doped epitaxial layer over a heavily doped silicon substrate, the bipolar device could be optimized for high breakdown voltage of the collector-substrate junction, while still maintaining low collector resistance. The low collector resistance provided high device operating speeds at moderate currents. More recently, epitaxial processes have been used in fabricating advanced complementary metal-oxide-silicon (CMOS) VLSI circuits. In these circuits the device is built in a thin (3-7 μm), lightly doped epitaxial layer over a heavily doped substrate. This structure minimizes latch-up effects that a CMOS circuit may undergo when powered-up, or when subjected to a radiation burst. Other advantages of fabricating devices (both bipolar and MOS) in an epitaxial layer are that the doping concentration of the device can be accurately controlled, and that the layer can be made oxygen and carbon free. The epitaxial process however is not without its disadvantages. These include: a) increased processing complexity and wafer costs; b) defect generation in the epitaxial layer; c) autodoping; and d) pattern shift and washout.

In this chapter we present: a) the fundamentals of epitaxial deposition; b) doping in epitaxial films; c) defects in epitaxial films; d) process considerations for VLSI epitaxial depositions; e) epitaxial deposition equipment; f) the characterization of epitaxial films; g) selective deposition of epitaxial silicon; and h) molecular beam epitaxy of silicon.

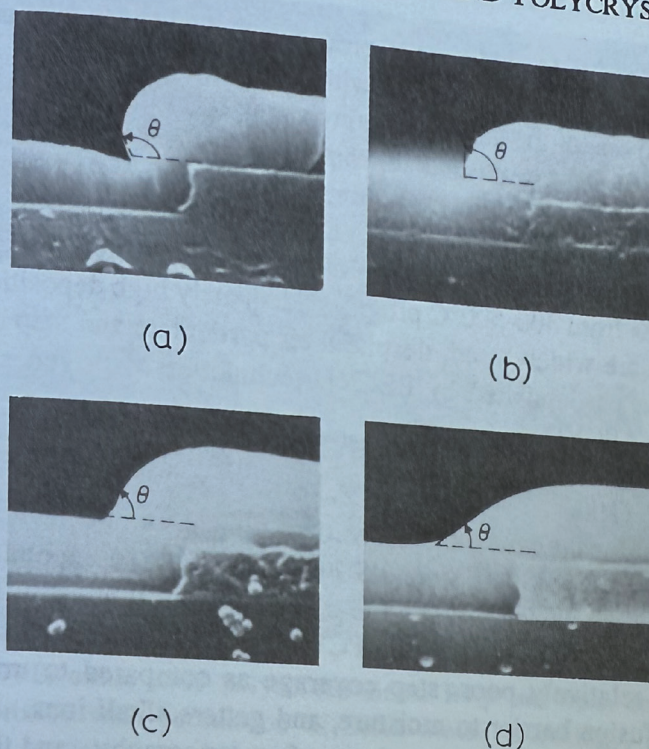


Fig. 19 SEM cross-sections (10,000X) of samples annealed in steam at 1100°C for 20 min for the following weight of phosphorus: (a) 0.0 wt.% P; (b) 2.2 wt.% P; (c) 4.6 wt.% P; (d) 7.2 wt.% P.³³ Reprinted by permission of the publisher, the Electrochemical Society, Inc.

decomposition, or by the high temperature reaction of $\text{SiCl}_2\text{H}_2\text{-N}_2\text{O}$ under LPCVD conditions, exhibit nearly conformal coverage. Conversely, during low temperature deposition of SiO_2 by APCVD, almost no surface migration takes place, and step coverage is dependent only on the arrival angle (and is quite poor, as noted earlier). On the other hand, PECVD produces reactants which arrive at the substrate with more energy (obtained from the glow-discharge) than in APCVD. This results in increased adatom migration. Thus, improved step coverage by PECVD SiO_2 films can be obtained compared to APCVD depositions made at the same temperature. Note that the mechanisms of this model can also be applied to analyzing the step coverage effects seen in evaporated and sputtered films.

CVD and Applications of Undoped and Doped SiO_2 Films

Both undoped and doped films of SiO_2 are easily deposited at low temperatures. Doping of TEOS and high temperature CVD SiO_2 films is more difficult. As we shall see, doping of the SiO_2 can produce a variety of desirable film properties for some applications.

Undoped CVD SiO_2

Undoped CVD SiO_2 is similar to its thermally grown counterpart in many respects, with some exceptions being its as-deposited density and etch rate, and a lower quality SiO_2/Si interface (higher density of interface states). Due to its poor interface qualities, CVD SiO_2 is therefore only used as a temporary structure if it is used in contact with single crystal silicon (e.g. as a capping layer over doped regions to prevent outdiffusion during thermal processes or as an ion-implantation mask). Its chief use, however, is as a permanent structure, whose function

is to increase the thickness of field oxides, or to provide isolation between conductors.

When the underlying conductor is able to withstand high temperatures (e.g. polysilicon or refractory metal silicides) one of the LPCVD methods may be utilized, because of their excellent uniformity, good step coverage, low particulate contamination, and high purity.

Often the film must be deposited over aluminum, and therefore the process must take place at less than 450°C. At these temperatures LPCVD reactions exhibit extremely low deposition rates (Fig. 20b). On the other hand the reaction of silane and oxygen mixtures at atmospheric pressure and temperatures from 300-500°C provides adequately high deposition rates. Therefore such APCVD processes are widely used, despite their particulate and step coverage problems. Undoped oxide can also be deposited by PECVD techniques, with generally improved step coverage as compared to APCVD.

Phosphosilicate Glass

Adding phosphorus dopant during the deposition, typically in the form of phosphine, PH_3 , forms phosphosilicate glass, or PSG. Since PSG consists of two compounds, P_2O_5 and SiO_2 , it is a *binary glass* (or binary silicate), and some of its properties are considerably different from those of undoped CVD SiO_2 . That is, APCVD PSG shows reduced stress and somewhat improved, though still relatively poor, step coverage as compared to undoped CVD SiO_2 . Moreover PSG is a diffusion barrier to moisture, and getters alkali ions. Finally PSG can be *flowed* at high temperatures to create a smoother surface topography, and thereby facilitate the step coverage of subsequently deposited films. The flow step is performed at 1000-1100°C, at pressures from 1-25 atm, and in gas ambients of H_2O , N_2 and O_2 . The glass becomes viscous and responds to surface tension forces, rounding sharp corners. The extent of flow is often measured as the reduction in slope angle of the flowed film surface over an underlying step (Fig. 19), and is a function of flow temperature and phosphorus concentration. Increasing temperature, duration of the flow step, or phosphorus concentration in the oxide will increase film flow. Note that for concentrations less than 6 wt% phosphorus, PSG does not readily flow.

It is relatively easy to incorporate the P_2O_5 into the PSG, as the $\text{SiH}_4:\text{PH}_3$ ratio in the gas flow controls the $\text{SiO}_2:\text{P}_2\text{O}_5$ ratio in the deposited film. PSG, however, becomes increasingly hygroscopic at high phosphorus levels. Thus, it is recommended that its concentration in the oxide film be limited to 6-8 wt% P to minimize phosphoric acid formation, and consequent Al corrosion. Rapid thermal processes have also been reported to successfully flow PSG. It should be noted, however, that if PSG is to be used as a final passivation layer (in which no glass flow

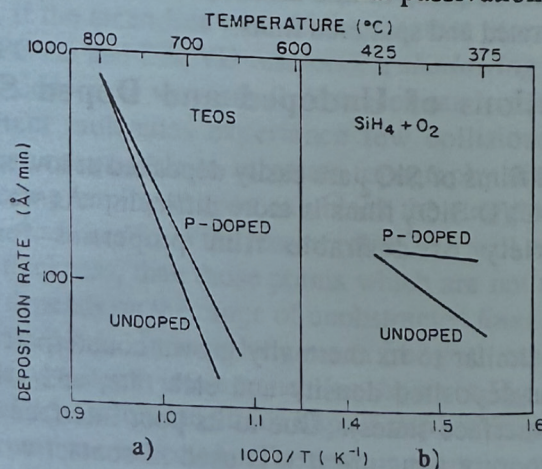


Fig. 20 Arrhenius plots for the deposition of (a) LPCVD TEOS, and (b) LPCVD SiO_2 (P-doped and undoped)³³. Reprinted with permission of the publisher, the Electrochemical Society, Inc.

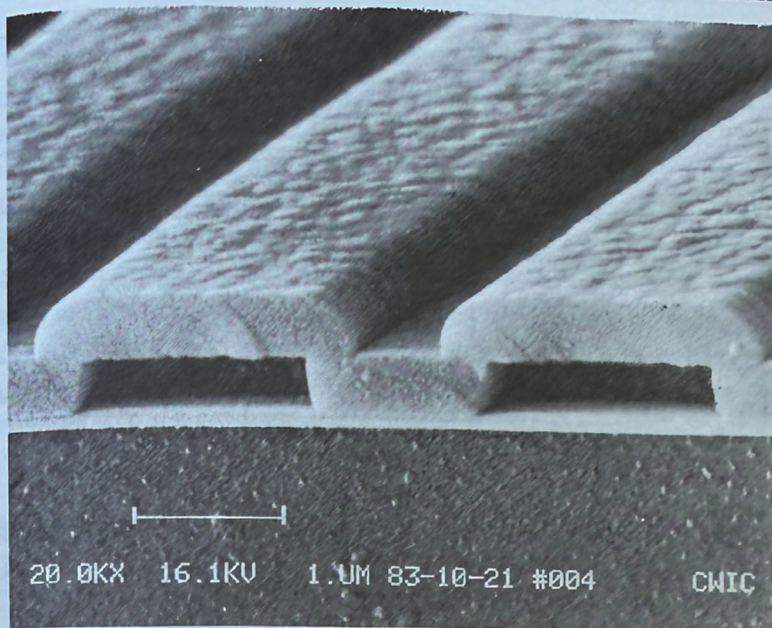


Fig. 21 SEM of PECVD oxide over polysilicon lines. Poly has been removed by wet etch to show detail¹². Reprinted with permission of Solid State Technology, published by Technical Publishing, a company of Dun & Bradstreet.

is performed), the maximum permitted phosphorus content is 6 wt%. This is a precaution taken to again minimize the risk of phosphoric acid formation, particularly when in contact with Al.

PSG has been deposited in PECVD systems by the reaction of SiH_4 , N_2 , O_2 , and PH_3 with Ar as a carrier gas. It is reported that the films are more conformal (Fig. 21), crack resistant, and pinhole free than APCVD films³⁴. The phosphorus content is a function of the SiH_4/PH_3 ratio, deposition temperature and $\text{N}_2\text{O}/(\text{SiH}_4 + \text{PH}_3)$ ratio³⁵. The plasma PSG films can be flowed under conditions similar to those for flowing APCVD PSG films.

Borophosphosilicate Glass

Some VLSI processes would benefit from being performed at lower temperatures than those necessary for PSG reflow (1000-1100°C) because such high temperatures result in excessive diffusion of shallow junctions. Furthermore, radiation-hard MOS gate oxides cannot be exposed to high temperature processing (>900°C). But flowable glass is still very desirable for easing film coverage over abrupt steps in the substrate topography. Glass flow temperatures as low as

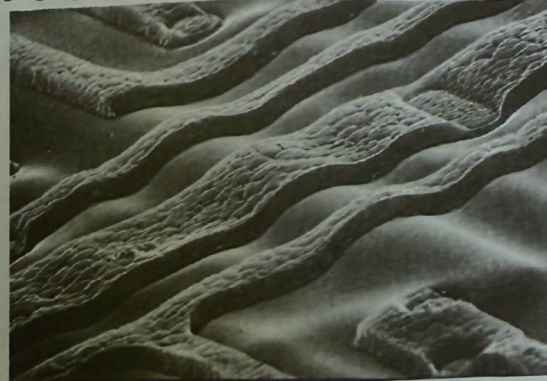
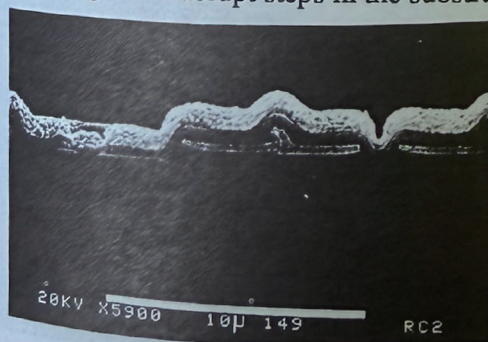


Fig. 22 Micrographs showing BPSG as the interlevel dielectric under the metal. Reprinted with permission of Semiconductor International².

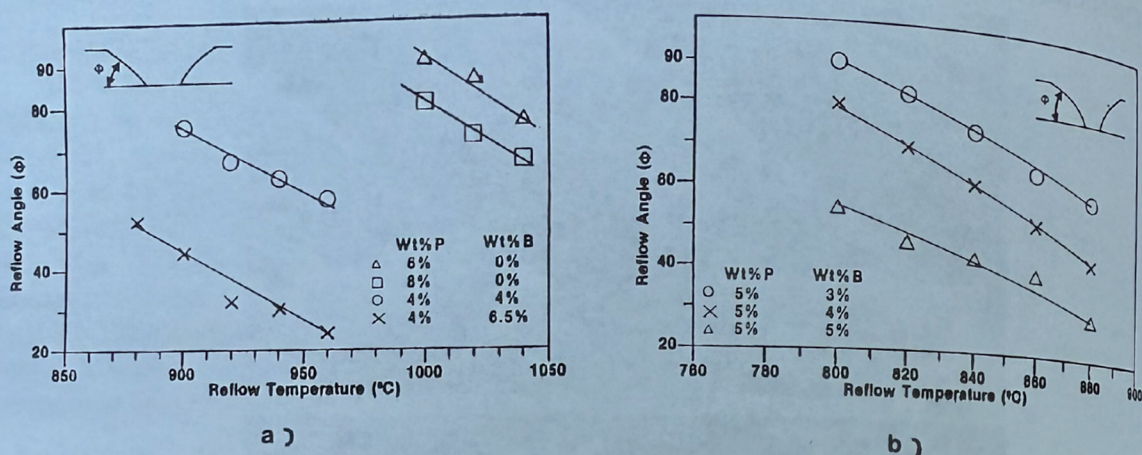


Fig. 23 (a) Reflow angle vs. reflow temperatures in a nitrogen ambient (30 min). (b) Reflow angle vs. reflow temperatures in a steam ambient (30 min). Reprinted by permission of Solid State Technology, published by Technical Publishing, a company of Dun & Bradstreet³⁷.

700 $^{\circ}\text{C}$ can be obtained by adding boron dopant (e.g. B_2H_6) to the PSG gas flow to form the ternary (three component) oxide system $\text{B}_2\text{O}_3\text{-P}_2\text{O}_5\text{-SiO}_2$, borophosphosilicate glass, or BPSG³⁶ (Fig. 22).

BPSG flow depends upon film composition, flow temperature, flow time, and flow ambient. It has been reported that an increase in boron concentration of 1 wt% in BPSG decreases the required flow temperature by $\sim 40^{\circ}\text{C}$ ³⁶. A plot of required flow temperatures vs. BPSG dopant concentrations in LPCVD films is shown in Fig. 23. In general, increasing the P concentration beyond $\sim 5\text{wt}\%$ does not further decrease BPSG flow temperatures. An upper limit on boron concentration is imposed by film stability. That is, BPSG films containing over 5 wt% boron tend to be very hygroscopic and unstable, and if used, should be flowed immediately following deposition. It has also been reported that rapid thermal annealing for 30 s at a temperature 100–175 $^{\circ}\text{C}$ higher than that used in a conventional furnace step will result in equivalent BPSG flow³⁶. The ambient gas of the flow cycle also affects the flow mechanism. By using a steam ambient instead of N_2 , the minimum required flow temperature is reduced by $\sim 70^{\circ}\text{C}$ ³⁷.

In addition to exhibiting these low temperature flow properties, BPSG (like PSG) is an alkali ion getter and exhibits low stress. Because of its doping, however, BPSG can also be an unwanted diffusion source to underlying silicon. It is found that BPSG is primarily a source of phosphorus, and the phosphorus outdiffusion is increased at higher boron concentrations.

Besides being useful for isolation, passivation, and surface planarization, BPSG is also more attractive for use than PSG in a process known as *contact reflow*. Following anisotropic etching, contact holes have sharp upper corners which make them difficult to fill (Fig. 24a). By successfully rounding these sharp edges with a *second* thermal flow (or *reflow*) cycle (Fig. 24b), contact coverage by a subsequent metal film is significantly improved. (Note that two separate flow cycles are preferred to a single post-etch flow cycle, since the appropriate degree of flow desired in the second cycle is normally less than that required for the first flow step). The ambient is also usually inert, rather than oxidizing, in order to avoid SiO_2 growth in the contacts during the reflow step. Because flow depends on BPSG composition, precise control of dopant uniformity across substrates is necessary to ensure uniform flow and consequent control of contact size.

BPSG deposition reactions for APCVD⁴, LPCVD³⁸, and PECVD^{39, 40} processes have all been reported. If hot-wall LPCVD reactors are used, they must be equipped with distributed feed gas systems so that adequately uniform BPSG films can be deposited. During deposition, the

source gases for B and P compete with one another for inclusion into the final deposited film. This makes for a complex relation of reactant gas composition to eventual film doping³⁶.

The chemical composition of BPSG (and PSG), can be determined by several techniques, including the following: a) *wet chemical colorimetry*, which is the most accurate, analyzes the dissolved BPSG film; b) *x-ray photoelectron spectroscopy* (see Chap. 17), which is useful for determining the phosphorus content of the film; c) *Fourier transform infrared spectroscopy* (see Chaps. 1 and 5) which can measure boron levels quite accurately, but phosphorus levels less well accurately (due to the presence of a partially obscured phosphorus-oxygen absorption band); and d) *film etch rates in buffered HF*. Since the etch rate of BPSG in buffered HF depends on the concentration of both B and P in the film, a determination of the etch rate can provide a rapid, qualitative comparison of the composition between BPSG samples.

PROPERTIES AND CHEMICAL VAPOR DEPOSITION OF SILICON NITRIDE

Silicon nitride films are amorphous insulating materials that find three main applications in VLSI fabrication: 1) as final passivation and mechanical protective layers for integrated circuits, especially for parts encapsulated in plastic packages; 2) as a mask for the selective oxidation of silicon; and 3) as a gate dielectric material in MNOS devices. Silicon nitride also has a high dielectric constant (6-9 vs ~4.2 for CVD SiO_2), making it less attractive for interlevel insulation, because of the resultant higher capacitance between conductor layers.

Silicon nitride is highly suitable as a *passivation layer* because of its following properties: a) it behaves as a nearly impervious barrier to diffusion (in particular, moisture and sodium find it very difficult to diffuse through the nitride film); b) it can be prepared by PECVD to have a low compressive stress, which allows it to be subjected to severe environmental stress with less likelihood of delamination or cracking; c) its coverage of underlying metal is conformal; and d) it is deposited with acceptably low pinhole densities.

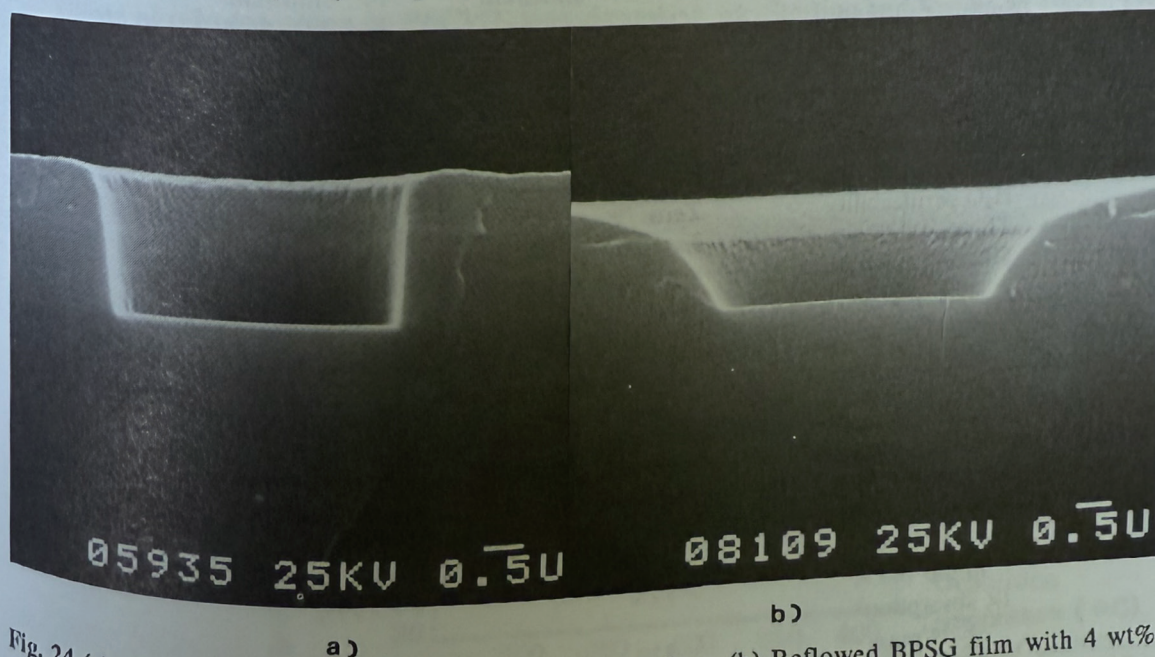


Fig. 24 (a) SEM of dry-etched contact window before reflow. (b) Reflowed BPSG film with 4 wt% P and 4 wt% B. Reflow was 930°C in N_2 for 25 min³⁷. Courtesy of Applied Materials, Inc.