Chapter 2. Microstructural Evolution in Thin Films of Electronic Materials

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2.1 Modeling of Microstructural Evolution in Thin Films

Sponsors

Joint Services Electronics Program
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Contract AFOSR 85-0154

Project Staff

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

We are developing analytic models for normal, secondary and epitaxial 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 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 computer simulations for two-dimensional normal grain growth and secondary grain growth.

We are developing analytic models and computer simulations in parallel with experimental studies in model systems. Computer

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simulations have allowed us to explain microstructrual features which are generally characteristic of thin films, including: (1) stagnation of normal grain growth, (2) development of lognormal distributions of grain sizes and (3) abnormal grain growth which leads texture development or epitaxy. Grain growth models also provide a theoretical context for research on microstructure engineering using impurities, ion bombardment, substrate-surface-topography and precipitates.

Publications

Thompson, C.V. "Coarsening of Particles on a Planar Substrate: Interface Energy Anistropy and Application to Grain Growth in Thin Films." *Acta Metall.* 36:2929 (1988).

Thompson, C.V. "Observations of Grain Growth in Thin Films." In *Microstructural Science for Thin Film Metallizations in Electronic Applications,* 115. Eds. J. Sanchez, D.A. Smith, and N. Delanerolle. Warrendale, Pennsylvania: the Minerals, Metals, and Materials Society, 1988.

2.2 Reliability and Microstructures of Interconnects

Sponsors

Joint Services Electronics Program
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Semiconductor Research Corporation

Project Staff

Jaeshin Cho, Harold Kahn, Hai Longworth, Professor Carl V. Thompson

We are investigating the use of precipitates to produce metallic films and interconnects with engineered microstructures. We deposit initially layered alloy films (e.g., films deposited in a sandwich structure with a pure W layer between pure Al layers). When heated, precipitates form in the center of these films. These precipitates lead to a drag force which impedes grain boundary motion and supresses normal grain growth. Eventually, at elevated temperatures, a minor fraction of the grains begin to break free of the precipitates and grow abnormally. This can ultimately lead to very large grains and also changes in the crystallographic texture of films. With this technique, it is possible to control the grain sizes, the distribution of grain sizes, and the distribution of grain orientations over very broad ranges. We have now observed these effects in a number of aluminum alloy systems including Al-Cu-Cr, Al-Ag-Cr, Al-Mn-Cr, Al-Mn, and Al-W.

We are also developing new techniques which allow statistical characterization of failure of contacts and interconnects for silicon-based integrated cricuit technology. We are using these techniques to correlate failure rates and mechanisms with microstructures of interconnect lines and contact diffusion barriers. We are investigating techniques for controlling microstructures in order to improve contact and interconnect reliability, especially under conditions which can lead to electromigration.

We have recently shown that interconnect lines with bimodally distributed grain sizes have drastically reduced reliabilities. Also, for lines with monomodally distributed (uniform) grain sizes, increasing the grain size (relative to line width) results in an increase of both the median time to electromigration-induced failure and the lognormal standard deviation in the time to failure, see figures 1-3. The net result, in large populations of lines with monomodal grain size distributions, is little or no change in the time to the first failure. We have explained these results in terms of a "failure unit model" in which grain boundaries are taken to be the individual units which are responsible for the reliability of a line. The successful application of this model indicates the importance of the properties of individual grain boundaries in controlling interconnect reliability. We are now investigating the statistical reliability of lines with single, controlled grain boundaries in order to understand in detail the type of microstructural features which limit interconnect reliability.

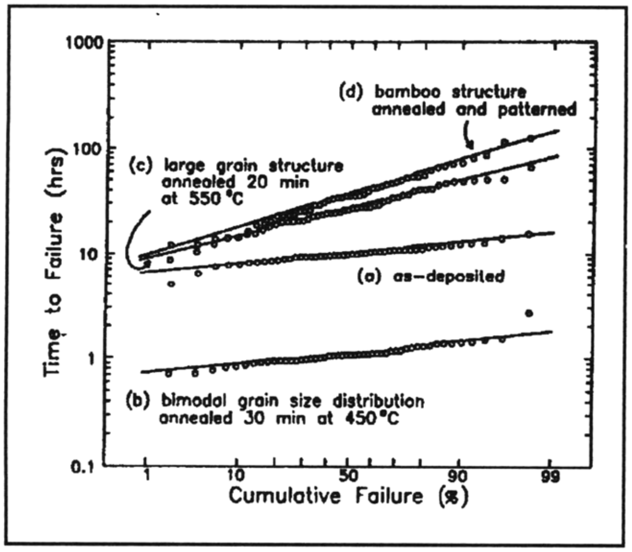

Figure 1. Distribution of failure times for 2.2-μm-wide, Al-2%Cu-0.3%Cr lines: (a) as-deposited (MTTF = 9.8 h, DTTF = 0.197), (b) after annealing for 30 min. at 450°C to develop a bimodal grain size distribution (MTTF = 1.08 h, DTTF = 0.223), (c) after annealing for 20 min. at 550°C to obtain mono-modally distributed large grains (MTTF = 26.3 h, DTTF = 0.465), and (d) after annealing for 20 min at 550°C before patterning, to obtain bamboo microstructures (MTTF = 35.0 h, DTTF = 0.580).

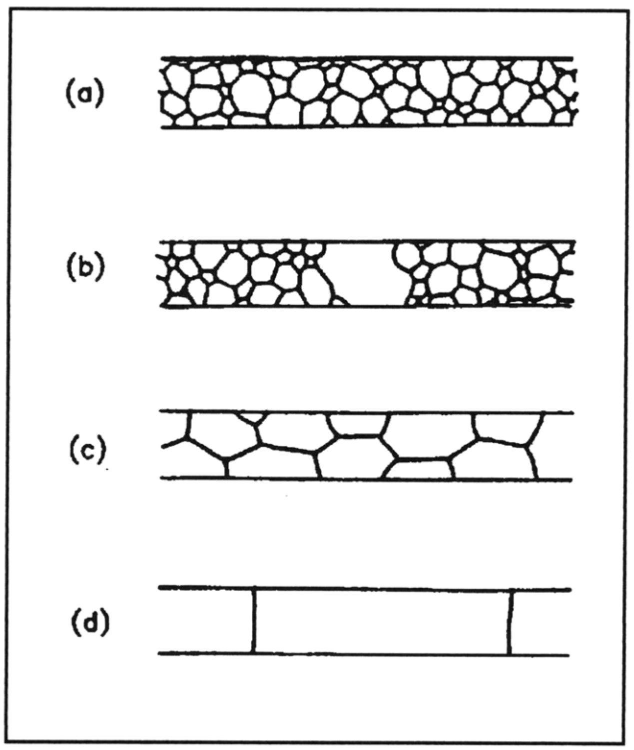

Figure 2. Sketches of the microstructures of the lines described in Figure 1, based on transmission electron microscopy.

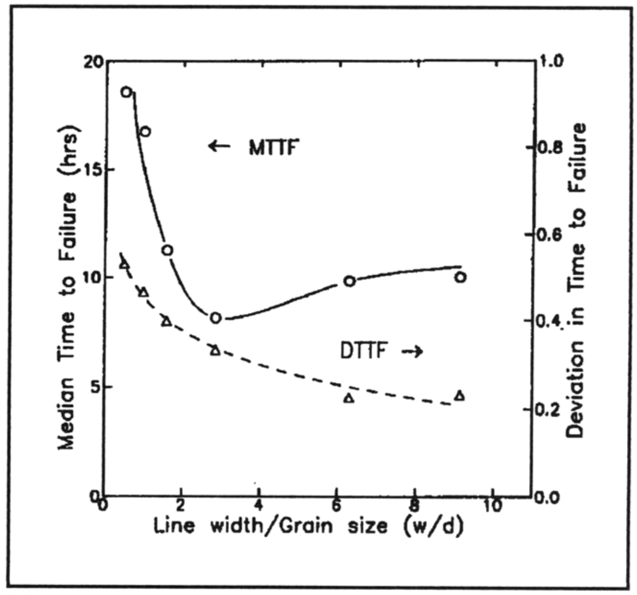

Figure 3. Median time to failure and deviation in the time to failure vs. linewidth/grain size ratio for Al-2%Cu-0.3%Cr lines with monomodally distributed grain sizes.

Publication

Cho, J., and C.V. Thompson. "The Grain Size Dependence of Electromigration Induced Failures in Narrow Interconnects." *Appl. Phys. Lett.* 54:2577 (1989).

2.3 Epitaxial Grain Growth

Sponsors

AT & T
U.S. Air Force - Office of Scientific Research
Contract AFOSR 85-0154

Project Staff

Jerrold A. Floro, Professor Carl V. Thompson, Professor Henry I. Smith

In the past year, we demonstrated that grain growth in polycrystalline films on single crystal substrates can lead to epitaxial films. This new approach to obtaining heteroepitaxial films can lead to ultrathin films with reduced defect densities compared to films deposited using conventional techniques. In epitaxial grain growth, ultrathin polycrystalline films are deposited on single crystal substrates. When these polycrystalline films are heated to elevated temperatures, epitaxial grains with low film-substrate interface energies grow and consume misoriented grains. Because the initial polycrystalline films are deposited at low temperatures, fully continuous ultrathin films can be obtained. Conventional Volmer-Weber epitaxy which is carried out at higher deposition temperatures can not be used to obtain equivalently thin epitaxial films. We have developed kinetic analyses for epitaxial grain growth and are testing these analyses through experiments on model systems, including Au and Ag films on mica and NaCl. The ultimate goal of our research is to develop a general understanding of when and how epitaxial grain growth can be used as a route to low-defect-density ultra thin heteroepitaxial films in film/substrate systems with large lattice mismatches.

2.4 Heteroepitaxy in Lattice Mismatched Systems

Sponsor

U.S. Air Force - Office of Scientific Research
Contract AFOSR 85-0154

Project Staff

Joyce E. Palmer, Jerrold A. Floro, Geoffrey Burns, Professor Carl V. Thompson, Professor Clifton G. Fonstad

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 accomodation well after film nucleation and the early stages of film growth. Alternatively, strain accomodation 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.

2.5 Kinetics of Thin Film Silicide Formation

Sponsor

International Business Machines Corporation

Project Staff

Lawrence A. Clevenger, Dr. En Ma, Dr. Roberto R. DeAvillez, Professor 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. 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 films reactions are being studied through thermal, TEM, and X-ray analysis of reactions in multilayer thin films.

We have found that in Pt/amorphous-Si, Ni/α-Si, V/α-Si and Ti/α-Si multilayer films, an amorphous silicide is the first phase to form. These phases are thermodynamically stable only if crystalline silicide formation is kinetically suppressed. We have also detected evidence for nucleation at the early stages of the formation of crystalline silicides. These results suggest that phase selection in thin film reactions is governed by nucleation barriers.

We have also observed explosive reactions in multilayer metal/α-Si films. These reactions can propagate in a room temperature ambient at velocities over 20 meters per second. This self-rapid-thermal-annealing process results in homogeneous films composed of the stable high temperature crystalline silicide.

2.6 Coarsening of Particles on a Planar Substrate

Sponsor

National Science Foundation

Project Staff

Yachin Liu, Professor Carl V. Thompson

Very small particles on a planar substrate can exchange material by atomic diffusion of the particle constituent on the substrate surface. This generally leads to an increase in the average particle size and spacing and can also lead to the development of restricted crystallographic orientations. This process can be very important in the early stages of the formation of a thin film. We have developed a theory to describe the evolution of particle sizes and orientations and are testing this theory by experimentally characterizing particle coarsening in model systems.

2.7 Thin Film Zone Melting Recrystallization of Silicon

Sponsor

International Business Machines Corporation

Project Staff

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

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.

We are also using ZMR to prepare thin film bicrystals in order to study the electronic properties of grain boundaries in silicon. We will correlate electronic properties with structural features, as revealed using high resolution electron microscopy.

2.8 Capillary Instabilities in Thin Solid Films

Project Staff

Eva Jiran, Professor Carl V. Thompson

Very thin metallic and semiconductor films ($\lesssim$200Å) 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_2. Film patterning allows independent study of both hole formation and hole growth.

2.9 Focused Ion Beam Induced Deposition

Sponsor

International Business Machines Corporation

Project Staff

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

It is now possible to produce ion beams with diameters as small as 500 Å. 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.

2.10 Protective Coatings for Integrated Circuits in an In Vitro Environment

Sponsor

National Institutes of Health

Project Staff

David J. Edell, Professor Carl V. Thompson

We are investigating the use of various coating materials to prevent Na diffusion into integrated circuits to be used in biomedical applications. We are correlating processing conditions, microstructural characteristics and diffusion barrier properties to develop standard methodologies for deposition and characterization of protective coatings.

2.11 Publications

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Atwater, H.A., and C.V. Thompson. "The Role of Point Defects in Ion-Bombardment-Enhanced and Dopant-Enhanced Grain Growth in Silicon Thin Films." *J. Nucl. Instrum. Meth. Phys. Res.* B 39:64 (1989).

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Clevenger, L.A., C.V. Thompson, and K.-N. Tu. "Controlled and Explosive Reactions in Nickel/Silicon Multilayer Thin Films." In *Materials Research Society International Meeting on Advance Materials* 10:431 (1989).

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Clevenger, L.A., C.V. Thompson, A.J. Judas, and J.L. Olson. "Metastable Reactions and Explosive Silicidation in Nickel/-Amorphous-Silicon Multilayer Thin Films." In *Selected Topics in Electronic Materials,* 23. Ed. B.R. Appleton et al. Materials Research Society, 1989.

Clevenger, L.A. *Controlled and Explosive Silicidation of Metal/Amorphous-Silicon Multilayer Thin Films.* Ph.D. diss. Dept. of Mater. Sci. and Eng. MIT, 1989.

Coffey, K.R., L.A. Clevenger, K. Barmak, D.A. Rudman, and C.V. Thompson. "Experimental Evidence for Nucleation During Thin Film Reactions." *Appl. Phys. Lett.* 55:852 (1989).

DeAvillez, R.R., L.A. Clevenger, and C.V. Thompson. "Relaxation Phenomena in Evaporated Amorphous Silicon Films." *J. Mater. Res.* 4:1057 (1989).

Im, J.S. *Experimental and Theoretical Investigation of Interface Morphologies Observed in Directional Solidification of Thin Si Films.* Ph.D. diss. Dept. of Mater. Sci., and Eng., MIT, 1989.

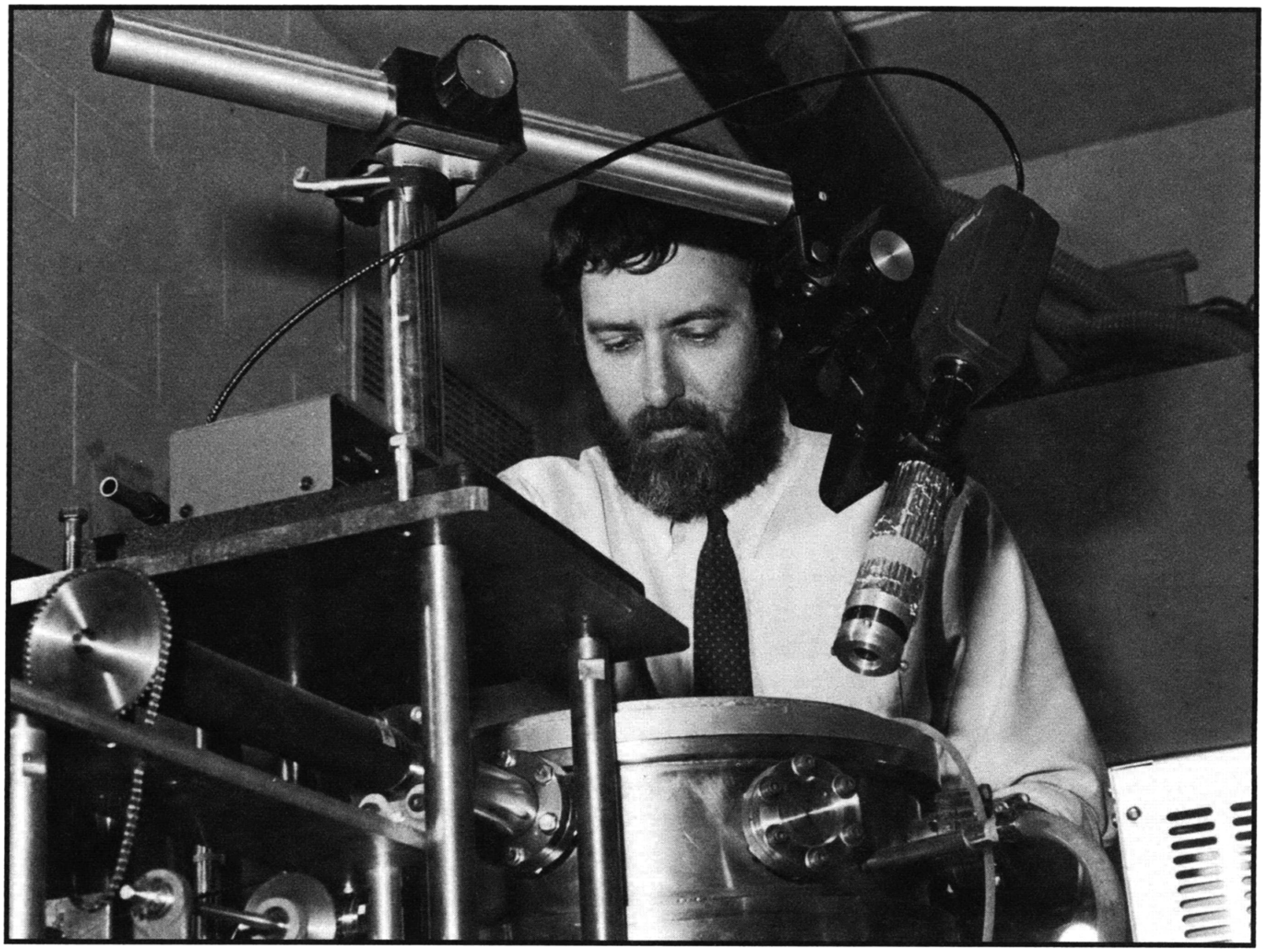
Palmer, J.E., G. Burns, C.G. Fonstad, and C.V. Thompson. "The Effect of As_4 Overpressure on Initial Growth of Gallium Arsenide on Silicon by MBE." *Appl. Phys. Lett.* 55:990 (1989).

Palmer, J.E. *Evolution of Microstructure in Ultra-Thin Films of GaAs and* CaF_2 *on Single Crystal Silicon.* Ph.D. diss. Dept. of Electr. Eng. and Comput. Sci., MIT, 1989.

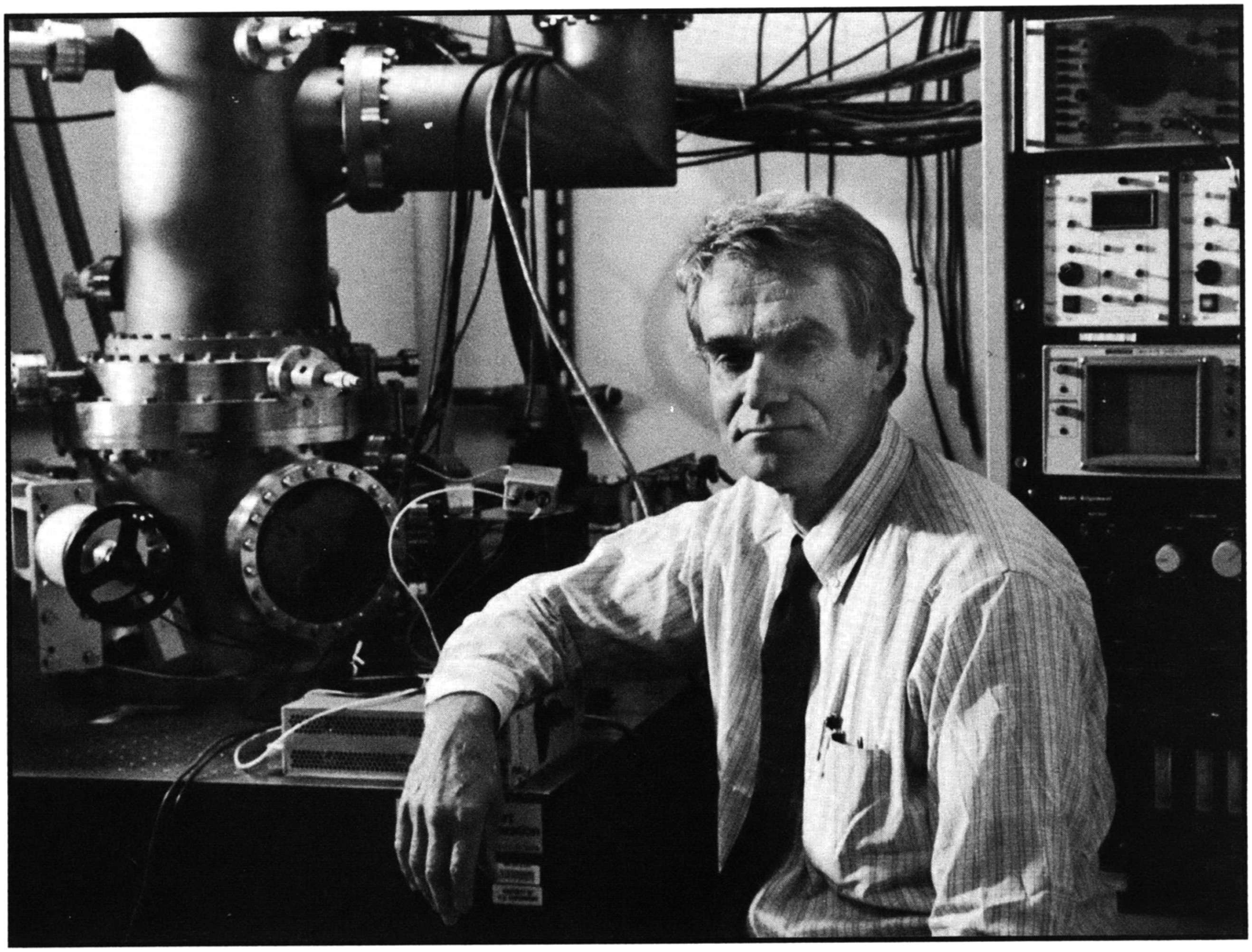
Phillips, J.M., J.E. Palmer, N.E. Hecker and C.V. Thompson. "The Effect of Annealing on the Structure of Epitaxial CaF_2 Films on Si(100)." *Proceedings of the Spring 1989 Materials Research Society Meeting,* Symposium D, San Diego, California, April 1989. Forthcoming.

Quek, H.M. *An Investigation of Graphoepitaxy in Thin Au and Bi Films.* S.M. thesis. Dept. of Mater. Sci. and Eng., MIT, 1989.

Spaepen, F., and C.V. Thompson. "Calorimetric Studies of Reactions in Thin Films and Multilayers." *Appl. Surf. Sci.* 38:1 (1989).



Professor Carl V. Thompson checks a zone meter that was constructed in his laboratory.



Principal Research Scientist Dr. John Melngailis uses focused ion beams for patterned deposition from adsorbed gas molecules and for patterned implantation or lithography.