Silicon Epitaxy and Particle Dynamics:
A Theoretical and Experimental Study

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Chemical vapor deposition (CVD) is a process which uses chemically reactive gases to deposit thin solid films on a surface. The use of these thin solid films is widespread in many industries such as microelectronics, magnetic materials, optical devices, automobiles and ceramics. In the silicon based semiconductor industry CVD is used to deposit a wide variety of films including polycrystalline silicon (polysilicon), epitaxial silicon, silicon oxides and silicon nitrides (1). When the CVD process is used to deposit epitaxial layers the process is known as epitaxy. Silicon epitaxy i.e., deposition of a single crystal silicon layer on a single crystal silicon substrate is extensively used in the microelectronics and semiconductor industries. Silicon epitaxy is a complex dynamical process involving simultaneous mass, momentum and energy transport and complex chemical reactions. Hence, the quality of the films produced will be determined by the interactions of various transport processes and the chemical reactions in the epitaxial reactor chamber, which in turn depend on process conditions such as flow rates, pressure, temperature, concentration of chemical species, reactor geometry, etc. In addition, during the epitaxy process the control of epitaxial film purity is critical to the establishment of electrical properties. In fact, the ability to accurately adjust the purity and thus the electrical conductivity of a film is the basis for operation of solid state electronic devices. The effect of impurities on the electrical properties of solids is analogous to their effect in electrolytes i.e., impurities can undergo ionization reactions and significantly alter the free charge concentration. In a similar manner, a semiconductor material can be doped with impurities that may result in an excess of occupied conduction band electron states (free electrons) or with an excess of unoccupied valence band electron states (holes).

Particle contamination of epitaxial reactors results in impurities in the epitaxial film, and is one of the major limitations for the efficient processing of semiconductors and wafers. Specifically, in fabrication of feature sizes of size less than 1 micron, as much as 75% of the yield loss can be attributed to particle contamination of the wafers (3). Since feature sizes less than 1 micron are becoming prominent in the microelectronics industry, contamination by sub-micron particles such as airborne viruses and other inorganic and organic species is also important. The major sources of particle contamination in silicon epitaxy process can be broadly classified into two classes. The first class is the clean room air, process gases and people in the clean room which lead to particles coming into the epitaxial reactor. In addition, the process gases which enter the reactors could be contaminated with particles emanating from other sources such as gas tubing, valves and other mechanical equipment. The second class is particle generation inside the reactor through chemical and physical processes.

The modern microelectronics and semiconductor industries have imposed severe demands on the quality of films produced by the silicon epitaxy process and the epitaxial film deposition techniques need to fulfill several general requirements such as high growth rate, good epitaxial thickness uniformity, minimum particulate generation and economic use of reactants. Due to the lack of detailed fundamental models, the industrial practitioners are frequently forced to rely on methods of trial-and-error as well as on statistical methods to create purely empirical models for meeting the industry demands. The empirical relations are system specific and not applicable if the reactants or the reactor geometry is changed. On the other hand, mathematical modeling and simulation provide an excellent economic alternative to trial-and-error based experimental techniques.

Several simulation models accounting for complex flow patterns as well as heat and mass transfer in 3-D CVD reactors have been developed (1,2). Models with complex multiple chemical reactions have also been used to predict epitaxial film deposition rates and film thickness uniformity (4,5). However, rigorous models for simulating both particle dynamics and transport in CVD reactors have not been developed. In this study robust silicon epitaxy and particle dynamic numerical models have been developed and measures to meet the industry demands are provided.

The governing set of equations for mass, momentum, energy balance and particle dynamics were derived in their dimensionless form using the standard assumptions for an atmospheric silicon epitaxy process. As computational efficiency and accuracy are important factors for the realistic implementation of the numerical models, a thorough evaluation of standard numerical techniques as well as a newly proposed numerical technique is examined. It is demonstrated that our newly proposed adaptive semi-implicit algorithm based on the concept of operator-splitting is the method of choice for solving the governing set of equations.

A detailed comparison of simulation and experimental results was made and the simulation model was used for optimization of commercially available horizontal reactors for epitaxial deposition of silicon (2). The computational model was used for designing new and novel reactor designs leading to high deposition rate and excellent thickness uniformity of epitaxial single crystal silicon (6). Detailed particle dynamic simulation models describing the particle generation, transport and growth by coagulation and condensation for the complete particle size spectrum have been developed. Several parametric studies have been performed and measures required for the prevention of particle contamination of wafers have been determined.

References

1. C. Kleijn and C. J. Hoogendoorn, *Chem. Eng. Sci*., **46**, 321 (1991).
2. S. Kommu, G. M. Wilson and B. Khomami, *J. Electrochem Soc.* **147**, 1538 (2000).
3. R. W. Davis, E. F. Moore and M. R. Zachariah, *J. Cryst. Growth.*, **132**, 513 (1993).
4. H. K. Moffat and K. F. Jensen, *J. Electrochem. Soc*., **135**, 459 (1988).
5. M. E. Coltrin, R. J. Kee, and J. A. Miller, *J. Electrochem. Soc*., **131**, 425 (1984).
6. S. Kommu, *Design and Optimization of Horizontal CVD Reactors*, Presented at the Annual AIChE meeting, Los Angeles (2000).