
Polycrystalline Silicon for Integrated Circuit Applications

Ted Kamins



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by

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Preface

Recent years have seen silicon integrated circuits enter into an increasing number of technical and consumer applications, until they now affect everyday life, as well as technical areas. Polycrystalline silicon has been an important component of silicon technology for nearly two decades, being used first in MOS integrated circuits and now becoming pervasive in bipolar circuits, as well. During this time a great deal of information has been published about polysilicon. A wide range of deposition conditions has been used to form films exhibiting markedly different properties. Seemingly contradictory results can often be explained by considering the details of the structure formed.

This monograph is an attempt to synthesize much of the available knowledge about polysilicon. It represents an effort to interrelate the deposition, properties, and applications of polysilicon so that it can be used most effectively to enhance device and integrated-circuit performance. As device performance improves, however, some of the properties of polysilicon are beginning to restrict the overall performance of integrated circuits, and the basic limitations of the properties of polysilicon also need to be better understood to minimize potential degradation of circuit behavior.

Because of the limited size of this monograph (constrained by publishing economics), the thorough treatment I had hoped to provide was not practical. As writing progressed, it became obvious that the amount of material published about polysilicon is too great to be covered exhaustively in a monograph of reasonable size. Although the amount of data available, especially that concerning electrical properties, is over-

whelming, much of it applies to very specific deposition or processing conditions. To provide a more generally useful treatment, I have tried to emphasize trends and models and place specific experimental data in the context of these models. If this treatment is successful, the framework provided in this volume can be used to plan experiments pertinent to specific deposition and processing conditions so that the detailed data needed for practical device fabrication can be rapidly obtained.

The material covered in this book is divided into six chapters, which are briefly described below:

Chapter 1: DEPOSITION

In a continuous-flow reactor, kinetics, as well as thermodynamics, affect the deposition process. Either gas-phase or surface mechanisms can limit the overall deposition process, and the choice of the limiting step should be compatible with the reactor geometry being used. Both atmospheric-pressure and low-pressure reactors can be used to deposit polysilicon. Introducing arsenic- or phosphorus-containing dopant gases during the deposition can decrease the deposition rate, while adding a boron-containing dopant gas can increase it.

Chapter 2: STRUCTURE

Initial nucleation of a polysilicon deposit on an amorphous surface depends on the deposition conditions and the nature of the surface. Surface migration of adsorbed atoms during the deposition of the film also influences its structure. Surface migration can be affected by deposition temperature, rate, and pressure. Complementary structural information is provided by various evaluation techniques, such as transmission-electron microscopy (for grain size and detailed microstructure) and x-ray diffraction (for quantitative comparison of films deposited under different conditions). The structure of undoped films is stable at high temperatures, while marked grain growth can occur in highly doped films even at moderate temperatures. Epitaxial regrowth of polysilicon on single-crystal silicon can also occur.

Chapter 3: DOPANT DIFFUSION AND SEGREGATION

Rapid diffusion of dopant atoms along grain boundaries dominates the diffusion of dopant atoms in polysilicon. Diffusion of dopants *within* polysilicon is differentiated from diffusion *from* polysilicon into underlying single-crystal silicon; in the latter case, residual oxide layers at the

interface or (in the opposite extreme) epitaxial regrowth can retard the diffusion of dopant from polysilicon. The n -type dopants phosphorus, arsenic, and probably antimony segregate to grain boundaries, especially at lower temperatures, limiting the amount of dopant available to contribute carriers to the conduction process; boron does not appear to segregate.

Chapter 4: OXIDATION

The oxidation of undoped polysilicon is controlled by the different oxidation rates of differently oriented crystallites. Doped films exhibit a complex dependence on the dopant concentration and the ability of the dopant to diffuse away from the surface during oxidation. Conduction through oxide grown on polysilicon depends on the surface morphology of the film.

Chapter 5: ELECTRICAL PROPERTIES

The resistivity of undoped polysilicon films is similar to that of intrinsic silicon and depends only weakly on the deposition conditions. The electrical properties of moderately doped films are determined both by dopant segregation to the grain boundaries and by carrier trapping at the grain boundaries. Trapping creates potential barriers, impeding carrier transport between grains and reducing the "effective mobility." Current flow is normally modeled by considering thermionic emission, but tunneling can be important in some cases. The nonuniformity of the grain size restricts detailed modeling of conduction in polysilicon. The conductivity of heavily doped films is limited by the solid solubility of the dopant in crystalline silicon.

Chapter 6: APPLICATIONS

The main application of polysilicon is for the gate electrodes of silicon-gate MOS integrated circuits, in which the high-temperature compatibility of polysilicon allows fabrication of self-aligned transistors with low parasitic capacitances. The polysilicon can also serve as an additional partial level of circuit interconnections. Lightly doped polysilicon can provide the high-value resistors needed for static memories and other applications. Polysilicon is being increasingly used in bipolar integrated circuits for contact to the base and emitter of the transistor. When used for the emitter contact, it can markedly improve the transistor gain. Devices, such as MOS transistors and diodes, may also be fabricated within the polysilicon layer itself.

I would like to express my appreciation to Stanford University's Center for Integrated Systems, which provided an environment conducive to writing this monograph during a year I spent there as Hewlett-Packard's resident industrial representative. At Stanford Professor John Linvill provided welcome encouragement to pursue this work, and Ms. Louise Peterson and Ms. Joyce Pelzl provided logistical assistance. During preparation of the monograph, presenting a course at Stanford covering the same material provided me with the opportunity to assess the effectiveness of the content and organization of the material.

I would like to thank Hewlett-Packard for providing me with the opportunity to spend time at Stanford, both to provide the liaison between the company and the university which is becoming increasingly important and to be actively involved in research projects there. I would especially like to thank Dr. John Moll of Hewlett-Packard for encouragement in selecting this monograph as one of the projects to pursue while at Stanford.

I would also like to acknowledge those, both at Stanford and elsewhere, who shared their information concerning polysilicon with me. At Stanford the research groups of Professors J. Plummer and R. Dutton and Professor J. Bravman, E. Crabbé, E. Demirlioglu, J. Hoyt, M. Ghannam and others provided useful discussion. The suggestions and encouragement of Dr. G. E. Davis of Northrop are especially appreciated. Dr. John Andrews from AT&T Bell Laboratories kindly allowed me to use about twelve figures that he had drawn for a course we taught together through the University of California. (These figures are used in Chapters 1 and 6.) I also appreciate the loan of original micrographs by Professor J. Bravman of Stanford University, Dr. Y. Wada of Hitachi, Dr. R. B. Marcus of Bell Communications Research, and Dr. H. Oppolzer of Siemens.

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Chapter 1

Deposition

1.1 Introduction

Silicon integrated circuits are playing an increasingly important role in the electronics industry. The content of integrated circuits in electronic products has increased continuously over the past decade until today it can dominate the value, as well as the cost, of a computer. One of the critical factors leading to this rapid increase in the use of integrated circuits in electronics has been the development of high-density, metal-oxide-semiconductor (MOS) integrated circuits, which allow complex logic or large, dense memories to be built on a single silicon chip. Key to the fabrication of these dense MOS chips is the use of polycrystalline silicon as a gate-electrode material. The use of polysilicon allows realization of a self-aligned structure, greatly improving the device characteristics by reducing parasitic capacitance. It also permits more complex structures to be fabricated because of its compatibility with high-temperature silicon integrated-circuit processing.

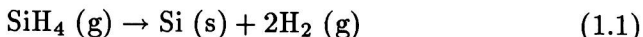
Although the first widespread application of polysilicon was in MOS integrated circuits, its availability led to its use in bipolar circuits as well, where it has similarly improved device performance and allowed increased density. Today, virtually all advanced bipolar integrated circuits include one or even two layers of polysilicon. Polycrystalline silicon is also used in other devices and is increasingly being employed in novel ways within both MOS and bipolar integrated circuits. For example, the storage regions and even the access transistors of dynamic, random-access memories are being placed in wells etched in the silicon surface

and refilled with polysilicon.

In addition to integrated-circuit applications, polysilicon is being employed in solar cells, and a considerable amount of understanding has been gained by research motivated by solar-cell applications. However, the material used for solar cells often differs substantially in grain size and method of formation from that important for integrated-circuit applications. Although most of the basic considerations in this volume are common to the two types of material, our discussion will be directed toward the type of polysilicon used for integrated-circuit applications.

1.2 Thermodynamics and kinetics

Polycrystalline silicon is generally deposited by chemical vapor deposition, utilizing the thermal decomposition of silane (SiH_4) to form elemental silicon and molecular hydrogen by the overall reaction



In the open-flow reactors important for chemical vapor deposition of thin films for electronic applications, gases are continuously introduced into the reactor and unused gases and reaction products are continuously removed. Because of the continuous gas flow, the deposition process is influenced by kinetic factors, as well as by the thermodynamics of the decomposition reaction itself.

From a list of the possible species present and thermochemical data, the *equilibrium* concentrations of the various gaseous species can be determined. Available computer programs calculate these quantities by minimizing the free energy of the overall system. The equilibrium constant K of a reaction can be calculated from the relation

$$\ln K(T) = -\frac{\Delta G(T)}{RT} \quad (1.2)$$

where G is the Gibb's free energy of the reaction found from the sum of the free energies of formation of the products minus that of the reactants. The amount of product formed from a given amount of reactant can then be determined if the reaction proceeds fully to equilibrium. The deposition rate (product per unit time) can similarly be determined from the input gas flow rate (reactant per unit time). In actual reactors, however, the gases are not in the reaction zone long enough

for equilibrium to be established, and *kinetic* factors limit the amount of material deposited to less than that expected solely from equilibrium considerations. In practical deposition systems thermodynamic considerations only set an upper bound on the amount deposited. Kinetic factors are often of more practical concern because they can depend strongly on the geometry of the reactor and the operating conditions, over which we have control.

1.3 The deposition process

The overall deposition process can be viewed as the sum of a series of microscopic steps. First, the silane enters into the reaction chamber by forced convection and flows to the vicinity of the wafer. It approaches the wafer by diffusing through a boundary layer near the wafer and may decompose partially or completely in the gas phase. When the silane and reaction intermediates reach the wafer surface, they adsorb and may be able to diffuse on the surface before completely decomposing to silicon and hydrogen. The resulting silicon atoms diffuse to stable sites, generally at steps formed by partially completed layers of silicon previously deposited. Subsequently arriving silicon atoms surround the first atom, complete bonds, and bind it firmly into the deposited layer. (The initial stage of deposition, in which nucleation occurs on an amorphous layer, will be discussed separately in Chapter 2.) Simultaneously, hydrogen atoms or molecules liberated by the decomposition reaction diffuse on the surface. Two hydrogen atoms can encounter each other, combine, and desorb as a hydrogen molecule.

The overall deposition process thus includes the following individual steps (and possibly others):

- Forced convection
- Boundary-layer diffusion
- Surface adsorption
- Decomposition
- Surface diffusion
- Incorporation

Any of these individual steps can limit the overall deposition process so that the temperature and pressure dependences of the deposition process reflect those of the rate-limiting step. Proper process design often requires selecting the rate-limiting step to optimize the uniformity of deposition in a given reactor by choosing the proper set of operating conditions. For ease of discussion, the entire series of individual steps can be divided into gas-phase processes and surface processes, although as we shall see, this division is somewhat idealized.

1.4 Gas-phase and surface processes

1.4.1 Convection

Most CVD reactions important in the electronics industry are carried out in *open-flow reactors*. The reactor may operate at atmospheric pressure, with the gas forced through it by a slightly higher pressure of the incoming gases, or it may operate at reduced pressure, with the gas flow caused by pumping at the outlet (exhaust) end of the reaction chamber.

At low velocities temperature gradients can determine the nature of the gas flow, and *free convection* established by the temperature gradients must be considered along with *forced convection* caused by the gas flowing through the reactor [1.1,1.2]. When free convection dominates, the gas motion is established by the largest thermal gradients in the system, with the gas flowing from the hottest region to the coolest. When a heated plate forms one boundary of the reaction zone (as in the cold-wall, atmospheric-pressure reactor to be discussed in Sec. 1.5.2), free convection dominates at low gas velocities. The gas flow is approximately circular from the center of the heated plate to the center of the opposite cool wall and then along the relatively cool walls and back across the heated plate. Obtaining uniform deposition in a reactor dominated by the irregular gas flow of free convection is difficult, and reactors are operated so that free convection does not control the gas flow.

As the gas velocity through the reaction chamber increases, forced convection is superposed on the free-convection pattern to produce a spiral gas flow. At higher velocities, forced convection dominates, and the gas flows primarily parallel to the walls. If the walls of the reactor are uniformly heated, as in the hot-wall, low-pressure reactor to be dis-