

## Chapter 2. Microstructural Evolution in Thin Films of Electronic Materials

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## 2.1 Grain Growth in Thin Films

### Sponsors

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### Project Staff

Sergio Ajuria, Hui Meng Quek, Professor Carl V. Thompson III, Professor Henry I. Smith

Polycrystalline metallic and semiconductor films are used in a wide variety of electronic and magnetic devices and circuits. The grain size, grain orientations, and grain size dis-

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tributions strongly affect the properties of these films. We are studying microstructural 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 film thickness, deposition conditions, substrate topography, laser illumination, ion-bombardment, dopant concentrations, as well as other parameters, on grain growth.

## 2.2 Modelling of Microstructural Evolution in Thin Films

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### Project Staff

Professor Carl V. Thompson III, Harold J. Frost, Jerrold A. Floro, Yauchin Liu

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 anisotropy play especially important roles in these processes. We have 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 also developed a computer model for two-dimensional normal grain growth and are extending this model for treatment of secondary grain growth.

## 2.3 Post-Nucleation Heteroepitaxy in Lattice Mismatched Systems

### Sponsors

U.S. Air Force - Office of Scientific Research  
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### Project Staff

Joyce E. Palmer, Jerrold A. Floro, Yauchin Liu, Tow Chong, Professor Carl V. Thompson III, Professor Clifton G. Fonstad, Jr., Professor Henry I. Smith

Heteroepitaxial growth of films with poor lattice matching with 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 and the early stages of film growth. 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 post-nucleation epitaxial processes in continuous and discontinuous films. Model systems include GaAs-on-silicon and epitaxial metals on alkali halide crystals.

## 2.4 Thin Film Zone Melting Recrystallization of Silicon

### Sponsor

International Business Machines, Inc.

### Project Staff

James S. Im, Chenson K. Chen, Professor Carl V. Thompson III

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.

## 2.5 Capillary Instabilities in Thin Solid Films

### Project Staff

Eva Jiran, Professor Carl V. Thompson III

Very thin metallic and semiconductor films ( $\lesssim 200 \text{ \AA}$ ) 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, 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  $\text{SiO}_2$ . Film patterning allows independent study of both hole formation and hole growth. These eventually lead to complete beading.

## 2.6 Kinetics of Thin Film Silicide Formation

### Sponsor

International Business Machines, Inc.

### Project Staff

Lawrence Clevenger, Professor Roberto DeAvillez, Professor Robert C. Cammarata, Andreas Judas, John Olson, Professor Carl V. Thompson III, King N. Tu, Professor Ulrich Gosele

Currently, there is considerable 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. One method of silicide formation is through reaction of metallic thin films with silicon substrates or polycrystalline silicon films. This application raises fundamental questions about the rate and products of thin film metal-silicon reactions. There are four critical parameters in analysis and modeling 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 the kinetics of thin film reactions are being studied through thermal, TEM, and x-ray analysis of reactions in multi-layer thin films.

## 2.7 Reliability and Microstructures of Interconnects

### Sponsors

Semiconductor Research Corporation  
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### Project Staff

Jaeshin Cho, Hal Kahn, Hai Longworth, Professor Carl V. Thompson III

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 diffusion 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.

## 2.8 Focused Ion Beam Induced Deposition

### Sponsors

Charles Stark Draper Laboratory  
Defense Advanced Research Projects Agency  
(DARPA)  
International Business Machines, Inc.  
Nippon Telegraph and Telephone, Inc.

### Project Staff

Jaesang Ro, Andrew D. Dubner, Dr. John Melngailis, Professor Carl V. Thompson III

It is now possible to produce ion beams with diameters as small as 500Å. This permits use of focused 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.

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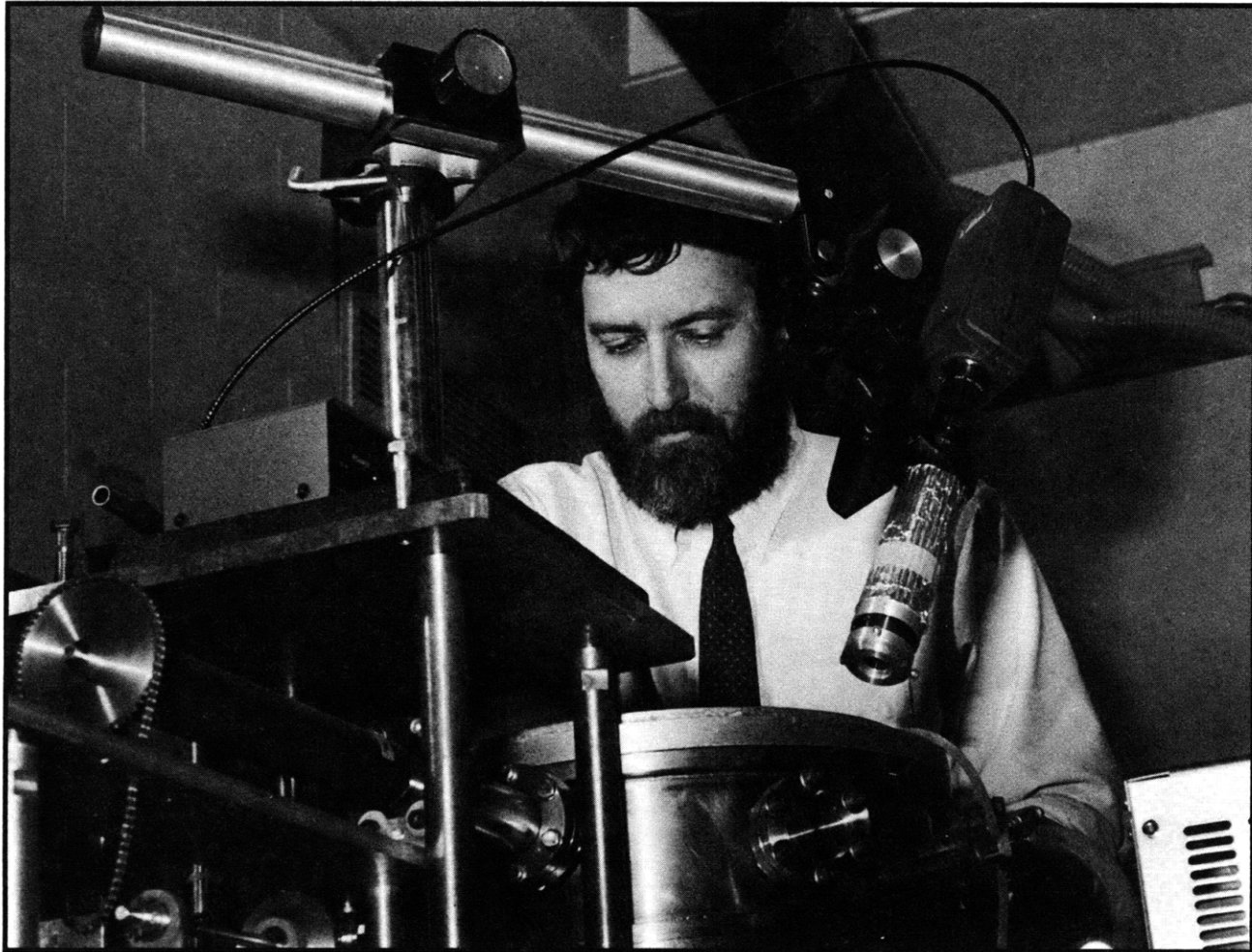
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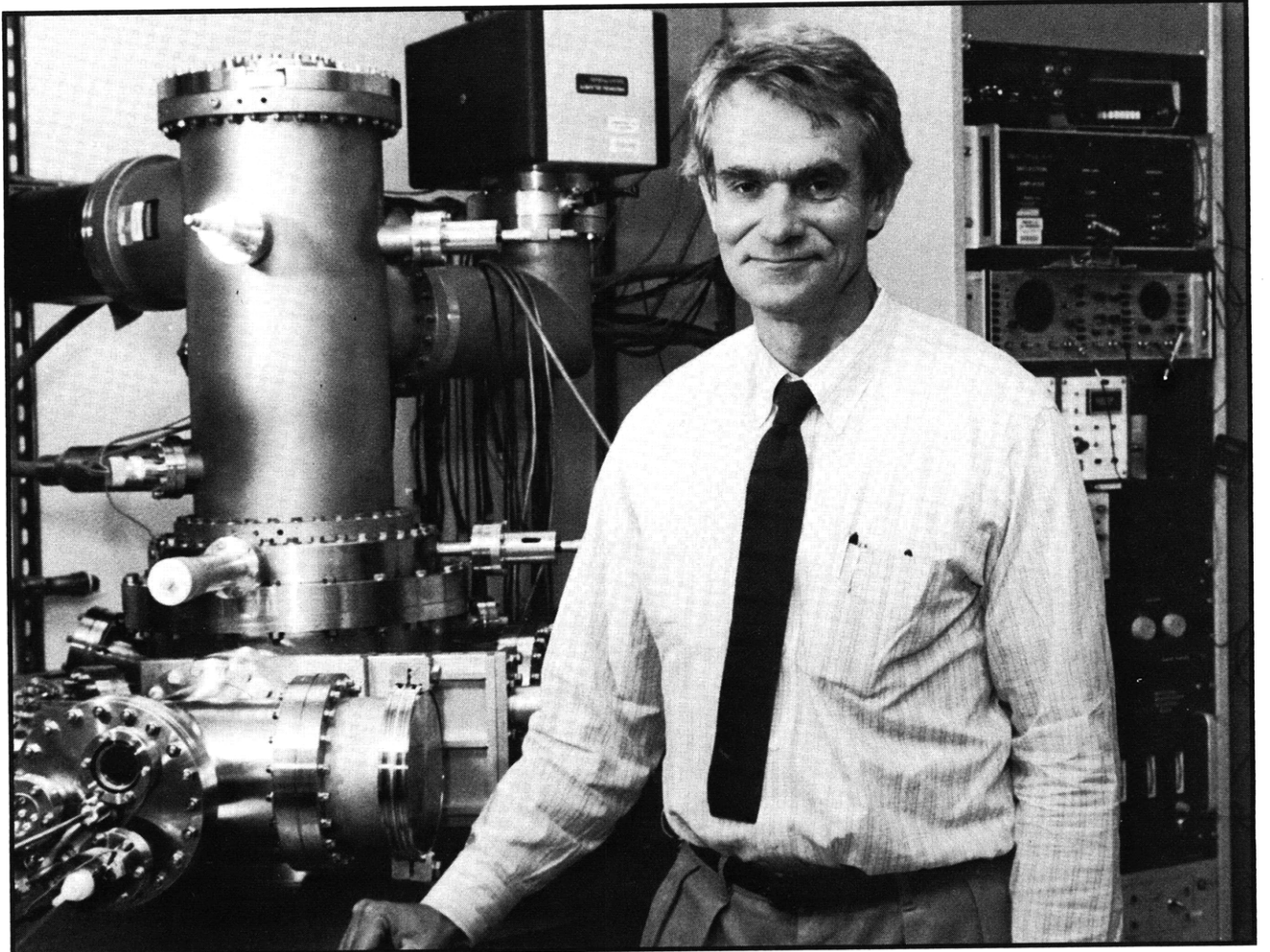
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