# 2.0 Kinetic Phenomena in Thin Film Electronic Materials

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# 2.1 Grain Growth in Thin Films

National Science Foundation (Grant ECS 85-06565) U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154)

Sergio Ajuria, Hui M. Quek, Carl V. Thompson, Henry I. Smith

Polycrystalline metallic and semiconductor films are used in a wide variety of electronic and magnetic devices and circuits. Grain sizes, grain orientations, and grain size distributions strongly affect the properties of these films. We are studying microstructrual evolution through normal and secondary grain growth in thin films. Secondary grain growth often leads to very large grains (up to 500 times the film thickness) with restricted crystallographic orientations. We are studying the effects of

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film thickness and deposition conditions, as well as other parameters, on thermal grain growth. We are also investigating grain growth under laser irradiaton and during alloy formation.

## 2.1.1 Dopant Enhanced Grain Growth in Silicon Thin Films

Semiconductor Research Corporation (Contract 87-SP-080) U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154) International Business Machines, Inc. (Faculty Development Award)

Hyoung -J. Kim , Carl V. Thompson

Polycrystalline silicon films are used as gates in metal oxide semiconductor field effect transistors, as base and emitter contacts and diffusion sources in bipolar transistors, in sensors, and as active device films in thin film transistors. Performance in all of these applications is affected by the microstructure of the films. Microstructural evolution, specifically grain growth, is strongly affected by electronically active dopants. The rates of both normal and secondary grain growth are increased when electron donors (P and As) are added to silicon. This rate enhancement can be reduced or eliminated through codoping with boron. We have developed a model which accounts for the dependence of grain boundary atomic mobilities on the free electron concentration. The concepts developed here are also being applied to other solid state kinetic processes in silicon.

## 2.1.2 Ion Bombardment Enhanced Grain Growth in Thin Films

U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154) National Science Foundation (Grant ECS 85-06565)

Harry A. Atwater, Jerrold A. Floro, Carl V. Thompson, Henry I. Smith

We have demonstrated that ion bombardment of thin films leads to grain growth at temperatures well below those required for thermally induced grain growth. In germanium, silicon, and gold films it has been shown that the grain size increases with ion dose, independent of ion flux and with only a very weak temperature dependence. It appears that grain growth is promoted through ion-bombardment-induced generation of point defects at grain boundaries. A transition state model for grain boundary motion during ion bombardment has been developed. This model is being tested and extended for application to other ion-assisted solid state kinetic processes. We are also investigating the effects of ion bombardment on microstructural evolution during film deposition.

## 2.1.3 Graphoepitaxy by Grain Growth in Thin Films

U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154) National Science Foundation (Grant ECS 85-06565)

Hui M. Quek, Sergio Ajuria, Henry I. Smith, Carl V. Thompson

Surface-energy-driven secondary grain growth in thin films on amorphous substrates normally leads to films with grains having restricted or uniform texture but random inplane orientations. By using sub-micron lithographic techniques to pattern amorphous substrates, we have shown that artificial surface topography can be used to control the in-plane orientation of secondary grains. Use of artificial surface topography to control crystalline orientation in thin films is known as graphoepitaxy. We are optimizing this process through development of improved patterning techniques. We are also investigating techniques for patterning the top surface of polycrystalline films in order to investigate whether graphoepitaxy can occur due to top-surface patterning.

## 2.1.4 Modeling of Microstructural Evolution in Thin Films

U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154) National Science Foundation (Grant DMR 85-06030)

Carl V. Thompson and Harold J. Frost

We are developing analytic models for normal and secondary grain growth in continuous thin films as well as particle coarsening in discontinuous films. The effects of surface or interface energy anistropy play especially important roles in these processes. We have also developed computer models for film formation by crystal nucleation and growth to impingement under a variety of conditions. The topology and geometry of grain structures have been shown to strongly depend on the conditions of film formation. We have developed a computer model for two-dimensional normal grain growth and have extended this model for treatment of secondary grain growth.

## 2.2 Post-Nucleation Heteroepitaxy in Lattice Mismatched Systems

U.S. Air Force - Office of Scientific Research (Contract AFOSR 85-0154) National Science Foundation (Grant ECS 85-06565)

Joyce E. Palmer, Tow Chong, Carl V. Thompson, Clifton G. Fonstad, Henry I. Smith

Heteroepitaxial growth of films with poor lattice matching on single crystal substrates often leads to films with high bulk as well as interface defect densities. When atom by atom or layer growth occurs, bulk defects are generally generated during strain accommodation well after film nucleation. Alternatively, strain accommodation can occur through formation of low energy interfaces during competitive growth of grains or nuclei which initially have a variety of orientations. We are investigating these postnucleation epitaxial processes in continuous and discontinuous films. Model systems include GaAs-on-silicon and epitaxial metals on silicon.

# 2.3 Thin Film Zone Melting Recrystallization of Silicon

International Business Machines, Inc. Sony Company

James S. Im, Hisashi Tomita, Carl V. Thompson, David A. Smith

Techniques for producing device-quality single-crystal films of semiconductors on insulator (SOI) are of interest for multilayer or multimaterial integrated circuits, display devices and low-cost, high-efficiency solar cells. Such films can be obtained through directional solidification of confined thin films (zone melting recrystallization, ZMR). While there are analogies to bulk crystal growth, in ZMR there are also phenomena and mechanisms unique to thin-film solidification of radiatively heated silicon. Direct observation of dynamic and static liquid-solid interfaces complements theoretical modeling of solidification. We are studying these phenomena in order to develop means of controlling and optimizing thin film growth by ZMR.

# 2.4 Capillary Instabilities in Thin Solid Films

National Science Foundation (Grant ECS 85-06565)

Eva Jiran, Carl V. Thompson

Very thin metallic and semiconductor films (< 200 Å) are being used in an increasing variety of applications. Most solid films are used on substrates with which they would, in equilibrium, form non-zero contact angles. Therefore, even solid films tend to become discontinuous or bead in order to reduce their total film/substrate interface energy. This phenomena occurs in both continuous and patterned films. The rate of solid state beading is a strong function of the dimensions of a film or line as well as the microstructure of the film or line. For example, the beading rate rapidly increases with decreasing film thickness. We are experimentally characterizing the kinetics of beading of thin films of gold on SiO<sub>2</sub>. Film patterning allows independent study of both hole formation and hole growth. These eventually lead to complete beading.

# 2.5 Kinetics of Thin Film Silicide Formation

International Business Machines, Inc.

Robert C. Cammarata, Lawrence Clevenger, Carl V. Thompson, King N. Tu

There is considerable current interest in the use of refractory metals or refractory metal silicides as interconnects, as gate materials in MOS devices and for low contact resistance diffusion barriers at metal-silicon contacts in integrated circuits. These applications raise fundamental questions about the rate and products of thin film metal-silicon reactions. One method of silicide formation is through reaction of metallic thin films with silicon substrates or polycrystalline silicon films. There are four critical parameters in analysis and modelling of these reactions; interdiffusivities, free energy changes, surface energies and interface reaction constants. Of these, the first two parameters are fairly well understood and can be predicted. The purpose of this project

is to develop a better understanding and predictive capability for the last two parameters. Surface energies are being determined through silicide precipitation experiments and interface reaction rate constants are being determined through thermal and X-ray analysis of interface limited reactions of thin films.

## 2.6 Reliability and Microstructures of Interconnects

Semiconductor Research Corporation (Contract 87-SP-080) Joint Services Electroncs Program (Contract DAAL03-86-K-0002)

Jaeshin Cho, Hal Kahn, Hai Longworth, and Carl V. Thompson

We are developing new techniques which allow statistical characterization of failure of contacts and interconnects for silicon-based integrated circuit technology. We are using these techniques to correlate failure rates and mechanisms with microstructures of interconnect lines and contact barriers. We are also investigating techniques for controlling microstructures in order to improve contact and interconnect reliability, especially under conditions which can lead to electromigration. For example, very large grained (100  $\mu$ m), 0.75  $\mu$ m-thick, electromigration-resistant films have been made using layered deposition and post-deposition annealing of Al- 2% Cu - 0.3% Cr films.

## 2.7 Focused Ion Beam Induced Deposition

Charles Stark Draper Laboratories, Inc. (Contract DL-H-261827) Defense Advanced Research Projects Agency (Contract MDA 903-85-C-0215) International Business Machines, Inc. Nippon Telephone and Telegraph, Inc.

Jaesang Ro, Andrew D. Dubner, John Melngailis and Carl V. Thompson

It is now possible to produce ion beams with diameters as small as 500Å. This permits use of focussed ion beams for high spatial resolution implantation, sputtering and deposition. In principal, the latter can be used in integrated circuit mask repair or high resolution direct writing of interconnects. We are investigating the mechanisms of ion-beam-induced chemical vapor deposition from metal-bearing gases.

#### Thesis

Atwater, H.A., *Ion Beam Enhanced Grain Growth in Thin Films,* Ph.D. diss., Dept. of Electr. Eng. and Comp. Sci., MIT, 1987.

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