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Gold metallization for aluminum nitride

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Abstract

A metallization scheme for gold on AlN is investigated that incorporates three layers sputter-deposited in succession on the AlN substrate, without breaking vacuum: 20 nm of Ti to promote adhesion, a 100 nm thick Ti–Si–N barrier layer, and 230 nm Au. The stability of the scheme was studied after annealing in vacuum up to 800 °C for 30 min and at 400 °C in Ar ambient for 300 h, using 2 MeV $^4He^{++}$ backscattering spectrometry, sheet resistance measurements, and adhesion tests. It is shown that the incorporation of the diffusion barrier prevents the interaction of the Ti from the adhesion layer with the gold layer and thereby preserves the integrity of the metallization scheme. This metallization scheme may be applicable to other substrate materials.

Keywords: Gold; Metals; Aluminium nitride

1. Introduction

Aluminum nitride (AlN) offers an attractive alternative to alumina (Al_2O_3) as a substrate material for electronic packaging [1]. Its high thermal conductivity (200 W mK^{-1} [2]) and its thermal expansion coefficient (4.5×10^{-6} $°C^{-1}$ [2]) that closely matches that of silicon (2.5×10^{-6} $°C^{-1}$ [3]) result in minimal thermally induced stress and excellent thermal management for multichip modules as well as for advanced, high lead count, single chip packaging. Its better dielectric properties than those of alumina allow faster switching times, thereby making it possible to locate signal lines directly onto the AlN substrate.

Ground planes and interconnecting lines require a metallization of low electrical resistivity. This requirement is emphasized when high frequency signals are involved. The metallization should also be electrically and structurally stable and adhere even at elevated temperatures as packaging densities and heat dissipation demands are rapidly growing. Adhesion usually requires a reaction, while a reaction is not desirable when long-term stability is sought. Being contradictory in nature, it is practically impossible to satisfy both requirements with a metallization scheme that consists of a single layer. Gold is usually desirable because of its low resistivity, superior electromigration resistance, and inertness; but the latter property also deleteriously affects adherence. Combinations of gold as a top layer with a layer of a reactive element, e.g. Ti, to promote adhesion with the substrate have been widely studied [4–12] and are commercially applied [13]. These metallizations, however, are known to fail at temperatures between 300 and 400 °C [4–9] because the Ti adhesion layer reacts with the gold overlayer. When annealed in air, the affinity of oxygen with Ti acts as a Ti sink and titanium oxide accumulates at the surface. This process depletes the Ti layer and finally results in a loss of adhesion.

In this paper we show that a Ti\TiSiN\Au scheme improves the stability and adhesion of a gold metallization to AlN. The increased stability accomplished with this scheme is attributed to the presence of the $Ti_{27}Si_{20}N_{53}$ layer. This layer, originally developed as a diffusion barrier between silicon and Cu [14], is shown here to prevent the migration of Ti from the adhesion layer to the surface during annealing in an ambient of a nominally inert gas, thereby maintaining good adhesion at higher temperatures than the plain Ti\Au metallization tolerates.

2. Sample preparation and characterization

Polished AlN substrates with a roughness of less than 20 nm were obtained from The Carborundum Company. The substrates were cut into 8×8 mm^2 pieces, degreased in

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organic solvents in an ultrasonic bath (trichloroethylene, acetone, and methanol, sequentially) followed by an etch of 10 s in water-diluted HF etch prior to loading into the deposition chamber.

All films in this study were deposited by r.f.-sputtering using a planar magnetron cathode of 7.5 cm in diameter. The substrate plate was placed 7 cm below the target and was neither cooled nor heated externally. The sputtering system is equipped with a cryopump and a cryogenic baffle that yields a background pressure of 4×10^{-7} Torr prior to the sputter deposition. The different layers were deposited sequentially in the same chamber without breaking vacuum. They were all deposited at 10 mTorr total pressure and 300 W rms forward sputtering power. The Ti adhesion layers and the Au overlayers were deposited in Ar discharges. The Ti–Si–N films were deposited in a discharge of Ar/N_2 gas mixture. The flow ratio of N_2 to Ar (0.036) and the total gas pressure (10 mTorr) were adjusted by mass flow controllers and monitored with a capacitive manometer in a feedback loop.

Three sets of AlN samples were prepared: one set of AlN\Au(200 nm), another set of AlN\Ti(20 nm)\Au(200 nm), and a third set of AlN\Ti(20 nm)\$Ti_{27}Si_{20}N_{53}$(100 nm)\Au(230 nm) in which a $Ti_{27}Si_{20}N_{53}$ layer was introduced as a diffusion barrier between the Ti adhesion layer and the gold overlayer.

Of each of the first two sets, one sample was kept as reference and the others were annealed at 400 °C for 120 h (5 days). The heat treatment was carried out in an open-ended quartz-tube furnace. A nominally inert atmosphere was maintained by a gas flow fed directly from a cylinder of conventional-grade argon. Of the third set, one sample was kept as reference, others were annealed for 30 min at 600, 700, 750 and 800 °C in an evacuated tube furnace (5×10^{-7} Torr), or at 400 °C in Ar ambient for 300 h (12.5 days).

Before and after the thermal annealing, the samples were characterized by 2 MeV $^4He^{++}$ backscattering spectrometry to determine compositional profiles and monitor interdiffusion or reactions in the samples. The sheet resistance of as-deposited and annealed samples were measured at room temperature with a four-point probe. The thickness of the films were obtained from the widths of the corresponding signals in the backscattering spectra of the as-deposited films.

Adhesion tests were performed on all samples using a 3M 250 tape (40 g mm^{-1} adhesion strength). Two cuts down to the substrate in the form of a cross were made in the film using a sharp razor blade. The tape was then applied over the cut and afterwards removed by pulling at 180° (parallel to the surface) [15].

3. Results and discussion

Adhesion tests performed on the as-deposited samples gave good results for all the Ti-containing samples (sets #2 and #3). Poor adhesion was found only in AlN\Au sample (set #1).

Fig. 1(a) depicts the backscattering spectra obtained from samples of the first set where gold was deposited directly on the AlN substrate. No reaction is evidenced between the gold and the substrate after five days of annealing in Ar at 400 °C. However, the adhesion of the gold was so poor that it peeled off upon mere touching with tweezers. The sheet resistance decreases upon this annealing from 0.53 Ω/□ to 0.33 Ω/□.

Fig. 1(b) shows the backscattering spectra obtained from samples of the second set where a 20 nm thick layer of Ti is used to promote the adhesion of the gold film to the AlN substrate. Five days of annealing at 400 °C in an Ar ambient results in Ti diffusing through the gold overlayer to the surface and in a discoloration of the sample. This Ti migration also results in a partial loss of adhesion as the gold overlayer was partly removed when tested with Scotch tape. The same Ti diffusion was observed by Poate et al. [4] and by Speight and Cooper [5] in Ti\Au bilayers annealed in air and was explained by the creation of an oxidation sink for the Ti on the gold surface. This process results in an accumulation of TiO_x on the surface that should appear as a peak in the backscattering spectrum at the surface energy of Ti. The absence of this peak in our case can be explained by the small quantity

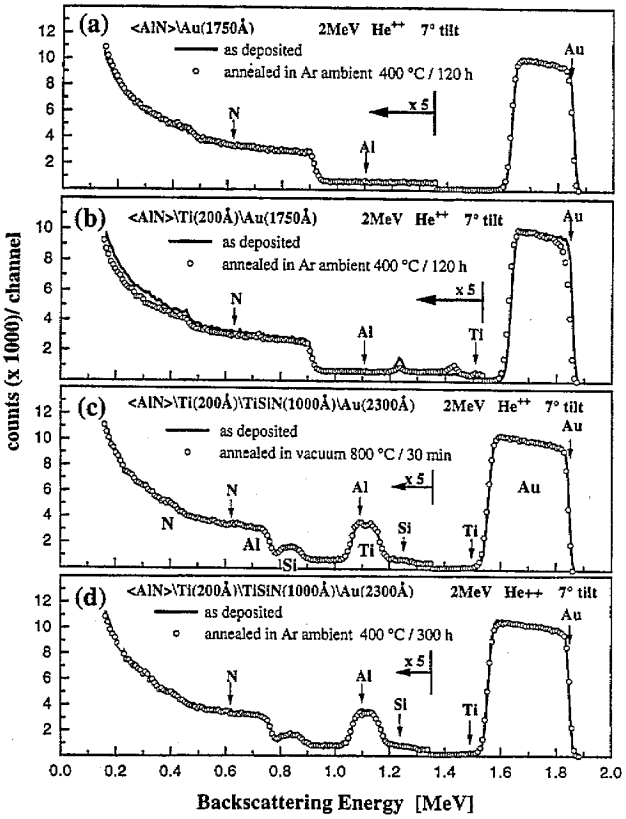

Fig. 1. 2MeV $^4He^{++}$ backscattering spectra: (a) AlN\Au sample before and after annealing in Ar at 400 °C for 120 h; (b) AlN\Ti\Au sample before and after annealing to 400 °C for 120 h; (c) AlN\Ti\TiSiN\Au sample before and after annealing in vacuum at 800 °C for 30 min; (d) AlN\Ti\TiSiN\Au sample before and after annealing in Ar at 400 °C for 300 h.

Table 1
Sheet resistance measured with a four-point probe and the calculated resistivity

Sample	Annealing conditions			Au layer	Sheet resistance		Adhesion	
	Temp. (deg.)	Duration (h)	Ambient	thickness (nm)	As-deposited (Ω/□)	Annealed (Ω/□)	As-deposited	Annealed
AlN/Au	400	120	Ar	175	0.53	0.33	bad	bad
AlN/Ti/Au	400	120	Ar	175	0.53	0.4	good	partial
AlN/Ti/TiSiN/Au	400	300	Ar	230	0.4	0.2	good	good
AlN/Ti/TiSiN/Au	600	0.5	vacuum	230	0.4	0.28	good	good
AlN/Ti/TiSiN/Au	700	0.5	vacuum	230	0.4	0.29	good	good
AlN/Ti/TiSiN/Au	800	0.5	vacuum	230	0.4	0.29	good	good

of Ti available for that process and the non-uniform distribution of the oxide on the surface. An indication of this non-uniformity is seen in the rounded top of the high-energy edge of the Au signal in Fig. 1(b). It is therefore evident that the use of a Ti layer to promote the adhesion of gold to an AlN substrate is limited to low temperatures by the Ti migration process. The sheet resistance for this sample decreases from 0.53 to 0.4 Ω/□.

To reduce this migration, a 100 nm thick $Ti_{27}Si_{20}N_{53}$ layer was introduced between the Ti and the gold layers in the third set of samples. The resulting metallization scheme was first tested by annealing in vacuum (10^{-7} Torr). Fig. 1(c) shows that the backscattering spectrum of a sample annealed for 30 min at 800 °C exactly overlaps that of the as-deposited sample. The spectra of samples annealed in vacuum for 30 min at 600 or 700 °C yield the same overlap and are not shown. No diffusion or reaction is therefore evidenced by backscattering spectrometry upon vacuum annealing up to 800 °C, proving that the $Ti_{27}Si_{20}N_{53}$ layer acts as a barrier to the Ti transport. The sheet resistance decreases from the as-deposited value of 0.4 to 0.29 Ω/□ after annealing to 800 °C.

Backscattering spectra of the same metallization annealed at 400 °C in Ar ambient for 300 h contains no evidence of Ti diffusion (Fig. 1(d)). Adhesion tests done on samples annealed in vacuum or Ar show complete adhesion. No peeling of the layer is observed. This result, though qualitative, clearly demonstrates the benefit of incorporating the TiSiN diffusion barrier. The sheet resistance decreases from 0.4 to 0.2 Ω/□ after 300 h Ar annealing at 400 °C.

The sheet resistance and the results of the pull test are summarized in Table 1. The initial sheet resistance of all the as-deposited samples corresponds to a Au resistivity of 9.2 μΩ cm and much exceeds the resistivity of pure bulk gold (2.2 μΩ cm [16]). For this calculation, we assumed that the electrical current flows through only the Au layer and thus multiplied the measured sheet resistance by the thickness of the Au layer. This approximation is validated by the small amount of Ti present in comparison with Au, and the high resistivity of the barrier layer (1800 μΩ cm as-deposited and 1100 μΩ cm after 700 °C/60 min [17]). The high resistivity of the Au film may be accounted for by impurities introduced into the gold overlayer and its microstructure. The quantity of these impurities is too small to be detected by backscattering spectrometry.

In all cases the sheet resistance decreases upon annealing, but the amount of reduction differs. The differences can be explained by several possible mechanisms: (1) the grain growth upon annealing causes a reduction of the resistivity

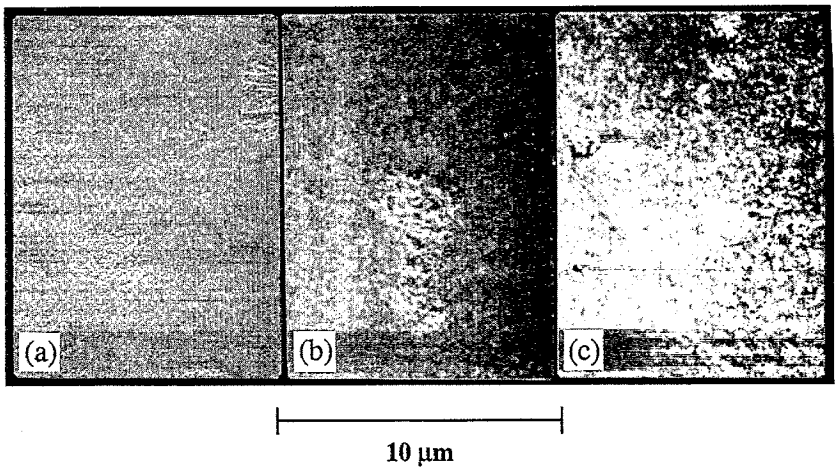

Fig. 2. Scanning electron micrographs (tilt angle, 45°) of AlN\Ti\TiSiN\Au samples before and after annealing in vacuum: (a) as-deposited; (b) annealed at 700 °C for 30 min; (c) annealed at 800 °C for 30 min. The patterns seen on the as-deposited sample manifest the roughness of the polished ceramic. After annealing in vacuum at 700 °C the surface become granular. The same granularity is found after annealing at 800 °C along with some hillocks and holes.

which may differ for the various cases; (2) the impurities may redistribute upon annealing; (3) Ti can react with the gold. In the AlN\Ti\Au reference sample the resistivity decreases, least upon annealing. This may be attributed to the presence in the gold layer of some Ti as it reacts or diffuses through the gold to the interface during the annealing. While some Ti will end up as TiO_x on the surface, some may remain in the gold and impede the resistivity lowering. The long annealing duration, favoring the growth of large grains, may be responsible for the lowest resistivity found in the AlN\Ti\TiSiN\Au sample.

Fig. 2 displays scanning electron micrographs obtained from samples as-deposited and annealed for 30 min at 700 and 800 °C in vacuum. A slight roughening of the surface morphology appears after annealing at 700 °C, while after 800 °C annealing the surface is disrupted locally by what appear to be holes and hillocks. Energy dispersive analysis of X-rays of these hillocks and holes reveals that they are composed of gold. Similar hillocks were observed by Kim and Hummel [11] on plain Ti\Au metallization annealed to 500 °C in air. The explanations given therein were: relief of stress that would be adequate to explain either the formation of holes or the formation of hillock, but not the appearance of both, and the tendency of the underlayer to oxidize. That latter cause should be of lesser significance for annealing in high vacuum. Hillocks in trenches were observed by Pokela et al. [18] for a <Si>\TaSiN\Au sample after annealing it for 30 min at 750 °C in vacuum. The area occupied by the hillocks and the holes is, however, too small to cause a visible change in the backscattering spectra.

4. Conclusions

We show that the incorporation of a 100 nm thick $Ti_{27}Si_{20}N_{53}$ layer as part of a Ti\$Ti_{27}Si_{20}N_{53}$\Au trilayer metallization scheme can suppress the diffusion of Ti to the surface or a reaction with Au during annealing in a conventional inert gas ambient, thereby preserving the adhesion and the integrity of the metallization scheme at a temperature of 400 °C at which the plain Ti/Au metallization fails.

The bond between the gold overlayer and the Ti–Si–N barrier layer never broke in our tests. This suggests the possible use of the Ti–Si–N\Au bilayer combination in conjunction with adhesion-promoting materials other than titanium, and substrates other than AlN.

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