

Chapter 2. Microstructural Evolution in Thin Films of Electronic Materials

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2.1 Coarsening of Particles on a Planar Substrate

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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. We have shown that Au particles on amorphous SiN membranes annealed in air undergo a coarsening process which is described well by the theory for interface-reaction-limited coarsening. We have also shown that differences in the gaseous ambient strongly affect the coarsening rate.

2.2 Epitaxial Grain Growth

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Jerrold A. Floro, H. Inglefield, Professor Carl V. Thompson

We have 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,

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including Au and Ag films on mica and NaCl. Experiments on epitaxial grain growth are providing a means of characterizing the film-substrate interface energy, as a function of crystal orientation.

2.3 Modeling of Microstructural Evolution in Thin Films

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U.S. Air Force - Office of Scientific Research

Project Staff

Professor Carl V. Thompson, Harold J. Frost,
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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. We have shown that topology and geometry of grain structures strongly depend on the conditions of film formation.

We have also developed a computer model for two-dimensional grain growth. This simulation has been modified to account for the important effects that the surfaces of a film have on grain growth. We have shown that when formation of grain boundary surface grooves leads to stagnation of normal grain growth, lognormal grain size distributions with average grain size two to three times the film thickness result. This is in agreement with well-established experimental observations. We have also successfully modeled abnormal grain growth caused by anisotropy of the surface energy of grains.

2.4 Properties of Grain Boundaries in Zone Melted Silicon Thin Films

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Dr. Paul Evans, David A. Smith, Professor Carl V. Thompson

We are using zone melting recrystallization (ZMR) of thin silicon films on oxidized silicon wafers to prepare thin film bicrystals in order to study the electronic properties of grain boundaries in silicon. We are correlating electronic properties with structural features, as revealed using high resolution electron microscopy. We have found that in these samples, (100) tilt boundaries with tilts up to 25.5 degrees are electrically inactive. This surprising result indicates that even polycrystalline ZMR films might be useful for silicon-on-insulator (SOI) majority carrier devices.

2.5 Kinetics of Thin Film Silicide Formation

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Professor Carl V. Thompson, Dr. En Ma, Dr. H. Miura, King-N. Tu

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 the 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: (1) interdiffusivities, (2) free energy changes, (3) surface energies, and (4) interface reaction constants. Of these, the first two parameters are fairly well understood and predictable. 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 multilayer thin films.

We have used differential scanning calorimetry, transmission electron microscopy, electron beam microanalysis, and thin film x-ray diffractometry to study the thermodynamics and kinetics of reactions in multilayer thin films. In Pt/amorphous-Si (Pt/a-Si), Ni/a-Si, V/a-Si and Ti/a-Si multilayers, amorphous silicides are the first phases to form, even though these phases are thermodynamically stable only if crystalline silicide formation is kinetically suppressed.

We have demonstrated that calorimetric analysis of multilayer films can be used to detect and analyze crystalline silicide nucleation during reactions in multilayers. Evidence for crystal nucleation has been observed in the cases listed above as well as in Co/a-Si and Ni/Al multilayers in which crystalline phases are the first phases to form. We have accumulated experimental and theoretical evidence which suggests that nucleation is preceded by interdiffusion and that it is the kinetic constraints of these sequential processes which govern phase selection during interfacial reactions.

We have also observed explosive reactions in multilayer metal/a-Si films and fully crystalline Ni/Al multilayers. 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 product phase.

2.6 Reliability and Microstructures of Interconnects

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Project Staff

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

We are developing new techniques which allow statistical characterization of failure of contact vias and interconnects for integrated circuits. We are using these techniques to correlate failure rates and mechanisms with microstructures of interconnect lines, contact diffusion barriers and via plugs.

We are also 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 in interconnect lines with uniform microstructures, increasing the grain size results in an increase of both the median time to electromigration-induced failure and the lognormal standard deviation in the time to failure. The net result, in large populations of lines, 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.

This interpretation is further supported by the observation that interconnects with bimodal grain size distributions (leading to grain size discontinuities) have greatly reduced reliabilities. On the other hand, lines which are completely free of grain boundary triple junctions have greatly improved reliabilities compared to lines with comparable grain sizes but also with triple junctions. We are now investigating the development of electromigration-induced damage in lines with individual grain boundaries of controlled types and locations. This will allow characterization of the failure mechanisms and rates for the fundamental units that control the reliability of interconnect systems.

2.7 Focused Ion Beam Induced Deposition

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IBM Corporation

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

2.8 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.

2.9 Publications

- Cammarata, R.C., C.V. Thompson, C. Haydelden, and K.N. Tu. "Silicide Precipitation and Silicon Crystallization in Nickel Implanted Amorphous Silicon Thin Films." *J. Mater. Res.* 5: 2133 (1990).
- Cho, J., and C.V. Thompson. "Electromigration-Induced Failures in Interconnects with Bimodal Grain Size Distributions." *J. Electron. Mater.* 19: 1207 (1990).
- Clevenger, L.A., and C.V. Thompson. "Explosive Silicidation in Nickel/Amorphous-Silicon Multilayer Thin Films." *J. Appl. Phys.* 67: 2894 (1990).
- Clevenger, L.A., and C.V. Thompson. "Nucleation Limited Phase Selection During Reactions in Nickel Amorphous-Silicon Multilayer Thin Films." *J. Appl. Phys.* 67: 1325 (1990).
- Clevenger, L.A., C.V. Thompson, R.R. De Avillez, and E. Ma. "Nucleation Controlled Phase Selection in Vanadium/Amorphous-Silicon Multilayer Thin Films." *J. Vac. Sci. Tech. A* 8 (3): 1566 (1990).
- De Avillez, R.R., L.A. Clevenger, C.V. Thompson, and K-N. Tu. "Quantitative Investigation of Titanium/Amorphous-Silicon Multilayer Thin Film Reactions." *J. Mater. Res.* 4: 593 (1990).
- Frost, H.J., C.V. Thompson, and D.T. Walton. "Simulation of Thin Film Grain Structures: I. Grain Growth Stagnation," *Acta Metall. Mater.* 38: 1455 (1990).
- Jiran, E., and C.V. Thompson. "Capillary Instabilities in Thin Films." *J. Electron. Mater.* 19: 1155 (1990).
- Kim, H.-J., and C.V. Thompson. "The Effects of Dopants on Surface-Energy-Driven Secondary Grain Growth in Silicon Films." *J. Appl. Phys.* 67: 757 (1990).
- Ma, E., and C.V. Thompson. "Self-Propagating Explosive Reactions in Al/Ni Multilayer Thin Films." *Appl. Phys. Lett.* B7: 1262 (1990).
- Thompson, C.V. "Grain Growth in Thin Films." *Ann. Rev. Mater. Sci.* 20: 245-68 (1990).
- Thompson, C.V., J. Floro, and H.I. Smith. "Epitaxial Grain Growth in Thin Metal Films." *J. Appl. Phys.* 67 (9): 4-99 (1990).

Theses

- Cho, J. *Effect of Microstructure of Aluminum Alloys on the Electromigration-Limited Reliability of VLSI Interconnects*, Ph.D. diss. Dept. of Mater. Sci. and Eng., MIT, 1990.
- Dubner, A.D. *Mechanisms of Ion Beam Induced Deposition*. Ph.D. diss. Dept. of Mater. Sci. and Eng., MIT, 1990.
- Jiran, E. *Capillary Instabilities in Thin, Solid Films*. Ph.D. diss. Dept. of Mater. Sci. and Eng., MIT, 1990.