Defect dominated charge transport in amorphous Ta$_2$O$_5$ thin films


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(Received 23 December 1999; accepted for publication 11 April 2000)

Ta$_2$O$_5$ is a candidate for use in metal–oxide–metal (MOM) capacitors in several areas of silicon device technology. Understanding and controlling leakage current is critical for successful implementation of this material. We have studied thermal and photoconductive charge transport processes in Ta$_2$O$_5$ MOM capacitors fabricated by anodization, reactive sputtering, and chemical vapor deposition. We find that the results from each of these three methods are similar if one compares films that have the same thickness and electrodes. Two types of leakage current are identified: (a) a transient current that charges the bulk states of the films and (b) a steady state activated process involving electron transport via a defect band. The transient process involves either tunneling conductivity into states near the Fermi energy or ion motion. The steady state process, seen most commonly in films $<300$ Å thick, is dominated by a large number of defects, $\sim 10^{19}$ – $10^{20}$ cm$^{-3}$, located near the metal–oxide interfaces. The interior of thick Ta$_2$O$_5$ films has a substantially reduced number of defects. Modest heating ($300$–$400$ °C) of Ta$_2$O$_5$ in contact with a reactive metal electrode such as Al, Ti, or Ta results in interfacial reactions and the diffusion of defects across the thickness of the film. These experiments show that successful integration of Ta$_2$O$_5$ into semiconductor processing requires a better understanding of the impact of defects on the electrical characteristics and a better control of the metal–Ta$_2$O$_5$ interface. © 2000 American Institute of Physics. [S0021-8979(00)03514-3]

I. INTRODUCTION

The continued scaling of dielectric thicknesses for gate and memory in advanced complementary metal–oxide–semiconductor (CMOS) technology is pushing the tunneling limit of SiO$_2$. The thickness of the insulator needed for these applications could be reduced if a suitable material with a higher dielectric constant than SiO$_2$ ($\epsilon_r$$\sim$4) were available. One potential replacement for SiO$_2$, at least in some areas such as dynamic random access memory (DRAM) or embedded DRAM (eDRAM) capacitors, is Ta$_2$O$_5$ ($\epsilon_r$$\sim$23).

Ta$_2$O$_5$ has been actively investigated for more than 50 years and is an established dielectric material in discrete capacitors made from anodized, porous tantalum. Films of Ta$_2$O$_5$ (as opposed to anodized, bulk Ta) were first made by anodization of tantalum films. A comprehensive review of the anodized film literature can be found in the 1975 review by Westwood et al.$^1$ More recently, the potential use of Ta$_2$O$_5$ as a thin film dielectric material in silicon devices has promoted an even greater interest in this material. The preferred method for making films for device integration is by oxide deposition since this allows more flexibility in choice of electrode materials. A more recent review containing references to measurements of deposited Ta$_2$O$_5$ films, fabricated by both chemical vapor deposition (CVD) and physical vapor deposition (PVD) sputtered films can be found in an article by Channiere et al.$^2$

Successful integration of Ta$_2$O$_5$ into silicon devices requires a more detailed understanding of electron transport mechanisms in this material than is currently available. In particular, there has not been a detailed comparison of the performance of Ta$_2$O$_5$ films made by the various methods nor has there been a comparison of the number of defects in films made by different methods. Earlier studies of anodized films$^1$ report many of the features described in this article such as defect states in the band gap,$^3$–$^6$ reactive metal electrodes,$^7$ and transient conductivity,$^1$,$^3$,$^9$ but similar studies of deposited Ta$_2$O$_5$ films have not been made. This article addresses aspects of charge transport in Ta$_2$O$_5$ that are common to all processing methods (PVD, CVD, and anodization). We hope that this broad approach will allow us to gain a better understanding into the nature of Ta$_2$O$_5$ as well as the aspects of Ta$_2$O$_5$ that limit device performance.

II. EXPERIMENT

In this study we have characterized the charge transport in a variety of Ta$_2$O$_5$ thin films made by three different methods: PVD reactive sputtering, CVD, and anodization. None of the Ta$_2$O$_5$ films, regardless of the deposition method, showed x-ray diffraction peaks that would indicate long-range structural order. We note that short-range order on the scale of 10 Å has been reported for anodic Ta$_2$O$_5$ films.$^{10}$ The Ta$_2$O$_5$ films were grown between 100 and 1000 Å thick and studied in a metal–oxide–metal (MOM) geometry. We will use the words "thin" and "thick" to refer to films thinner or thicker than 300 Å. The base metal electrodes were continuous metal films of TiN, TaN, Ta, or Pt. For most of the results reported in this paper, 200-µm-diam circular top metal electrodes were applied in a separate vacuum sys-

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tem from the growth, using e-beam evaporation and a shadow mask. In a few cases, electrodes were applied using thermal evaporation through a shadow mask, sputter deposition through a shadow mask, or blanket metal deposition followed by photolithography. Top electrodes were composed of one of the following metals: Al, Ag, Au, Co, Cr, Cu, Pd, Pt, Ta, or Ti. In films intended for photoconductivity, the top electrodes were made thin enough to transmit 10%–50% of the light intensity. Separate depositions of the thin metal films onto quartz substrates were made to directly measure the absorption spectrum from each type of metal.

Anodized Ta$_2$O$_5$ was made from ~2000 Å tantalum films sputter deposited on silicon (100) wafers. The anodization was performed in 0.01 M citric acid solution with a platinum foil counter electrode. The wafer sections were only partially submersed in the solution, with electrical contact being made to the exposed section with a gold-coated copper clip. A constant current (~0.2 mA/cm$^2$) was applied to the samples until the desired voltage was reached. The samples were held at the final voltage for several hours before being removed from the bath, rinsed, and dried with compressed air. The thickness of the Ta$_2$O$_5$ layer is linearly related to the final anodization voltage with the proportionality constant being approximately 20 Å/V at room temperature. The thickness of each Ta$_2$O$_5$ layer, and its refractive index, were measured with a Rudolph Research AutoEL ellipsometer at 633 nm assuming zero extinction. The measured indices of refraction were 2.15 ± 0.05.

PVD films were grown by reactive sputtering from Ta targets using a pulsed-direct-current (dc) power supply (ENI Corp, RPG-50). The sputter gas was typically a 50/50 Ar/O$_2$ mixture at a pressure of 5 mTorr. Pulsed–dc reactive sputtering is more efficient than radio-frequency (rf) sputtering and avoids the target poisoning effects caused by an oxide growth on the target characteristic of dc sputtering. For many of the films, the bottom metal electrode and the top metal electrode were deposited in a separate vacuum system. For some films a complete metal–oxide–metal stack was grown in situ and a top electrode of Al was subsequently patterned by photolithography. Film properties were weakly dependent on the substrate temperature during deposition. Most Ta$_2$O$_5$ films were grown with the substrate at 300 °C and all films were grown in the range 25–550 °C. PVD films were measured with no postdeposition anneal. Thickness was monitored by ellipsometry as described above or by Rutherford backscattering spectroscopy (RBS).

CVD films were grown in a number of different reactors including a Novellus Systems Concept II, Applied Materials DCSxZ CVD chamber or Applied Materials HTF chamber. The film thickness was typically 100 Å and the process used either tantalum penta-ethoxide [Ta(OCH$_3$)$_5$] (TaTEO) or tantalum tetra(ethoxy)dimethylaminoethoxide [Ta(OC$_2$H$_5$)$_4$(OC$_2$H$_5$N(CH$_3$)$_2$] (TaTDMAE) as the precursors. The deposition temperature was 380–450 °C at a pressure of 3–10 Torr and a N$_2$–O$_2$ mixture as the carrier gas. As-grown CVD films are quite leaky and all CVD films underwent a postdeposition anneal. Typical annealing parameters were a down stream microwave plasma anneal at 300 °C in a 50% mixture of O$_2$ gas and N$_2$ gas for 2 min. The thickness was measured as above.

Electrical characteristics of the Ta$_2$O$_5$ films were studied as a function of electric field, time, temperature (100–500 K), and incident light energy (photoconductivity). Current voltage ($I–V$) data were taken in a constant voltage mode using a probe station shielded from ambient light. Typical $I–V$ curves were made by stepping the voltage and waiting 5–15 s before recording the current with a Keithley 6517 or a Hewlett Packard 4140B electrometer. Contact to the bottom electrode of the capacitor array was usually made by passing a large current through two capacitors to form a short. Voltages and fields are plotted with respect to the sign of the voltage on the top electrode. The terms ““forward”” and ““reverse”” bias refer to positive and negative voltages on the top electrode respectively in analogy with the $I–V$ characteristics of Schottky diodes. Temperature control was by a water-cooled, heated stage on the probe station capable of operation between 290 and 500 K or by a low-temperature probe station (MMR Technologies, Inc.) capable of operation between 100 and 500 K. Capacitance was measured using an Hewlett Packard 4192A impedance analyzer. Using the thickness derived from ellipsometry, the dielectric constant averaged 23±3 for films with nonreactive electrodes.

Photoconductivity measurements were made using an ISA SPEX TRIAX 180 0.19 m f/3.9 grating monochromator with either a 100 W tungsten–halogen or 30 W deuterium light source. Using three different gratings and filters for removing overlapping orders, we were able to cover the spectral range from 200 to 2000 nm with a spectral resolution between 7 and 28 nm. The optical output power spectrum was measured using calibrated silicon and germanium photodetectors. The monochromator output was coupled to the variable-temperature MMR probe station using either visible or ultraviolet (UV) fiber-optic bundles, and was focused on the sample to give a 1-mm-diam spot. The resulting photon flux incident on the sample varied from $10^{12}$ photons/cm$^2$/s at the UV end of the spectrum to greater than $10^{16}$ photons/cm$^2$/s in the infrared. The photocurrent at any particular wavelength was found to be linearly proportional to the incident photon flux. Therefore, at each wavelength the measured photocurrent per unit area was normalized by the corresponding photon flux and transmission of the semitransparent metal electrode to give photoelectrons per incident photon. The photocurrent was measured in both dc and alternating-current (ac) modes. The instrumentation for the dc mode was the same as used for the $I–V$ curves. The ac mode used a light chopper (4–50 Hz) with a Keithley 427 current amplifier acting as the preamplifier for a PAR HR-8 lock-in amplifier. The photoconductivity spectra was the same for either mode, but the ac mode provided a more convenient method to discriminate against the slowly varying transient dark current, which was found to be largely independent of light.

III. RESULTS

A. Thick films

Over the course of measuring the dark $I–V$ characteristics of numerous samples, we observed that the lowest leak-
Fig. 1. (a) $|J|$ vs $E$ for thick (1200 Å) PVD and anodized films measured 10–15 s after changing the voltage. Both films are in the transient regime over most of the range of measurement. The solid line is a scan that starts at $-2.5 \text{ MV/cm}$, proceeds to $+2.5 \text{ MV/cm}$, and back to $-2.5 \text{ MV/cm}$ to show the hysteresis. The cusps are where the current changes sign as shown in the linear-scale insert. (b) $|J|$ vs time for the anodized film. Data for charging and discharging using both forward and reverse bias are shown.

The explicit time dependence of the current is shown in Fig. 1(b) where the magnitude of the current at room temperature is plotted as a function of time after a 2.5 MV/cm electric field step using the 1200 Å anodized film shown in Fig. 1(a). The solid symbols are the current observed on charging the capacitor; the open symbols are current observed on discharging the capacitor. Both polarities of charging and discharging are included. The $RC$ time constant of the capacitor displacement current is much less than 1 s and is not a factor in these data. The time dependence is a power law, $J = \text{const} \cdot t^{-m}$, with $m = 0.92$ at room temperature as indicated by the solid line in Fig. 1(b). The reverse bias charging curve is roughly parallel to the discharge curves, but is slightly displaced indicating slightly more charge passes via the transient current on charging than on discharging. The forward bias charging curve has a shallower slope and an up-turn after $10^5$ s. We have seen this in multiple films and suspect that the up-turn is related to dielectric breakdown, but we have not investigated this phenomenon in detail. At elevated temperatures, typically 400–500 K, we have measured an exponent of the power law of about 1. We have observed that the power law persists to the smallest time interval we were able to measure (30 μs).

A consequence of the slow transient behavior is that one can freeze a polarization into a capacitor. For example, if one applies a field at high temperature, say 500 K, and cools in a field to room temperature, a subsequent warming at zero bias will result in substantial thermally stimulated current of the opposite sign of the polarization. This demonstrates that the transient current has a finite activation energy at temperatures above room temperature. Details of this transient behavior will be a topic of a future publication.

B. Thin films

A comparison of the thinnest films (~100 Å) made by the three different techniques are shown in Fig. 2, along with data from a commercial Ta$_2$O$_5$ anodized capacitor. For each deposition technique, the best example with the lowest leakage current was chosen. The top contact was Pt for all films with varying bottom electrodes as noted in the figure caption. Remarkably, despite the differences in how the Ta$_2$O$_5$ films were produced, the $I-V$ curves are similar with a diode-like, asymmetric shape. In reverse bias, all the films show relatively flat $I-V$’s and transient currents with about the same hysteresis as in the thick films. It is important for the top contact to be both nonreactive, and have a high work function in order to see transient current in reverse bias with thin films. In forward bias, there is a rapidly rising current with an exponential rise similar in shape to a forward biased Schottky diode. This current is not transient and is a true dc leakage current in the sense that charge is transported across the film. We will refer to this type of nonhysteretic current with a large field dependence as steady state current. These data and the thick film data shown above in Fig. 1 show that for the films we studied, the lowest leakage examples are
FIG. 2. $I-V$ curves for PVD, CVD, and anodized films of similar thicknesses plus a commercial anodized Ta$_2$O$_5$ capacitor (Kemet, Inc.). The dotted line shows the thick PVD film results of Fig. 1. Except for the commercial capacitor, all the films have a Pt top contact. The bottom contacts were Ta for the anodized film, TiN for the CVD film, and a Pt for the PVD film. The thicknesses and deposition temperatures varied as follows: (a) anodized film—110 Å, 25 °C, (b) CVD film—100 Å, 400 °C, and (c) PVD film—100 Å, 550 °C. The commercial capacitor (Kemet, Inc.) had a value of 1 mF and was rated at 4 V. Its thickness was estimated to be 200 Å from a measurement of the breakdown voltage (10 V), and its area was estimated to be 1000 cm$^2$ from the capacitance and an assumption of the dielectric constant ($\varepsilon_r$ = 23). The top electrode of the Kemet capacitor was MnO$_2$, formed at temperatures $>250$ °C, and the bottom contact was Ta. All scans start at zero bias with 15 s between points.

equivalent if one compares films with similar thicknesses and electrodes. This is a strong indication that the underlying physics of charge transport is the same in all films, regardless of the method of preparation.

The qualitative difference in the temperature dependence of the conductivity in the transient and steady state regimes is illustrated in Fig. 3 where the current as a function of bias is plotted for different temperatures. This is the same CVD film shown in Fig. 2, which was 100 Å thick with TiN bottom and Pt top contacts. The data were taken by using the loop scan shown earlier in Fig. 1(a). The $I-V$ scans start at $-1.5$ MV/cm, increase to $+1.5$ MV/cm, and return to $-1.5$ MV/cm. The cusps indicate current changing sign and highlight the hysteresis. Notice that the forward bias portion of the data has little or no hysteresis compared to the reverse bias. The temperature dependence of the forward bias current will be shown in more detail in Sec. III F. It is nonlinear on an Arrhenius plot but tends toward 0.75–0.9 eV at the high end of the temperature range we investigated (500 K).

C. General optical properties

The photoconductivity spectra consist of absorption from both the fundamental band gap (above 4.0 eV) and the defect-related gap states (below 4.0 eV). One point of this article is to relate the shape and magnitude of the defect photoconductivity spectra to the variations observed in the $I-V$ curves. However, since the photocurrent collection efficiency depends on the sample thickness and the dc bias voltage applied to the sample, we must use the magnitude of the band-gap photocurrent to normalize the intensity of the defect photocurrent. To linearly relate the magnitude of the defect photoconductivity to the band-gap photoconductivity, the photon energy of the normalization must be selected such that absorption in the film is less than 10% for all thicknesses considered. The photoconductivity spectrum is distorted above the band-edge region for films that are thick enough to substantially attenuate the light as it passes through the film.

To fully characterize the nature of the band-edge photocurrent, we measured the transmission spectrum of a 2000 Å PVD film deposited on a quartz disk. The resulting absorption coefficient is shown in Fig. 4 The theoretical curve in the figure is the absorption spectrum calculated from the power-law absorption edge typical of amorphous materials. The best fit to our data is for $n = 2.2$ and $E_g = 4.0$ eV in the expression

$$\alpha = \text{const} \cdot (E - E_g)^n / E^2,$$

where $\alpha$ is the absorption coefficient, $E$ is the photon energy, and $E_g$ is the band gap. This expression reduces to $n = 2$ if both band edges are parabolic, as is observed for many amor-
phous materials. To compare these results with the band-edge photocurrent, we have converted typical photocurrent data from a 110 Å anodized film into the absorption coefficient format by the relation

\[ \alpha = -A \cdot \ln(1 - I_{pb})/w, \]

where \( A \) is a constant to account for the photoelectron collection efficiency, \( I_{pb} \) is the photocurrent in electrons/incident photon, and \( w \) is the sample thickness. In the limit of small sample thicknesses, the photocurrent is proportional to the absorption coefficient. The best fit for the data in Fig. 4 is \( A = 12.8 \), implying that the maximum photoconductive yield (photoelectrons per absorbed photon) is \( 1/A = 7.8\% \) at the electric field of 0.7 MV/cm corresponding to this particular measurement. This yield is reduced by a factor of 2 if it is assumed that the light makes a double pass through the sample as a result of the reflective Ta substrate. Note in Fig. 4 that the photoconductive yield falls off approximately exponentially with photon energy above 4.7 eV, presumably due to the faster recombination or trapping rate of highly excited electron–hole pairs.

We find that the spectral shape of the band edge photocurrent is almost identical for similar thickness amorphous samples grown by PVD, CVD, and anodization. This is to be contrasted with the wide range of optical band gap values (3.9–5.28 eV) quoted for \( \text{Ta}_2\text{O}_5 \) in the literature.\(^5\) When we examine some of the cases where the optical absorption or transmission data are presented, however, we note that vastly different definitions of the band gap were used,\(5,12–14\) and the differences in the definitions account for the differences in the published values of the band gap. Using the definition in Eq. (1) and the published data, the range of band gap values reduces from 4.1 (thermal oxidation of Ta or \( e\)-beam evaporation of \( \text{Ta}_2\text{O}_5 \),\(^3\) 4.2 (polycrystalline CVD),\(^12\) 4.4 (anodized Ta), and 5.28 eV (amorphous CVD)\(^14\) to 4.1, 4.0, 3.8, and 4.3 eV, respectively. This corresponds to an average value from the literature of 4.05±0.18 eV, compared to our value of 4.0 eV.

In general, because of work function differences between the two metal electrodes, photocurrent can be observed at zero bias in thin films when the top electrode differs from the bottom electrode, indicating band tilting at zero bias. A measurement of the open circuit photovoltage (OCPV), the voltage at zero photocurrent, allows one to measure the work function offsets of the two metal electrodes. Zero photocurrent occurs when the bands of the insulator are flat. In the case of a Pt top electrode (work function \( \phi_m \sim 5.7 \) eV) and a TiN bottom electrode, the OCPV is about +0.7 V. The OCPV decreases as the work function of the top electrode is decreased and reaches zero when the top electrode is Ti or Ag (\( \phi_m \sim 4.4 \) eV). The swing in the flat band condition is about half the difference in the work function, indicating that the Fermi level of the top electrode is not completely pinned. For comparison, covalent semiconductors like GaAs or Si show little variation of the Fermi level pinning point with type of metal, whereas ionic materials like SiO\(_2\) show approximately a 1:1 scaling of barrier height with electronegativity.\(^15\) Since we only looked at the OCPV in films with a TiN bottom electrode, the swing in the flat band condition with top electrode metal does not establish whether or not the bottom electrode is pinned at the defect level. We will discuss this further in Sec. IV.

It is important to note that the photoconductivity of anodized films has previously been reported for a variety of electrode configurations.\(^1–6\) The results for the three types of \( \text{Ta}_2\text{O}_5 \) films studied here (PVD, CVD, and anodized) agree very well with the published anodized results when one takes the film thickness and the composition of the metal electrodes into account. No attempt was made to verify the observation of weak electroluminescence that also has been reported in the anodized \( \text{Ta}_2\text{O}_5 \) literature.\(^3\)

D. Defects and film thickness

In this section we will show how the dark conductivity and the photoconductivity scale with film thickness. We have illustrated that thick films show transient conductivity in both biases, while thin films show a diode-like \( I–V \) curve if the top contact is nonreactive and has a large work function like Pt. The transition from thick film behavior (transient conductivity) to thin film behavior (steady state conductivity) in the forward bias leakage as a function of film thickness is illustrated in Fig. 5. All films were produced by anodization and have a Pt top contact and a Ta bottom contact. The transition from transient to steady state current in forward bias occurs at approximately 300 Å.

The thickness dependence of the photoconductivity using these same samples is shown in Fig. 6. For optimum signal-to-noise ratio, the data were taken under conditions that minimized the dark current, yet still provided adequate photocurrent. The photocurrent is strongly field dependent. For thin samples, ample photocurrent could be achieved at zero bias due to the band tilting discussed above. For the thick films an applied bias was required to achieve enough signal. Typically, a reverse bias in the range 1–2 MV/cm was used to maintain a sufficiently small dark current. The photocurrent spectra were recorded at least 10 min after any dc voltage change; thus the transient dark current was only a small correction to the dc photocurrent and not present in the ac photocurrent. The data for a thick 620 Å film are plotted as-measured in Fig. 6 and the photocurrent from the remain-
ing films were normalized to equal the 620 Å film at 4.3 eV, where the absorption in the film is less than 10% for all cases. The normalization was always less than a factor of 2 and was necessary to account for differences in the overall photocurrent collection efficiency.

Comparing the data in Figs. 5 and 6 one can see that the dark current at 3 MV/cm increases by a factor of 10⁶ on going from thick Ta₂O₅ to thin Ta₂O₅; this is accompanied by a corresponding increase in the photocurrent at 3.0 eV by a factor of 10. The photocurrent as a function of film thickness is plotted in Fig. 7. The photocurrent varies approximately inversely with thickness as shown by the straight line. The below band-gap photocurrent is a measure of the number of defects averaged over the thickness of the film. These data suggest that the defects in the Ta₂O₅ films are located near the metal–insulator interfaces and that their density is vastly reduced in bulk Ta₂O₅. The transition from transient to steady state current in forward bias at approximately 300 Å suggests that the defect region is on the order of 150 Å, if we assume both interfaces are equivalent. Thus, the properties of thin films will be more dominated by these defects than thick films or bulk samples. This can also been seen by noting that the photocurrent data in Fig. 4 correspond to an absorption coefficient due to gap states in the 110 Å film of 100–1000 cm⁻¹ between 2.8 and 3.8 eV. If we were to extrapolate this level of absorption to the bulk limit, we would expect bulk Ta₂O₅ to be amber colored, whereas it is invariably transparent and colorless.

To confirm that the defect density is much greater in thin films than in bulk samples, we measured the transmission spectrum of a 750-μm-thick piece of bulk polycrystalline Ta₂O₅ in the visible spectral range. The sample was colorless but slightly cloudy due to scattering and had approximately 50% optical transmission between 0.8 and 3.5 eV, corresponding to an upper limit of 10 cm⁻¹ for the gap-state absorption coefficient. The transmission spectrum of the bulk sample was flat in the vicinity of the 2 eV feature seen in the thinnest films of Fig. 6. This means that if the same defects are present in the bulk film, the absorption is at least an order of magnitude lower, i.e., < 1 cm⁻¹ corresponding to a defect concentration < 10¹⁷ cm⁻³ in bulk Ta₂O₅. This upper bound of 10¹⁷ cm⁻³ defects in bulk Ta₂O₅ can be contrasted with the 10¹⁹–10²⁰ cm⁻³ defects we estimate in the following section for thin films.

E. Defects by heating with a reactive bottom electrode

We have shown that the electrical characteristics of films produced to date tend to be independent of how the film was grown if they have the same thickness. We have also demonstrated that the density of defects in the films scales as the inverse of the film thickness. Here we intentionally add defects to the film by heating a thick film in the presence of a metal electrode that can reduce Ta₂O₅. Anodized films are convenient for this experiment since the Ta/Ta₂O₅ interface will be blurred by oxygen diffusion into Ta. A second method of introducing defects is to use reactive top electrodes, such as Al, Ti, or Ta. This method will be explored in Sec. III F.

We showed in Fig. 2 that thick films show transient conductivity regardless of the type of metal used for the electrodes, and we demonstrated in Sec. III D that thick films have much less visible light photoconductivity than thin films. Figure 8 shows I–V curves of a 615 Å anodized film
pure tantalum foil. \(^{16}\) Other potential changes to the \(\text{Ta}_2\text{O}_5\) high suggesting few cancies brought about by heating \(\text{Ta}_2\text{O}_5\) in the presence of \(\text{Ta}\) consistent with the argument that the increase in oxygen vacancy versus the square root of the field. This steady state current is expected in a 615 Å film from Eq. 5.

The heavy solid line in Fig. 9 is a plot of the absorption lines of the thin samples and the heated thick samples. Figure 10 shows the photoconductivity for a 100 Å CVD film with a TiN bottom electrode, a 110 Å anodized film with a Ta bottom electrode, and a 170 Å PVD film with a Pt bottom electrode. A 615 Å anodized film after heating to 390 °C is also shown for comparison (from Fig. 9). All films had Pt top contacts. The spectra are normalized as in the previous photoconductivity figures and are comparable over the entire range. Note that due to low light intensity, the data in the range 3.2–3.9 eV are less accurate (as apparent from the scatter), so the differences in this region may not be significant. If we assume that the density of states giving rise to the band-edge absorption maximum above 4.5 eV is \(3 \times 10^{22}\) cm\(^{-3}\) (1 electron/Ta), the maximum defect density is about \(10^{20}\) cm\(^{-3}\). It is interesting that both the heated film and the as-grown thin films have about the same defect concentrations. This suggests that one can treat the defects as a region of constant defect density that occupies a fraction of the film thickness. As the thickness is changed, or the sample is heated, the fraction of the film occupied by the defects changes. Eventually a defect band is created that can transport charge across the film.

An interesting correlation can be made if we plot the fraction of the film occupied by the defects (measured by the photoconductivity) against the forward bias current taken from the \(I\text{–}V\) plots. Figure 11 shows such a plot. The \(x\) axis is the ratio of the photocurrent at 3 eV for various thicknesses or annealing temperatures to the maximum photocurrent at 3 eV from the 110 Å film of Fig. 6 or the 390 °C film of Fig. 9. This photocurrent ratio is a measure of \(x/w\), the fractional thickness of the film occupied by defects, if we assume that the defects are located in a region of constant defect density as described in the preceding paragraph. The \(y\) axis is the current density of the sample measured in forward bias at 3 MV/cm. Data are plotted for each of the samples in that was heated to various temperatures for 1 h in air, then cooled to room temperature, before the top Pt electrode was applied by \(e\)-beam evaporation. Notice that the heating produces a diode-like \(I\text{–}V\) with large currents in forward bias similar to the \(I\text{–}V\) curves of the thin samples shown in Figs. 2 and 3. The two samples heated to the highest temperatures, 390 and 325 °C, show steady state conductivity in reverse bias (at high fields \(E < -2\) MV/cm) as well as forward bias.

It is interesting to note that the forward bias current in these samples is roughly linear when plotted as \(\log[I]/(\log[|E|])\) versus the square root of the field. This steady state current is consistent with the argument that the increase in oxygen vacancies brought about by heating \(\text{Ta}_2\text{O}_5\) in the presence of Ta has resulted in enough defects to create a defect band across the thickness of the film. It is important to note that this heating technique, when limited to temperatures less than 400 °C, did not result in additional oxide growth at the Ta/\(\text{Ta}_2\text{O}_5\) boundary (to within the accuracy of ellipsometry measurements) consistent with results for anodized \(\text{Ta}_2\text{O}_5\) on pure tantalum foil.\(^{16}\) Other potential changes to the \(\text{Ta}_2\text{O}_5\) films from heating, such as the introduction of small crystalline inclusions,\(^{17,18}\) were not explicitly investigated but the overall uniformity of the annealed \(\text{Ta}_2\text{O}_5\) films remained high suggesting few (if any) pinhole type defects were introduced by the heating. The heated films showed no x-ray diffraction peaks, implying that any crystalline ordering was confined to length scales of order 50 Å or less.

Photoconductivity data from the same series of heated samples are plotted in Fig. 9. The data are normalized at the film with Pt bottom contact. The three thin sample were a 100 Å CVD film with a TiN bottom contact, a 110 Å anodized film with a Ta bottom contact, and a 170 Å PVD film with Pt bottom contact. The data for the thick film were taken from Fig. 9. The film was a 615 Å anodized sample with a Ta bottom contact that was heated to 390 °C before the top contact was applied.

Because of the diffusion of oxygen into tantalum and the creation of oxygen vacancies in \(\text{Ta}_2\text{O}_5\).\(^{16}\)

As can be seen from a comparison of Figs. 5 and 8, the \(I\text{–}V\) curves of the thin samples and the heated thick samples are very similar and suggest that the defect density may be approximately the same. Figure 10 shows the photoconductivity for a 100 Å CVD film with a TiN bottom electrode, a 110 Å anodized film with a Ta bottom electrode, and a 170 Å PVD film with a Pt bottom electrode. A 615 Å anodized film after heating to 390 °C is also shown for comparison (from Fig. 9). All films had Pt top contacts. The spectra are normalized as in the previous photoconductivity figures and are comparable over the entire range. Note that due to low light intensity, the data in the range 3.2–3.9 eV are less accurate (as apparent from the scatter), so the differences in this region may not be significant. If we assume that the density of states giving rise to the band-edge absorption maximum above 4.5 eV is \(3 \times 10^{22}\) cm\(^{-3}\) (1 electron/Ta), the maximum defect density is about \(10^{20}\) cm\(^{-3}\). It is interesting that both the heated film and the as-grown thin films have about the same defect concentrations. This suggests that one can treat the defects as a region of constant defect density that occupies a fraction of the film thickness. As the thickness is changed, or the sample is heated, the fraction of the film occupied by the defects changes. Eventually a defect band is created that can transport charge across the film.
Ta₂O₅ are shown in Fig. 12. In the figure, calculated free energies of reaction for a variety of metals with Ta is a reactive metal as observed in the previous section and trends predicted by Fig. 12 should be the same. Notice that thermodynamically should reduce the Ta₂O₅ film. The calculations assume that Ta₂O₅ is crystalline, which is more stable than amorphous Ta₂O₅, however we expect that the density of defects. The lines are guides to the eye.

F. Defects with reactive top electrodes

A second way to add defects to the Ta₂O₅ layer is to deposit reactive metals as the top electrodes, i.e., metals that thermodynamically should reduce the Ta₂O₅ film. The calculated free energies of reaction for a variety of metals with Ta₂O₅ are shown in Fig. 12. In the figure, ΔG’s were calculated for the reactions 5M+nTa₂O₅=5MO₃+2nTa at 600 K using HSC Chemistry software (Outokumpu Research, Pori, Finland). Work functions are from Sze. These calculations assume that Ta₂O₅ is crystalline, which is more stable than amorphous Ta₂O₅, however we expect that the trends predicted by Fig. 12 should be the same. Notice that Ta is a reactive metal as observed in the previous section and that Cr has borderline reactivity. These calculations predict that thin MOM capacitors with the reactive metals (metals with ΔG<0) are more likely to have oxygen vacancy defects in the oxide.

If the number of defects is sufficient to create a defect band, the I–V curves of samples with reactive metals as top electrodes should have qualitatively different I–V behavior than those made with nonreactive top electrodes. Data 100 Å CVD film of Ta₂O₅ are shown in Fig. 13. The different top metal contacts were all applied on a room temperature substrate through a shadow mask in an e-beam evaporation system. The I–V scans were taken with a delay of 5 s between points and start at the extreme negative field. The zero crossing cusps, seen in the scans made with Pt–Au, Co and Cu top contacts, indicate hysteresis and transient conductivity.

FIG. 11. The current at 3 MV/cm, taken from Figs. 5 and 8 plotted as a function of the ratio of the photocurrent at 3 eV to the maximum photocurrent at 3 eV (110 Å film of Fig. 6 or 390 °C film of Fig. 9). The photocurrent ratio is a measure of the fraction of the film thickness occupied by a high density of defects. The lines are guides to the eye.

Figs. 5 and 8. For both the annealing data and the data as a function of thickness the transition from transient conductivity to steady state conductivity (a change of about six orders of magnitude in current density) occurs over a narrow region of x/w of about 30%–40%. This is not a metal–insulator transition because the final state is not ohmic, but suggests it is a transition from conductivity by isolated defects to defect band conduction.

Photocurrent measurements of the samples from Fig. 13 are shown in Fig. 14. The results again divide into two groups, reactive and nonreactive top electrodes, but this time the film with CrAu is clearly in the reactive group. It should be noted that the data in Fig. 14 do not extend into the UV and thus are normalized to 1 near 3.5 eV. Samples with nonreactive top contacts (Ag, Cu, Co, Au, Pt) have the same photoconductivity as the thin samples shown in Fig. 10. Notice that the optical threshold for photoconductivity in Fig. 14 does not depend on the metal work function. This indicates that the photoconductivity (which is measured at zero or reverse bias) is not a result of internal photoemission from the top metal Fermi level to the conduction band.

FIG. 12. Calculated chemical stability of Ta₂O₅ with respect to potential metal electrodes.
Photoconductivity in samples with a reactive top contact (Al, CrAu, Ti, or Ta) are dramatically different. The signals are at least an order of magnitude higher and have a much lower onset, about 1.2 eV, consistent with earlier observations of a defect band.\textsuperscript{3,4} It is significant that the reactive samples have an onset that is less than half the 4.0 eV $Ta_2O_5$ band gap. To observe steady state photocurrent, it is necessary to have a conduction path for both the electron and the hole created by the light. In the case of band gap photoconductivity, the valence and conduction bands satisfy this condition. For isolated defects one requires two below-band-gap photons to excite the electron–hole pair to the conduction and valence band. For a defect band, one needs only to excite a carrier to the nearest band edge to create an electron–hole pair. In this case one half of the pair is in the defect band, while the other is in the valence or conduction band. This implies that the defect band is 1.2 eV from either the conduction or valence band. As we will show in Sec. IV B, the defect band is most likely near the conduction band.

The temperature dependence of the leakage current for two of these CVD samples is shown in Fig. 15. The two examples plotted are a film with nonreactive Co top contacts, and a film with reactive Ti top contacts. The closed symbols are the current in reverse bias while the open symbols are the current in forward bias. The data of Fig. 15 represent, for the most part, steady-state rather than the transient current. We know that transient current measured under these conditions is of order $10^{-8}$–$10^{-9}$ A/cm$^2$. Since the lowest current values in Fig. 15 approach these values, the lowest current points may be partially due to the transient response. Notice that in the sample with reactive Ti contacts and larger values of steady-state current, the temperature dependence is clearly non-Arrhenius. In all samples and for both signs of bias, the trend is toward an activation energy of 0.75–0.9 eV at low temperatures, the current is primarily steady-state and tends toward a 0.9 eV activation energy as indicated by the dotted line. At low temperatures, the current may have a transient component and the temperature dependence tends toward zero activation energy. The solid lines are guides to the eye.

FIG. 14. Normalized photocurrent from a 100 Å CVD film with different top electrodes for photon energies below 3.5 eV. The bottom electrode is TiN. The photocurrent spectra are different depending on whether the top contact is made of a reactive metal (Al, CrAu, Ti, Ta) or a nonreactive metal (Ag, Cu, Co, Au, Pd, Pt).

FIG. 15. The temperature dependence of the leakage current in a thin 100 Å CVD film with a TiN bottom contact and either Al (reactive, closed symbols) or Co (nonreactive, open symbols) top contacts. At high temperatures, the current is primarily steady-state and tends toward a 0.9 eV activation energy as indicated by the dotted line. At low temperatures, the current may have a transient component and the temperature dependence tends toward zero activation energy. The solid lines are guides to the eye.

expect that the reverse bias Co data would show an up-turn if the temperature were taken higher.

IV. DISCUSSION

The $Ta_2O_5$ MOM capacitors that we studied showed two types of charge transport, transient and steady state. Transient conductivity is, to first order, insensitive to light but steady state dark conductivity can be correlated with the observation of defect states in the gap by photoconductivity. These two types of charge transport appear to be independent, but potentially they could result from the same type of defect in $Ta_2O_5$. We will discuss each type of charge transport in detail and speculate on the types of defects that might give rise to these phenomena.

A. Transient conductivity

Transient conductivity showing a power-law current relaxation is a well-known phenomenon in insulators. It goes by several names including dielectric relaxation\textsuperscript{20} and either Curie-von Schweidler\textsuperscript{21} or Kohlraush\textsuperscript{22} behavior. Transient conductivity has been reported numerous times in $Ta_2O_5$ anodized films.\textsuperscript{1,8,9} It is a well-known feature of perovskite-type ferroelectric oxides\textsuperscript{23–29} and has been reported in anodic $Al_2O_3$\textsuperscript{22} and evaporated $SiO_2$.\textsuperscript{30,31} In the ferroelectric materials, the transient behavior has been attributed to proton motion,\textsuperscript{22,32} and indeed, proton transport in $Ta_2O_5$ has been demonstrated by the construction of an electrochromic device.\textsuperscript{33} An electronic mechanism of transient conductivity ferroelectric oxides involving hopping of charge carriers between defect pairs has also been proposed.\textsuperscript{21} Transient conductivity is usually identified as a property of disordered or amorphous films, but numerous examples of transient conductivity of approximately the same magnitude can be found in polycrystalline films.\textsuperscript{26,27} Transient conductivity is not observed in bulk, single-crystal ferroelectrics.\textsuperscript{21,24} The transient current in epitaxial $Pb(Zr,Ti)O_3$ is insensitive to above band gap light,\textsuperscript{34} in agreement with our observations for $Ta_2O_5$. 

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We find, in agreement with the results cited above, that the characteristics of transient conductivity are slow power-law time decays and hysteresis, both of which are only weakly temperature dependent below room temperature. For example, a Ta₂O₅ film cooled to 100 K has nearly the same hysteresis as that observed at room temperature. Above room temperature there is a finite activation energy associated with transient conductivity as revealed by the observation of thermally stimulated current following cooling the samples from 500 K in a field. When measured 5–15 s after applying a field step of about 0.1 MV/cm, transient current is typically of order 10⁻⁹–10⁻⁸ A/cm². The time dependence of the current scales approximately as a power-law, \( J = \text{const} \times t^{-m} \), where \( m \) is approximately 1, over the entire range of accessible times, \( 3 \times 10^{-5}–10^{3} \) s. Transient current has the same sign as the displacement current of a capacitor, but is much slower. Instead of charge residing on the metal electrodes, some charge bleeds into the bulk of the film over times much longer than the displacement current relaxation time \( (RC) \). Transient conductivity reported in the literature for both Ta₂O₅ and other dielectric materials is remarkably similar to the results we report here. Polycrystalline (Ba,Sr)TiO₃ films have a nearly identical transient response,²⁷ while a range of prefactors for the \( t^{-m} \) power law is reported for other perovskites.²⁴

Transient conductivity has little temperature or field dependence compared to steady state conductivity, therefore it is only visible under those conditions where the steady state conductivity is small. We have found two situations where transient current is easily observed. One example is a thick film where the defect band does not extend across the film. In this case, transient current will be the only current observed, independent of whether one has a reactive or a non-reactive electrode.

The second example where transient current is observed is in thin films where the top electrode of the capacitor has a large work function like Pt. In thin films the defect band extends across the film as evidenced by the large current in forward bias and the large number of defects seen in the gap by photoconductivity. If the top electrode work function is large, however, a Schottky-type barrier exists between the defect band and the metal electrode. This situation is schematically illustrated in Fig. 16 where we show the energy diagram of a thin Ta₂O₅ film with a Pt top electrode. In forward bias, current can flow via the defect band, but in reverse bias, the barrier afforded by the larger Pt work function results in too few thermally activated carriers for current via the defect band. Instead charge bleeds into the bulk of the film into states near the Fermi level, and the same transient current observed in thick films is observed. It should be noted that in the thin samples studied here, regardless of the bottom electrode material, steady state forward bias leakage is always observed. This suggests that the Fermi energy of the bottom metal is pinned at the defect band as drawn in Fig. 16. This is discussed further in Sec. IV B. Neither the mechanism nor the sign of the carriers of transient conductivity is presently understood.

There are two possibilities, electronic and ionic. In the electronic model the transient conductivity results from hopping or tunneling conductivity into deep electronic traps near the metal Fermi energy. The power law decay of the current on charging or discharging a Ta₂O₅ capacitor is consistent with hopping over barriers with a distribution of heights or tunneling into states with a distribution of distances. The weak temperature dependence of the transient conductivity may be evidence that tunneling is the charge transport mechanism and it also indicates that the charge tunnels into states located near the metal Fermi level. If the transient conductivity is electronic in origin, however, one would expect that these defects would be emptied or filled by UV light, contrary to what we observe. We note that there are exotic examples of deep traps that are strongly coupled to the lattice where filling or emptying the trap moves the energy of the trap out of the band gap. The result is a photobleaching effect where the trap in one charge state is light insensitive.³⁵

A simple explanation for the lack of response of transient conductivity to UV light is that the current comes from ion motion as has been previously suggested for Ta₂O₅ and ferroelectric materials.²²,²⁹,³⁶ The choices of possible ionic species here include, among others: \( \text{H}^+, \text{O}^{2-}, \text{Ta}^{5+}, \text{Na}^+ \) (or other alkali impurities). Clearly \( \text{Ta}^{5+} \) and \( \text{O}^{2-} \) species are mobile at room temperature at the breakdown field because that is how anodic films are formed. During the anodization process, \( \text{O}^{2-} \) ions move toward the Ta/Ta₂O₅ interface while \( \text{Ta}^{5+} \) ions move toward the Ta₂O₅/electrolyte interface. The ratio of the oxygen/tantalum mobility during anodization is about 2:1.³⁷ However, the problem of the ion description of transient current is the small value of the activation energy. There are examples of ion motion with low activation energies such as the motion of interstitial ions,³⁸ but the examples are few. The low activation energy rules out all ionic.

FIG. 16. Schematic energy diagrams of the defect band in Ta₂O₅ showing zero, forward and reverse bias. The defect band is located about 1.2 eV below the conduction band. The Fermi level of the bottom electrode is shown pinned at the defect band. In forward bias, steady state conduction occurs via an activated process within the defect band. In reverse bias, if the top electrode has a large work function as depicted here, there are not enough carriers to allow conductivity via the defect band. Instead, transient conductivity occurs via isolated states near the top electrode Fermi level.
species with the possible exception of protons.

While the transient and steady state currents clearly have different mechanisms of charge transport, the two types of current could be different manifestations of the same defects. For example, if the transient mechanism is electronic, the isolated states near the Fermi level could be the tail of the same distribution that produces the defect band. If the transient conductivity is ionic, a possible scenario is that the defects themselves are charged and move in a field. A precedent for this type of model is the redistribution of interstitial Cu in Si by an electric field. Finally we note that metal–oxide–semiconductor (MOS) capacitors have been a useful tool to probe mobile charge species in SiO₂. However MOS capacitors using Ta₂O₅ on Si are difficult to fabricate and interpret due to the parasitic SiO₂ at the interface. Si is marginally stable in contact with Ta₂O₅ as shown in Fig. 12. This reaction may be kinetically inhibited since measurements show that Si/Ta₂O₅ is stable to 830 °C.

Our experiment with TiN or Ta as a bottom electrode. Our observation of a zero open circuit photovoltage in the case of all reactive top contacts suggests that the top and bottom contacts are pinned at the defect band interface. The reason why the bottom Pt/Ta₂O₅ interface should have more defects than the top Ta or Pt interface is not clear. We have made preliminary observations that Fermi level pinning may be influenced by the surface roughness of the bottom electrode. With better film synthesis, it may be possible to form a Pt/Ta₂O₅/Pt structure where neither metal is pinned and the current is transient for both signs of bias regardless of the film thickness. It is important to note that the observation that the bottom Fermi level is pinned near the defect band means that the activation energy in forward bias does not come from a Schottky type barrier where the metal Fermi level is below the defect band. Instead, the observed activation energy results from an charge transport within the defect band.

B. Steady state conductivity

Steady state conductivity is clearly electronic in origin due to the large magnitude of the currents involved. Two experiments indicate that the charge is predominately carried by electrons. First, we have observed that changing the top electrode to a metal with a larger work function generally decreases the leakage current in reverse bias. This is consistent with electrons being the dominant charge carrying species. In a second experiment, we heated a 615 Å anodized film before applying the top contacts (Fig. 8) and observed that the forward bias leakage current increased 6 orders of magnitude. In this case we know that heating has altered the bottom interface because no top metal contact is present during heating. The increase in current in forward bias is again consistent with electron emission from the bottom electrode.

We now turn to the nature of the barriers at the top and bottom interface. A sketch of a band diagram that is consistent with our findings for a thin film with a Pt top electrode is shown in Fig. 16. The top interface is the most straightforward to interpret. Changing the top metal clearly changes the open circuit photovoltage indicating varying amounts of band tilt at zero bias due to differences in the electrode work functions. The change in the flat band condition when changing from a Pt top electrode to an Ag top electrode is about half the change in the work function. Neither of these metals is expected to remove oxygen from the oxide. Therefore, in reverse bias, nonreactive top electrodes have a thermal barrier to electron conduction via the defect band and thus one observes predominately transient conductivity. In the case of a Pt top electrode, the Pt Fermi level is 0.7 eV below the defect band.

We have less data on changing the bottom electrode. Our films all had TiN, TaN, Ta, or Pt bottom contacts. Ta creates oxygen defects, so one might expect that the metal Fermi level is pinned near the defect band. TiN and TaN are nonreactive, but both may have similar work functions to Ta, so one does not necessarily expect a change in barrier height by using these metals as bottom electrodes. Pt, on the other hand, has a large work function and is not reactive. If the bottom Fermi level is free to move as is the case on the top, a Pt/Ta₂O₅/Pt MOM capacitor should have the same thermal barriers and low leakage currents in both directions. Instead the I–V curve on the thin PVD capacitor with a Pt bottom electrode (Figs. 2 and 10) shows the same shape of the I–V curve and the same photoconductivity as all the other capacitors with TiN or Ta as a bottom electrode. (We have not made a similar symmetric Pt/Ta₂O₅/Pt capacitor using CVD.) From this we conclude that the Fermi level of the bottom electrode is pinned at the defect band as depicted in Fig. 16 because of the large number of defects at the bottom interface. The reason why the bottom Pt/Ta₂O₅ interface should have more defects than the top Ta or Pt interface is not clear. We have made preliminary observations that Fermi level pinning may be influenced by the surface roughness of the bottom electrode. With better film synthesis, it may be possible to form a Pt/Ta₂O₅/Pt structure where neither metal is pinned and the current is transient for both signs of bias regardless of the film thickness. It is important to note that the observation that the bottom Fermi level is pinned near the defect band means that the activation energy in forward bias does not come from a Schottky type barrier where the metal Fermi level is below the defect band. Instead, the observed activation energy results from an charge transport within the defect band.

One can also use the behavior of MOM capacitors with reactive metal electrodes to show that transport within the defect band is via an activated process rather than band conduction. A reactive metal top electrode such as Al or Ti on a thin MOM capacitor results in a symmetric I–V curve with high current in both directions as shown in Fig. 13. An identical result can be obtained if one heats a thick anodized film with reactive Ta top and bottom electrodes. Our observation of a zero open circuit photovoltage in the case of all reactive top contacts suggests that the top and bottom contacts are pinned at the defect band. Despite the fact that there are no Schottky barriers at either the top or the bottom interface, the electric field dependence is not ohmic (see Sec. IV C) and the temperature dependence has the characteristic “hockey stick” shape of Fig. 15. This suggests that the temperature dependence is a characteristic of defect band transport, not the interface.

Finally, it is important to clarify the evidence suggesting that the defect band is near the conduction band rather than near the valence band. The photoconductivity of samples with reactive electrodes (Fig. 14) indicates that the onset of photocurrent is below half the band gap indicating that a defect band has formed about 1.2 eV from the conduction or valence band. We also know from the measurements of the open circuit photovoltage that in films with a Pt top contact, the Fermi level is approximately 0.7 eV below the defect band. This argues in favor of the defect band being near the conduction band as shown in Fig. 16. If the reverse were true, there would be about a 0.5 eV barrier for hole emission from Pt with positive bias on the top metal giving rise to significant forward bias leakage currents in thick films, con-
C. Charge transport in the defect band

The influence of impurities and native defects on charge transport in semiconductors is a mature field that has received a great deal of attention. In the case of insulators, one typically extends the simplest semiconductor models by assuming that the traps have coulombic potentials, which give screened hydrogen-like wave functions in the effective mass approximation. The best-known theory for trap-dominated transport in an electric field is the Frenkel–Poole model. The location of the defect band near the conduction band is also consistent with local density approximation (LDA) calculations of Sawada and Kawakami who find that localized oxygen vacancies in Ta2O5 create a defect state 0.8 eV below the conduction band. If one allows that LDA generally underestimates the band gap by 50%, these calculations are consistent with our measurement of 1.2 eV and previous measurements of 1.5 eV.

V. CONCLUSIONS

We have identified two types of charge transport in Ta2O5 thin films—a steady state current that comes from a large number of defects that are located near the metal–oxide interface and a transient current that results in power-law current decays and hysteresis. We conclude that the steady state current is associated with oxygen vacancies since we observe that heating the oxide film next to a reactive metal such as Ta increases both the steady state conductivity and the number of defect states in the gap. A similar increase in the steady state current and the defects can be observed if one deposits a reactive metal such as Al, Ti, or Ta as a top electrode. Steady state current occurs by means a defect band located about 1.2 eV below the conduction band. Transport within the defect band is temperature and field dependent and can be qualitatively described using the model of phonon-assisted tunneling.

Transient conductivity is best observed in the absence of steady state conductivity. The power-law current decay is a well-known phenomenon in metal–oxide films, however, the mechanism is not well understood, either here or in the literature. Ionic mechanisms have been proposed, and are supported by our observation that transient conductivity is insensitive to above band gap light. However, the ionic models do not explain the weak temperature dependence of the transient behavior below room temperature. It is also not clear whether or not the mechanism of transient conductivity is coupled to the same type of defect that gives rise to steady state conductivity.

ACKNOWLEDGMENTS

The authors would like to especially acknowledge frequent and detailed conversations with R. J. Cava, G. A. Thomas, D. R. Hamann, B. Vyas, K. A. Ellis, J. J. Krajewski, S. M. Zahurak, and P. B. Littlewood. We would also like to acknowledge encouragement and help from M. A. Alam, J. D. Bude, P. W. Diadato, J. P. Chang, K. Chu, C.-T. Liu, L. Manchanda, D. P. Monroe, R. L. Opila, L. F. Schneemeyer, T. S. Siegrist, L. Stirling and C.-Y. Sung. We thank R. S. Roth for providing the bulk Ta2O5 used for the absorption measurement.