MBE GROWN COPPER-ALUMINUM ALLOY FILMS

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This document reports on the design and construction of a Molecular Beam Epitaxy system to grow and characterize aluminum/copper films, for electromigration studies. The growth of Al/Cu films in an evaporation system and reduction of the oxygen content of these films is discussed. Also, a novel approach to the modeling of electromigration in circuit metallization is presented.
This report documents contractor work completed during the period from Feb 87 to Dec 90 in conjunction with an ongoing in-house study of electromigration in Copper Aluminum metallization. Described are several unique mechanical designs incorporated into the Molecular Beam Epitaxy system located in the RL/ERDR (RADC/RBRE) facility. These designs include a pneumatic shutter control and a rotating sample stage which changes sample orientation according to position. The report also presents a novel if not unique electromigration model.

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Project Engineer
1. INTRODUCTION

The purpose of this effort was to grow high purity Cu-Al alloy films using a Molecular Beam Epitaxy Deposition (MBED) system, and study the "Electromigration" phenomena in these films. The MBE deposition system was to be built at the RADC/RBRE facility.

Cu-Al alloy films are used as leads in Very High Speed Integrated Circuits (VHSIC). In order to both increase the operating speed of a device and the number of devices per unit wafer area the active elements and interconnecting metallization are made smaller. Smaller electronic devices, in general, can be operated faster. For example, the shorter the gate length of a Field Effect Transistor (FET) the higher the frequency at which it will operate. Decreasing the length and the cross sectional area of the interconnects results in less distributed capacitance and inductance. Thus high frequency signals can propagate with less distortion.

Circuit interconnects with smaller cross sectional areas will have higher current densities than large cross sectional area interconnects used in low speed IC's. At these higher current densities the atoms of the metal from which the films are fabricated start to migrate leaving holes in the interconnects. This decreases the cross sectional area which results in even higher current densities. This further aggravates the metal migration process leading to eventual failure of the interconnect. This process is known as "Electromigration". The material from the voids
created in the metal interconnects accumulate in hillocks along the interconnect.

It is interesting to note that the metal atoms do not always migrate in the direction of the electron flow in metal interconnects. In Al the metal atoms, indeed, seem to migrate in the direction of the electron flow however in some gold interconnects the metal atoms have been reported to migrate in a direction opposite the electron flow. This seems to indicate that the electronic current in the interconnect ionizes the metal atoms. Negative ions experience forces in the same direction as the negatively charged electrons and migrate in the direction of the electron current. However, positive metal ions experience forces opposite to the direction of the forces experienced by the electrons and, thus, migrate in the opposite direction. There probably is an additional electron drag effect electromigration component that propels the metal atoms in the direction of the electron flow.

Conventionally Cu-Al films are deposited in diffusion pumped vacuum systems. However diffusion pumped vacuum systems, usually, have background pressures no lower than $10^{-6}$ torr. Various impurities are introduced into the metal films from which the interconnects are fabricated at these high deposition pressures. These impurities can influence the electromigration process. The background pressures in MBE deposition systems is on the order of $10^{-9}$ to $10^{-10}$ torr. At these low background pressures there would be considerably fewer impurities introduced into the metal films during deposition.
The composition of the Al-Cu films can be determined from Auger analysis. The Perkin Elmer Model PHI-600 Auger microprobe located at RADC/RBRE was to be used for this purpose. One proceeds with these measurements as follows:

First, pure aluminum and pure copper films are grown. These films are used for the calibration of the Auger microprobe. Next, Cu-Al alloy films of various compositions are grown and Auger analysis of these films are performed. By comparing the Auger data of the pure aluminum and copper films with the auger data of the Cu-Al alloy films it is possible to obtain the composition of the alloy films.

This data can be correlated with the temperature of the Al and Cu evaporation sources in the MBE machine. Thus, by operating the sources of the MBE machine at appropriate temperatures, films can be grown with predictable compositions of Al and Cu. The film compositions can then be confirmed with Auger analysis. The uniformity of the films can, also, be obtained from Auger depth profile measurements.

Films grown with predictable compositions of Al and Cu can then be patterned into stripes by means of a photolithographic process. Chemical etching or the "Lift Off Method" can be used to pattern the films. Each of these methods might, also, have an influence on the electromigration properties of the films.

Chemical etching causes somewhat rugged edges on the film stripes. The roughness of the edges of the film stripes will influence the electromigration properties of the Al-Cu alloy films, since voids and hillocks tend to accumulate at imperfections in the
leads. Nucleation centers for both forming voids and the aggregation of migrating material might form at various corners of the rough edges of the film stripes.

The Lift Off method yields film stripes with much smoother edges. Thus, stripes fabricated with the Lift Off method will have different electromigration properties than chemically etched films.

2. CONSTRUCTION OF THE MBE MACHINE

An old Auger instrument was converted to an MBE machine. This involved the design, construction and testing of a source holder, evaporation sources, a liquid nitrogen filled shielding chimney, and redesign of the sample holder stage.

The source holder consists of a central 1.25 inch diameter seven inch long liquid nitrogen tank surrounded by six pie section shaped source chambers. A 3.25 inch outside diameter stainless steel tube forms the outside surface of the source chambers. The plates that separate the pie section chambers are cooled by conducting the heat to the liquid nitrogen in the central tank. The source holder is mounted on a standard 6 inch diameter conflat flange. Two tubes that are mounted in a vacuum insulated feedthrough penetrate through the flange. The tubes are used to fill and vent the liquid nitrogen tank.

Each source chamber has a door located opposite the end that is nearest to the flange. The door serves as a shutter for each source. Each shutter is actuated by a rod. Each rod has a turn buckle for length adjustment. It also has a flexible coupling. The rods protrude through the flange. Bellows are used as vacuum seals for
the rods. The bellows allow linear motion to be transmitted into the vacuum chamber. Thus, the shutters can be opened and closed from outside the vacuum chamber. The shutters are actuated by pneumatic cylinders mounted in a frame that is fastened to the outside of the flange. A pneumatic control panel with pneumatic single pole, double throw switches was also fabricated.

The sources are fused quartz bottles that contain the material to be evaporated. The opening of the source bottles face the shutters. The source bottles are surrounded by tungsten filament coils. Each filament coil is surrounded by a fused quartz tube. The source assemblies are located in the pie shaped source holder sections. The source holder flange is mounted on a six way cross, and the source holder is located inside the six way cross. The flange of the six way cross that is opposite the source holder flange is mounted at the rear of the main vacuum chamber of the converted Auger apparatus. The other flanges of the six way cross carry electrical and thermocouple feedthroughs for the sources.

The liquid nitrogen cooled shielding chimney consists of a cylindrical liquid nitrogen tank. It can hold about one liter of liquid nitrogen. The inside diameter of the chimney is 3.25 inches to match the source holder. It covers the path length from the evaporation sources to the substrate on which the films are to be deposited. This chimney serves to protect the main vacuum chamber of the Auger apparatus from contamination by the material evaporated from the sources. Two flexible stainless steel tubes and a twin lead liquid nitrogen feedthrough serve to supply liquid nitrogen and to vent the chimney.
The original sample holder assembly of the Auger apparatus was rebuilt. It consists of a carousel with six cylindrical sample carrier sockets with horizontal faces that are, normally, parallel to the tangent planes of the carousel. The carousel turns about a vertical axis. The sample carrier sockets have threaded holes that receive the sample carriers. The sample carriers on which the samples are mounted are screwed into the sockets. Each sample holder socket pivots about a horizontal axis parallel to a tangent of the carousel. The sample holder socket faces are vertical when facing the front of the main vacuum chamber of the Auger apparatus and the load lock. The sample loading arm grips the sample carrier. It transports the sample carrier from the load lock to the carousel. The arm is also used to screw the sample carrier into the sample holder socket. After the sample carrier is secured to the sample carrier socket the arm releases the sample carrier.

When the carousel is rotated ninety degrees the sample carrier sockets are tilted 30 degrees about a horizontal axis, parallel to the tangent of the carousel, to face the Auger sensors. By rotating the carousel another ninety degrees the sample carrier sockets are tilted back to a vertical position to face the deposition sources which are located at the back of the main vacuum chamber. All this had to fit into the rather small main vacuum chamber of the Auger apparatus.

Due to delays in the construction schedule in the RADC machine shop the MBE machine could not be completed by the time this project had ran its scheduled course.
3. THEORY OF ION MOTION IN A FILM STRIP

A simple equation of motion of a migrating ion in a film strip can, perhaps be described, as follows:

\[ m \ddot{x}_\mu + D \dot{x}_\mu = Z e E_\mu(x,y) - \frac{(B/6)J_\mu (x,y)}{\epsilon_0 (x-x_m)^4 + (y-y_m)^4 + \Delta}^{5/4} \]

\[ \mu = 1, 2 \]

where \( x_\mu \) is a position vector component of the ion, \( m \) is the mass of the ion, \( D \) is and effective frictional force due to scattering of the ion, \( Z \) is the level of ionization, \( e \) is the charge of an electron, \( E_\mu (x,y) \) is a position dependent electric field vector component in the film, \( B \) is a dimensionless constant describing the electron drag on the ions, \( \sigma \) is the conductivity of the metal, \( J_\mu(x,y) \) is a position dependent electron current density component in the film, \( G \) is a constant associated with the force that tends to keep the ion in their lattice positions, \( \epsilon_0 \) is the dielectric constant of free space, and \( x_\mu m \) is a component of the position in the lattice of the \( m \) ions.

The charge \( e \) is positive for positive ions and negative for negative ions. The first term on the left side of the equations of motion describe the inertial reaction of the ions, the second terms on the left side describe average frictional terms due to scattering of the ions, the first term on the right side describe the electrostatic forces on the (charged) ions, the second terms on the right describe the average electron current drag on the ions, and the last term on the right side is the force that tends to keep the ions in their lattice positions.

We assume that the contribution of the slow moving ions to the total current in the film is negligible. Thus, the current in the film
is assumed to be entirely due to electrons. We assume the following form for the electron current density:

\[ J_{\mu} = \alpha \mu g(x,y)(I/w) \]  

where \( g(x,y) \) is the dimensionless local fractional density of ions, \( I \) is the total current in the metal strip, and \( w \) is the width of the metal stripe. This assures that in voids, where the ion density is equal to zero, the current density is also equal to zero. We can, for simplicity, assume that the electric field and current density of the electron current are described by Ohm's law. We, therefore, assume the following form for the electric field in the film strip:

\[ e \mu = \frac{(J_{\mu}/\sigma) - (Ae/e_0)(x_{\mu} - x_{\mu n})}{[(x-x_n)^2 + (y-y_n)^2 + \Delta]^3/2} \]  

where the sum is over the imperfections in the film. Here \( A \) is a dimensionless constant associated with the ion-impurity interaction and \( x_n \) and \( y_n \) designate the position of the \( n \) imperfections in the film. The quantity \( \Delta \) assures that the electric field at the imperfection does not become infinite.

We shall use a numerical method to solve for the motion of the ions. This requires that we express the first and second derivatives of the position vector of the ion as first and second differences:

\[ x_{\mu} = \frac{(x_{\mu k+1} - x_{\mu k})}{\Delta t} \]  
\[ x_{\mu} = \frac{(x_{\mu k+1} - 2x_{\mu k} + x_{\mu k-1})}{(\Delta t)^2} \]
where $\Delta t$ is a time increment.

By substituting equation 3-2 into equation 3-3 and equations 3-4 and 3-5 into equation 3-1 and solving for the youngest term of equation 3-1 we obtain:

$$E_{ukm} = \hat{\alpha}_u [g(x_{km}, y_{km})/\sigma] -$$

$$(Ae/\varepsilon_0)(x_{km} - x_{kn})/[(x_{km} - x_n)^2 + (y_{km} - y_n)^2 + \Delta]^{3/2} \quad (3-7)$$

and

$$x_{\mu(k+1)m} = [2 + (d\Delta t/m)]x_{\mu km} + [1 + (D\Delta t/m)]x_{\mu(k-1)m} +$$

$$[\Delta t^2 /m][ZeE_{\mu km}(x_{km}, y_{km}) - \hat{\alpha}_u g(x_{km}, y_{km})(B\varepsilon_0/\omega) +$$

$$[G\varepsilon^2(\Delta t)^2/m\varepsilon_0](x_{ukm} - x_{um})/[(x_{km} - x_m)^4 + (y_{km} - y_m)^4 + \Delta]^{5/4}$$

$$\quad (3-8)$$

where the subscript $k$ designates the time $t = \Delta tk$, the subscript $m$ designates the $m$'th ion and $\sigma = 3.541 \times 10^7$ Siemens per meter is the conductivity of aluminum.

The local fractional ion density $g(x_{km}, y_{km})$ is assumed to be equal to the fraction of ions present at any given time $\Delta tk$ in the area belonging to a lattice site divided by the total number of ions in a rectangle with the length of a lattice site in the $x$ direction and the width $w$ of the total strip in the $y$ direction.

The following assumptions were made:

1. Values for the constants are $m/D = 100$ seconds, $A = 1$, $B = 0.5$, $G = 10^{-14}$ m$^2$, and $\Delta = 10^{-18}$ m$^2$.

2. The atoms are singly ioned, that is $Z = 1$.

3. The metal stripe consists of a single layer of ions.
4. Initially the ions are located at their grid positions, that is 
\[ x_{om} = x_m, \quad y_{om} = y_m. \]

5. The initial velocities of the ions are equal to zero, that is 
\[ x_{lm} = x_{om}, \quad y_{lm} = y_{om}. \]

6. The three dimensional nature of the films can be simulated by letting many ions occupy the same position.

Both \( x_{(k+1)m} \) and \( y_{(k+1)m} \) are calculated by an iterative method. The resulting positions of the first calculation are used to calculate the position after the second time interval and so on. This calculation can be performed for different currents \( I \) in the film strip of width \( w \).

We cannot, of course, follow every ion in the film. However we can assume a grid of ions located in a portion of the film that we shall analyze, see Fig. 1. We also assume a number of imperfections located in the film. We assume that the applied electric field \( E_{Ox} \) is in the \( x \) direction. A number of imperfections is assumed at random locations in the array of ions in the film strip.

![Fig 1](image)

**Fig 1.** An array model of 25 x 10 atoms in a metal film stripe of width \( w \). The randomly located imperfections are marked by stars.
We observe that the net effect of the electron drag, the applied field and the field due to an imperfection can dislocate some atoms. This is similar to the Franz Keldish effect where an electron is freed from a trapping state with the aid of an electric field. These ions then drift and accumulate around another imperfection leaving voids in some places after some time as shown in Fig. 2. It is interesting to compare Fig's 1 and 2. If we would let the situation progress further we would observe that the voids move. Thus, this model seems to agree, at least qualitatively with the observed data.

Fig 2. The progress of the ions after 160 time steps. Voids are shown by stars.

This result does not seem to depend strongly on the exact nature of the various forces experienced by the ions. We previously used a different model for the electron drag component and obtained similar results. Equation 3-8 represents basically two coupled difference equations with a nonlinear potential term and contains
both an "acceleration" and a "velocity" dependent "loss" term. The
difference equations used in various fractal models are usually of a
similar nature. Of course, the numeric coefficients and the
nonlinear potential terms differ case to case. Thus, one would
expect that the results, at least qualitatively, do not differ greatly
by changing the nonlinear potential somewhat.

4. FILM GROWN IN HYDROGEN RESIDUAL GAS

We have grown Al films in a conventional vacuum system having
a typical vacuum of 10^{-6} Torr at Syracuse University. We flushed
the vacuum system three times with a gas mixture of 20% hydrogen
and 80% nitrogen before each film deposition. That is, we evacuated
the vacuum system to about 10^{-4} torr and refilled the system with
the 20% hydrogen-80% nitrogen to a pressure of about one torr. We
repeated this procedure three times. The last time we pumped the
system out to 10^{-6} torr before refilling it with the combination of
gases.

The purpose of using hydrogen as the residual atmosphere in the
vacuum system is to reduce the oxygen in the residual atmosphere in
the vacuum system and in the deposited Al film. Indeed, in films
grown with this method no oxygen could be detected with Auger
analysis. About 20 Al films, each about 2 inches square in area
were grown. Some of the films were patterned into 10 μm wide
strips.
5. CONCLUSION

An old Auger apparatus was converted to an MBE machine, retaining the original Auger analysis equipment. Prototype Al-Cu alloy films were grown in a diffusion pumped vacuum system at Syracuse University. The vacuum system used was flushed three times with 20% hydrogen -80% nitrogen gas prior to film growth. This was done to provide a reducing residual hydrogen atmosphere in the vacuum system during film deposition. Films fabricated with this method did not contain detectable oxygen concentrations.
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