2. Kinetic Phenomena in Thin Film Electronic Materials

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2.1 Surface-Energy-Driven Secondary Grain Growth in Ultrathin (<1000Å) Films of Silicon and Germanium

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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 the film thickness. We have shown that in sufficiently thin films (<1000 Å) 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 secondary grain growth and grain boundary motion in semiconductors. We are also investigating the effects of high intensity illumination and ion bombardment on grain boundary motion. Controlled surface-energy-driven secondary grain growth may provide a low temperature means of producing device quality semiconductor films on insulating substrates.

2.2 Metastable Phase Formation in Lithographically Defined Particles of Semiconductors

National Science Foundation (Grant DMR81-19285)
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 small particles of liquid metals can be undercooled to 50-80% of their melting temperatures. These undercoolings are achieved due to the isolation of the heterogeneities which 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 metastable 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.

2.3 Zone Melting Recrystallization of Silicon and Germanium Films

Sony International Business Machines, Inc.
Hisashi Tomita, James S. Im, Harry A. Atwater, Stephen C. Schott, Henry I. Smith, Carl V. Thompson

Techniques for producing device-quality single-crystal films of semiconductors (SOI) are of interest for multilayer and multi-material integrated circuits 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. We are studying these phenomena in order to develop means of controlling crystal growth in ZMR. Use of lithographically defined patterning, in conjunction with ZMR, permits formation of single crystal silicon films without the use of substrate seeding.

2.4 Graphoepitaxy of Si, Ge and Model Materials

National Science Foundation (Grant ECS85-06565)
U.S. Air Force - Office of Scientific Research (Contract AFOSR-85-0154)
Chee C. Wong, Joyce E. Palmer, Stephen M. Garrison, Harry A. Atwater, 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 2000 Å . 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. Secondary grain growth in thin (~300 Å) and smooth Ge films results in grains with predominant (110) and (112) texture. When patterned with surface structures having square wave surface relief, however, SEDSGG leads to growth of grains with (100) texture which have [100] in-plane directions aligned with the grating direction. We have recently shown that when Au is deposited on SiO_2 at room temperature, secondary grain growth leads to large grains with uniform texture. When SiO_2 substrates are patterned with square-wave cross section surface structures, Au films have uniform (111) texture and a dominance of grains with [112] directions parallel to the surface relief. Greater control of these solid state forms of graphoepitaxy may allow the development of low temperature processes for obtaining device quality films on insulating substrates.

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

International Business Machines, Inc.
James S. Im, Carl V. Thompson, David A. Smith[1]

Ultrathin (<1000 Å) films of silicon are being prepared by zone melting recrystallization (ZMR). Use of film patterning in conjunction with ZMR should allow production of 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. Motion of individual boundaries between grains with different textures will also be studied. The misorientation dependence of grain boundary structure, composition and mobility will be studied. The results will be correlated with measurements of electronic properties.

2.6 Kinetics of Silicide Formation at Refractory Metal-Silicon Contacts

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There is considerable current interest in the use of refractory metals or refractory metal silicides 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 will be determined through silicide precipitation experiments and interface reaction rate constants will be determined through analysis of interface limited reactions of thin films.

2.7 Modeling of Grain Formation and Grain Growth in Thin Films

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

2.8 Grain Growth in Thin Films of Aluminum

Joint Services Electronics Program (Contract DAAG29-83-K-0003)
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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

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(T/T_m, T_m = the melting temperature), T/T_m = 0.5, or in relatively thick films (> 1 μm). We have demonstrated that secondary grain growth in 0.75 μm films of Al–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 to electromigration. We are investigating the effects of deposition conditions, film composition and annealing conditions on secondary grain growth in Al alloys. These alloys are widely used as interconnect materials in microelectronic circuits.

2.9 Thin and Narrow Metallic Interconnects

Joint Services Electronics Program (Contract DAAG29-83-K-0003)
Semiconductor Research Corporation
Jaeshin Cho, Hai Longworth, Carl V. Thompson

Thin film lines of Al and Al 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 energy minimization (e.g., grain boundary grooving, void formation and/or beading). Reduced interconnect dimensions (both width and thickness) 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 production of interconnects with improved reliabilities.

Publications

Atwater, H.A., H.I. Smith, and C.V. Thompson, "Enhancement of Grain Growth in Ultra-thin Germanium Films by Ion Bombardment," to appear in the Proceedings of the Fall Meeting of the Materials Research Society, Boston, Massachusetts, December 2-6, 1985.

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