2.0 Kinetic Phenomena in Thin Film Electronic Materials

Academic and Research Staff

Prof. C.V. Thompson, Prof. H.I. Smith, Dr. R.C. Cammarata, Mr. H. Tomita, Prof. J. Melngailis

Graduate Students

S. Ajuria, H. Atwater, J. Cho, L. Clevenger, A.D. Dubner, J. Floro, S.M. Garrison, J. Im, E. Jiran, H. Kahn, H.-J. Kim, H. Longworth, C. Maiorino, J. Palmer, H.M. Quek, J. Ro, C.C. Wong

Undergraduate Student

H. Meng

Support Staff

M.L. Wilson, M. Porter

2.1 Normal and Secondary Grain Growth in Ultrathin (<1000 Å) Films of Silicon and Germanium

National Science Foundation (Grant ECS 85-06505)
U.S. Air Force - Office of Scientific Research (Contract AFOSR-85-0154)
Semiconductor Research Corporation (Contract 87-SP-080)

Hyoung-June Kim, Joyce E. Palmer, Harry A. Atwater, Stephen M. Garrison, Hui M. Quek, Sergio Ajuria, Jerrold A. Floro, Carl V. Thompson, Henry I. Smith

Polycrystalline semiconductor films are used in a wide variety of electronic applications including use as gates in MOS devices, base and emitter contacts in bipolar devices, diffusion sources, sensors, thin film transistors and solar cells. In thin films of semiconductors, normal grain growth is driven by the reduction of the total grain boundary energy and usually leads to grains with sizes roughly equal to film thickness. We have shown that in sufficiently thin films (<1000Å) of silicon and germanium, a secondary grain growth process leads to the continued growth of some grains to sizes much larger than the film thickness. These secondary grains often have near uniform crystallographic texture. We believe that surface-energy-anisotropy is responsible for the selective growth of these grains. That is, grains with orientations that minimize surface energy grow at the expense of other grains. We have shown that the rate of secondary grain growth increases with decreasing film thickness and increasing temperature. Unlike metals, addition of impurities (e.g., P and As in Si) can also lead to an increase in the secondary grain growth rate. We have recently shown that grain boundary mobility in silicon is directly related to the Fermi energy. We are developing theoretical models for secondardy grain growth and grain boundary motion in semiconductors. We are also investigating the effects of rapid thermal annealing and ion bombardment on grain boundary motion.

2.2 Graphoepitaxy of Si, Ge and Model Materials

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

C.C. Wong, Joyce Palmer, Stephen Garrison, Harry A. Atwater, Hui M. Quek, S. Ajuria, Jerrold A. Floro, Henry I. Smith, Carl V. Thompson

Graphoepitaxy is a process in which an overlayer film is crystallographically oriented by an artificial surface pattern. Graphoepitaxy can involve vapor to solid, liquid to solid and solid to solid transitions. In experiments on graphoepitaxy we use lithographically defined surface features with periodicities as low as 2000Å. Recent research has focused on the use of artificial surface features in controlling surface-energy-driven secondary grain growth (SEDSGG) in model materials. Periodic patterns with square-wave cross sections increase the driving force for SEDSGG by increasing the surface area. The driving force is increased for grains with specific in-plane orientations as well as texture. We have demonstrated graphoepitaxial alignment during surface-energy-driven secondary grain growth in gold and germanium films. Greater control of these solid state forms of graphoepitaxy may allow the development of low temperature processes for obtaining device quality semiconductor films on insulating substrates.

2.3 Epitaxy via Surface-Energy-Driven Grain Growth

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

Joyce Palmer, Carl V. Thompson, Henry I. Smith

Grain growth in polycrystalline films on single crystal substrates can lead to formation of low defect density or single crystal films. We are investigating surface-energy-driven secondary grain growth in films deposited on a variety of insulating single crystal substrates. We are also further developing the theory of epitaxy by surface-energy-driven grain boundary motion.

2.4 Zone Melting Recrystallization of Silicon on Insulators

International Business Machines, Inc.
Sony International Business Machines, Inc.

James Im, Hisashi Tomita, Carl V. Thompson

Techniques for producing device-quality single-crystal films of semiconductors on insulators (SOI) are of interest for multilayer and multi-materials integrated circuits and low-cost, high-efficiency solar cells. Such films can be obtained through directional solidification of confined thin films (zone melting crystallization, 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. We are studying these phenomena in order to develop means of controlling crystal growth in ZMR. Direct observation of dynamic and static liquid-solid interface complements theoretical modeling of solidification.

2.5 Properties of Grain Boundaries with Controlled Orientations and Locations in Thin Silicon Films

International Business Machines, Inc.

Hyoung J. Kim, James S. Im, Carl V. Thompson, David A. Smith[1]

We are using lithographic patterning of films in conjunction with zone melting recrystallization (ZMR) to produce isolated grain boundaries with controlled misorientations and locations. Preparation of these thin film "bicrystals" should allow study of grain boundary structure and composition via transmission electron microscopy. These will be correlated with electronic characterization. Motion of individual boundaries between grains with different textures will also be studied. The misorientation dependence of grain boundary structure, composition, atomic mobility and electronic properties will be studied.

2.6 Metastable Phase Formation in Lithographically Defined Particles of Semiconductors

National Science Foundation (Grant DMR 84-18718)

Eva Jiran, Carl V. Thompson

When divided into a large number of small particles, materials can undergo phase transformations at substantial departures from equilibrium. It has been shown, for example, that dispersions of small particles of liquid metals can be undercooled to 50-80% if their melting temperatures. These undercoolings are achieved due to the isolation of the heterogeneities that catalyze crystal nucleation into a minor fraction of the particles. At high undercoolings, metastable phases can result from configurational freezing (transformation from a liquid to an amorphous solid), through mestastable phase nucleation, or due to undercooling-induced rapid solidification. We are using advanced lithography techniques to create samples composed of large numbers of small (including submicron), identical particles of semiconductors for studies of nucleation and metastable phase formation.

---

1 International Business Machines, Inc.

2.7 Kinetics of Silicide Formation at Refractory Metal-Silicon Contacts

International Business Machines, Thomas J. Watson Research Center

Robert C. Cammarata, Lawrence Clevenger,
Carl V. Thompson, K.-N. Tu[2]

There is considerable current interest in the use of refractory metals or refractory metal silicides as interconnects, as gate materials in MOS devices and as diffusion barriers at metal-silicon contacts in integrated circuits. One method of silicide formation is through reaction of metallic thin films with silicon substrates. This potential 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 interface reaction rate constants are being determined through analysis of interface limited reactions of thin films.

2.8 Grain Growth in Thin Films of Aluminum

Joint Services Electronics Program (Contract DAAL03-86-K-0002)

Cesar D. Maiorino, Hai Longworth, Carl V. Thompson

The thermal and electrical stability of metallic thin films and thin film lines are strongly affected by microstructure. Because grain boundary mobilities are high in metals, as compared to semiconductors, secondary grain growth can occur at relatively low homologous temperatures (T/Tm, Tm = the melting temperature), T/Tm = 0.5, and in relatively thick films ($\gtrsim 1 \mu m$). We have demonstrated that secondary grain growth in 0.75 μm films of A1-2%Cu-0.3%Cr can lead to grains with dimensions greater than 200 μm. Control of surface-energy-driven secondary grain growth in thin film lines with near unity aspect ratios may lead to total elimination of grain boundaries. Such lines would be highly resistant to thermally induced beading and electromigration. We are investigating the effects of deposition condictions, film composition and annealing conditions on secondary grain growth in A1 alloys. These alloys are widely used as interconnect materials in microelectronic devices and circuits.

2.9 Thin and Narrow Metallic Interconnects

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

Jaeshin Cho, Hai Longworth, Carl V. Thompson

---

2 International Business Machines, Inc.

Thin film lines of A1 and A1 alloys are used to interconnect devices in integrated circuits. Interconnects often fail due to damage resulting from current induced diffusion (electromigration), temperature-gradient-induced diffusion (thermomigration), and morphological changes driven by surface energy minimization (e.g., grain boundary grooving, void formation and/or beading). Reduced interconnect dimensions are sought in order to increase device densities and to improve device performance through reduction of parasitic capacitances. Decreased dimensions, however, can lead to increased rates of diffusion-induced failure. We are investigating the morphological and electrical stability of current-carrying submicrometer thick and wide metallic lines. Control of the microstructure of such lines should allow processing of interconnects with improved reliabilities.

2.10 Electromigration at Aluminum-Silicon Contacts in Integrated Circuits

Semiconductor Research Corporation (Contract 87-SP-080)

H. Kahn, Carl V. Thompson

Thin film lines of aluminum alloys are used to interconnect devices in integrated circuits. These interconnects must make contact with silicon through windows in silicon dioxide films. The properties of these contacts and their long term reliability greatly affect the functionality and utility of integrated circuits. Contacts fail via chemical-potential-driven or electromigration-induced interdiffusion. These failure mechanisms lead to leakage due to aluminum "spiking" through shallow junctions and/or due to increased contact resistance due to silicon precipitation. These problems are exacerbated by the shallow junctions, small area contacts, and reduced interconnect dimensions characteristic of very large scale integrated circuits. We have initiated a new program to investigate interdiffusion at aluminum-silicon contacts as well as contacts with diffusion barriers. We will correlate electronic characterization with microstructural features as revealed through electron microscopy. We anticipate development of new processing techniques for producing contacts with improved reliability for applications in very large scale integrated circuits.

2.11 Computer Modeling of Microstructural Evolution in Thin Films

National Science Foundation (Grant DMR 85-06030)

Carl V. Thompson, H.J. Frost[3]

In thin films final grain sizes and final grain shapes vary with crystal nucleation and growth rates during film formation. We have modeled two dimensional crystallization and have quantitatively shown that grain structures are easily topologically differntiable

[3] Dartmouth College

when films form under conditions of nucleation site saturation or when constant nucleation rates persist. These results provide a post-formation means of analyzing the conditions under which polycrystalline thin films have been produced. We are also modeling two-dimensional grain growth in computer-generated initial grain structures. Capillarity effects due to surface energy as well as grain boundary energy are accounted for. This allows modeling of normal grain growth and secondary grain growth and should provide insight into the conditions required for secondary grain growth.

2.12 Focussed Ion Beam Induced Deposition

Charles Stark Draper Laboratory (Contract DL-H-261827)
Nippon Telegraph and Telephone, Inc.

Andrew D. Dubner, Jaesang Ro, John Melngailis, 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.

Publications

Atwater, H.A., C.V. Thompson, and H.I. Smith, "Ion Beam Enhanced Grain Growth in Thin Films," In Proceedings of the Beam-Solid Interactions and Transient Processes Symposium of the Fall 1986 Materials Research Society Meeting.

Atwater, H.A., H.I. Smith and C.V. Thompson, "Enhancement of Grain Growth in Ultra-Thin Germanium Films by Ion Bombardment," Proc. Mat. Res. Soc. Symp. 51 (1986), p. 337.

Frost, H.J., J. Whang, and C.V. Thompson, "Modeling of Grain Growth in Thin Films," In *Annealing Processes-Recovery Recrystallization and Grain Growth*, 7th Riso International Symposium on Metallurgy and Materials Science, edited by N. Hanson, T. Lerrere and B. Ralph.

Frost, H.J. and C.V. Thompson, "Modeling of Thin Film Grain Structures and Grain Growth," Proceedings of the Computer Based Microscipic Description of the Structure and Properties of Materials Symposium, Fall 1985 Meeting of the Materials Research Society.

Frost, H.J. and C.V. Thompson, "The Effect of Nucleation Conditions on the Topology and Geometry of Two-Dimensional Grain Structures," to appear in Acta Metall.

Garrison, S.M., R.C. Cammarata, C.V. Thompson and H.I. Smith. "Surface-Energy-Driven Grain Growth During Rapid Thermal Annealing (<10ns) of Thin Silicon Films," to appear in J. Appl. Phys.

Kim, H.-J., and C.V. Thompson, "The Effects of Dopants on Surface-Energy-Driven Secondary Grain Growth in Ultrathin Si Films," In *Grain Boundary Structure and Related Phenomena*, Supp. to Trans. Jpn. Inst. Met. 27, 495 (1986).

Kim, H.-J. and C.V. Thompson, "Compensation of Grain Growth Enhancement in Doped Silicon Films," Appl. Phys. Lett. *48*, 399 (1986).

Kim, H.-J., and C.V. Thompson, "The Effects of Dopants on Grain Boundary Mobility in Silicon," In *Grain Boundary Structure and Related Phenomena*, suppl. to Trans. Jpn. Inst. Metals *27*, 495 (1986).

Smith, H.I., M.W. Geis, C.V. Thompson and C.K. Chen. "Crystalline Films on Amorphous Substrate by Zone Melting and Surface-Energy-Driven Grain Growth in Conjunction with Patterning," Proceedings of the Beam Solid Interactions and Phase Transformations Symposium of the Fall 1985 Meeting of the Materials Research Society.

Srolovitz, D.J. and C.V. Thompson, "Beading Instabilities in Thin Film Lines with Bamboo Microstructures," Thin Solid Films *139*, 133 (1986).

Thompson, C.V. and C.D. Maiorino, "Very Large Grained Aluminum Alloy Thin Films for Interconnects," Proceedings of the 18th International Conference on Solid State Devices and Materials, Tokyo, Japan, 1986, p. 491.

Thompson, C.V. and H.I. Smith, "Secondary Grain Growth in Thin Films," Proc. Phase Transistions in Condensed Systems Symp., fall meeting of the Mat. Res. Soc. (1985).

Thompson, C.V., H.J. Frost, and F. Spaepen, "The Relative Rates of Secondary and Normal Grain Growth," to appear in Acta Metall.

Thompson, C.V. and J. Cho, "A New Electromigration Test Structure for Rapid Statistical Evaluation of Interconnect Technology," in I.E.E.E. Electron Dev. Lett., *EDL-7*, 667 (1986).

Wong, C.C., H.I. Smith, and C.V. Thompson,"Room Temperature Grain Growth in Thin Au Films," in Grain Boundary Structure and Related Phenomena, suppl. to Trans. Jpn. Inst. Metals *27*, 641 (1986).

Wong, C.C., H.I. Smith and C.V. Thompson, "Surface-Energy-Driven Secondary Grain Growth in Thin Au Films," Appl. Phys. Lett. *48*, 335 (1986).

Theses

Garrison, S.M., "Kinetics of Secondary Grain Growth in Rapidly Thermal-Annealed Thin Silicon Films." M.S. Thesis., Dept. of Mat. Sci. and Eng., M.I.T., Cambridge, Mass., 1986.

Maiorino, C.D., "The Effects of Composition and Layering of Secondary Grain Growth in Aluminum Alloy Thin Films." Thesis, Dept. of Mat. Sci. and Eng., M.I.T., Cambridge, Mass., 1986.

Palmer, J.E. "Secondary Grain Growth in Ultrathin Films of Germanium on Silicon Dioxide," M.S. Thesis. Dept. of Electr. Eng. and Comp. Sci., M.I.T., Cambridge, Mass., 1985.

Prevost, Lawrence N., II, "Secondary Grain Growth in Thin Aluminum Lines." S.B. Thesis, Dept. of Electr. Eng. and Comp. Sci., M.I.T., Cambridge, Mass., 1985.

Wong, C.C., "Secondary Grain Growth and Graphoepitxy in Thin Au Films." Thesis, Dept. of Mat. Sci. and Eng., M.I.T., Cambridge, Mass., 1986.