Material Characteristics of Sputtered Ta and TaAl Thin Films Used in Thermal Ink Jet Devices

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Abstract

The materials properties of Ta and TaAl thin films are studied to better understand their behavior in the thin film heater stack used in bubble jet printers. For Ta films, the stress can vary dramatically depending on deposition conditions. Correlated with this stress variation are other morphological properties such as film structure and surface roughness, film density, modulus, and thermal expansion coefficient. The nature of the stress leads to different dry run failure modes for the devices. For the TaAl films, a broad maximum in the resistivity as a function of composition is observed.

Originally published in the *Proc. of IS&T's Tenth International Congress on Advances in Non-Impact Printing Technologies*, October 30-November 4, 1994, New Orleans, Louisiana.

Introduction

For thermal ink jet printer heads, thin films of tantalum and TaAl alloys play critical roles as the top overcoat and the heater material respectively. The Ta top layer is designed to provide several important functions: a protective barrier layer, a shock absorbing layer, and to some extent a thermal diffuser. The Ta layer is exposed to an extremely harsh environment, where it is subjected to attack from chemical, electrochemical, and cavitation-erosion processes, as well as repeated thermal cycling. To achieve the desired device lifetime, this layer must maintain its protective properties even after billions of heater fires. Equally important, is the stability of the heater material. The materials that are used to fabricate the thin film resistors in bubble-jet transducers must have stable and reproducible electrical and mechanical properties throughout the operation of the device. The most popular resistor materials that are currently in use for the resistor heaters are: sputtered TaAl alloys, heavily doped silicon, and sputtered HfB2. Each offers advantages and drawbacks but all of the heater thin films, typically 0.08 microns thick, are expected to survive billions of temperature cycles to 400 degrees C at heating rates of 10E8 C/sec. Given the extreme demands put upon both the top layer and the materials, it is essential to develop a thorough understanding of these materials by char-acterizing their properties. For the top Ta layer, it is known that stress can influence the adhesion, and this paper looks at the stress over a wide range of deposition parameters. For the heater materials, TaAl and HfB2 are generally not as well documented as heavily doped silicon. We present results for the TaAl system in particular.

The Ta Overcoat Layer Properties

It is well known that changing the deposition conditions can have a dramatic influence on the properties of metal thin films. For the Ta top, a crucial property is the film stress. The stress built in during deposition is the primary stress component for this Ta layer. If the film stress is too large, the films will either delaminate for films in compression, or crack and tear for films in tension. The stress level at which these failures occur depends on both the magnitude of the stress, and the thickness of the films. When the stress energy exceeds the elastic limit of the film, adhesion failure occurs. In the case of 1 micron films, the failure can occur at stress levels of about +/- 2000MPa.

The Ta films were deposited using an Innotec sputtering system in a DC magnetron configuration with a base pressure of about 10E-7 Torr. The sputtering gas was argon, and the substrates were 4" silicon wafers lying flat on platters held stationary below the targets. The crystallographic phase of the Ta films was determined using x-ray scattering, and was predominantly the desired beta phase. The thickness was measured across the disk, and observed to be uniform.

The stress was measured for Ta films sputtered onto silicon wafer substrates using a Flexus tool. This device determines the wafer curvature before and after film deposition and calculates the stress from the change in wafer curvature due to the film. Various deposition conditions were varied, including power, sputtering gas pressure, substrate bias, and sputtering time. The stress was observed to vary dramatically over an extremely wide range: -1500MPa (highly compressive) to +1500MPa (highly tensile). Even larger values appeared to result, however, for the thicknesses studied these films would delaminate and stress measurements were not possible. The conclusion is that the Ta overcoat is very susceptible to excessive stress if the deposition conditions are not properly controlled. Other Ta film properties were found to correlate with the stress, and varied with deposition conditions. In particular the film structure and roughness showed a strong correlation with stress. The highly tensile films exhibited large columnarmorphology of 50 microns in diameter, whereas for the highly compressive films, the columns were significantly reduced in size to about 10 microns in diameter. There is a gradually and monotonic variation from the large columns to the smaller, as the stress changes. Similar changes are observed for surface roughness. Again with the highly tensile films, the surface has greater roughness, and as the films go into compression, the surface becomes smoother. The RMS surface roughness in nanometers drops from about 3 nm for highly tensile films to less than 1 nm for moderately compressive films. There is some indication that at high compressive levels the surface roughness increases a little. The film density also correlates with stress. The highly tensile films have the lowest density at about 14.6 gm/cc, and this increases monotonically to about 16.5 gm/cc for the highly compressive films. Unlike these material properties, the Young's modulus peaks at zero stress, and slowly drops off with increasing stress (either tensile or compressive). The thermal expansion coefficient inversely follows the Young's modulus.

When dry run thermal failure tests of the Ta overcoats were performed on representative device structures, differences in the failure modes were observed depending on stress level and state. The highly tensile films would tear and crack, whereas the highly compressive films would blister. This difference in the nature of the failure is consistent with the type of stress. The low stress films were the most resistant to failure in this test.

Properties of the TaAl Heater Material

The TaAl films were also sputter deposited with the Innotec system onto 4" silicon wafers. In this case the platters would spin and rotate past the sputtering target, producing films with excellent composition and thickness uniformity. The standard deviation of the sheet resistance for four wafers in a typical deposition was 0.2% rms. The composition of the films was measured by Electron Microprobe Spectroscopy. The stress was again measured by the Flexus instrument. A composite target was used to cosputter the two metals. By varying the sputtering gas pressure, a wide range in composition could be achieved.

The electrical resistivity was found to vary with the composition, showing a very broad maximum between ratios of 1:2 and 2:1 for the two metals. For the films studied, the resistivity peaked at about 230 microohm-cm, and gradually dropped off to around 200 microohm-cm at the 20% and 80% levels. At the ends of the composition ranges (below 20% of either Al or Ta), the resistivity dropped below 200 microohm-cm.

The Ta rich films were measured to be in compression while the Al rich films were in tension. One reason for this effect could be that the thermal induced stress component of the Al rich films is large enough to drive them into tension on cooling from the deposition temperature. In other words, the Al rich films simply have a larger coefficient of expansion than the Ta rich films.

In addition to the resistivity, and stress, the stability of the microstructure was studied. In-situ Transmission

Electron Microscopy (TEM) was performed on films at the 2:1 and 1:2 ratios, i.e. films with compositions on the endpoints of the resistivity plateau. The films were studied in-situ during a 2 hour heating excursion from room temperature to 1200 degrees C. The microstructure was monitored both with micrographs and electron diffraction. The as-deposited films were confirmed to be amorphous. The Al rich films (1:2 ratio), were observed to stay amorphous up to about 650 degrees C. The other Ta rich films (2:1 ratio) were observed to stay amorphous up to 1200 degrees C, with no obvious change in microstructure. These observations are consistent with the phase diagram of the TaAl system.

Conclusion

The data presented in this paper offers additional evidence that both the Ta and TaAl films, with the proper deposition conditions and/or composition, are indeed good materials to use for thermal ink jet applications.