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PECULIARITIES OF TIME-DEPENDENT-DIELECTRIC BREAKDOWN CHARACTERISTICS OF PURE AND DOPED TA_2O_5 STACKS

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Abstract. *The effect of both the process-induced defects and the dopant on the time-dependent-dielectric breakdown in Ta_2O_5 stacks is discussed. The breakdown degradation is analyzed in terms of specific properties of high-k stacks which make their dielectric breakdown mechanism completely different from that of classical SiO_2. The relative impact of a number of factors constituting the reliability issues in Ta_2O_5-based capacitors (trapping in pre-existing traps, stress-induced new traps generation, the presence of interface layer at Si and the role of the dopant) is clarified*.

Keywords: *high-k stack; doped Ta_2O_5; Weibull distribution; hard breakdown*

1. INTRODUCTION

A considerable progress has been made in understanding the electrical and material properties of a number of high-*k* dielectrics, and the main purpose for their implementation in nanoelectronic devices (low leakage current for equivalent oxide thickness below about 1 nm) has been achieved. In order to fulfil also the criterion of dielectric reliability assurance, a deeper physical understanding of the dielectric breakdown (DB) mechanisms in these films is required. A special focus at present is on doped and multicomponent high-*k* dielectrics as a new step in high-*k* alternatives engineering. A little is known on the processes which are forerunners of the BD events in high-*k* stacks, on the effect of dopant in constituting the pre-existing traps and their impact on the BDs. The specific feature of high-*k* dielectrics, charge trapping, fundamentally defines the reliability of high-*k* stacks and dictates the allowed operating voltage for 10 years lifetime requirement.

The dielectric reliability is typically denoted by charge Q_{bd} or time t_{bd} to breakdown, and an important aspect of this reliability is the voltage dependence of these entities. It is generally accepted that MOS devices are required to work constantly for about 10 years. Increased voltage and temperature are commonly used to accelerate the breakdown pro-

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cess, since waiting for 10 years to measure failure would not be possible. One approach for understanding the high-*k* degradation mechanisms is using indirect methods such as those based on data for stress-induced leakage current (SILC) [1]-[5]. Essential disadvantage of this approach is the fact that SILC appears long before the breakdown events. Whatever the specific approach is, however, a correct way for obtaining adequate picture of the voltage dependence of the dielectric BD is to collect data with great experimental statistics using Q_{bd} and t_{bd} as variable entities. It was suggested that the degradation mechanism in high-*k* dielectrics is dominated by an "extrinsic" mechanism in contrast to so called "intrinsic" BD which is not related to process-induced or other extraneous defects. The intrinsic reliability, typically assigned to SiO_2, is a material property and it is sufficiently well understood. Having in mind the inherent property of high-*k* insulators to be a trap-rich materials the behaviour of the early (extrinsic) failures is very important for these dielectrics. Due to the strong trapping phenomena, however, the relation between the BD and SILC as a forerunner of BD known for SiO_2, could be no longer valid in high-*k* films and BD can occur without occurrence of any significant SILC and vice versa – a significant SILC can be created before the high-*k* dielectric is broken down [6]. So the pre-existing traps were identified as responsible for the domination of extrinsic BD mechanism in these films. Since the parameters of each high-*k* dielectric are a function of both its chemical composition and the fabrication process [3], [5], [7]-[11], Time-Dependent-Dielectric Breakdown (TDDB) characteristics are difficult to model from fundamental dielectric properties point of view. This circumstance hampers the interpretation of the degradation mechanism of a certain high-*k* film by analogy to another one. This imperatively means that the BD processes have to be studied individually for each high-*k* film. It is expected that from the acquisition of many experimental data some fundamental pattern could be found. On the other hand, the studies of BD characteristics of these dielectrics are strongly complicated by their double-layer structure due to the presence of inevitable lower-*k* interface region at Si, i.e. the film has to be treated as stacked layer. So the complexity of high-*k* materials defines entirely different mechanism causing BD from that in SiO_2, and the models developed for SiO_2 can not be easily implemented. Moreover, field acceleration models are not applicable and it is more correct to use voltage acceleration approaches.

This work addresses issues such as hard BD, the effect of traps on the breakdown characteristics of both pure and doped Ta_2O_5, and the role of the dopant in these processes. Ta_2O_5 is a leading high-*k* dielectric for storage capacitors in dynamic memories. The doping of Ta_2O_5 results in improved stack characteristics [5], [8], [12]-[14] allowing further scaling of equivalent oxide thickness (EOT), and in terms of leakage current and dielectric constant aspects the effect of various dopants is somehow clarified. Our previous studies [5], [8], [13], [14] revealed that the doping improves the overall electrical characteristics of the stack through a compensation of oxygen vacancies in Ta_2O_5. At the same time, the dopant initiates the generation of specific traps which affect the current behaviour during electrical stress.

2. EXPERIMENTAL PROCEDURE

P-type (100) Si wafers were used as substrates and MIS capacitors with pure, with lightly Al-doped Ta_2O_5, and with Hf-doped Ta_2O_5 were prepared. Ta_2O_5 film was depos-

ited by reactive sputtering of Ta target in an Ar + 10% O_2 mixture. Details on the deposition conditions are given elsewhere [15]. Al-doped Ta_2O_5 layers were deposited by rf sputtering of Al/Ta alloy target (5 at.% Al content) in Ar + 10 % O_2 atmosphere following the procedure described previously [16]. Hf-doped Ta_2O_5 was deposited on the Si as it is described in [17], (~ 0.7 nm thick Hf layer was deposited by sputtering on the top of ~7.5 nm rf sputtered Ta_2O_5). Post-deposition annealing was carried out at 400°C in pure N_2 ambient in order to mix Hf and Ta_2O_5 and to ensure diffusion of Hf into te matrix of Ta_2O_5.

The films are amorphous according to X-ray diffraction analysis, and the basic physical and electrical properties of the doped films have been reported elsewhere [5], [13], [17], [18]. The results suggest that the doping tends to create shallow traps which mediate the charge transport in doped films thereby changing the dominant conduction mechanism as compared to the pure Ta_2O_5. The overall thickness of the films including interfacial layer determined ellipsometrically is 7-8 nm (the interfacial layer is SiO_2-like one with a thickness of ~ 1 nm). The capacitors with back side electrode of 300 nm evaporated Al and sputtered W top electrode with gate area of $1x10^{-4}$ cm^2 were defined by photolithography. W was chosen as a metal gate on account of its good chemical stability on Ta_2O_5-based films. A post-metallization annealing was performed in a forming gas at 450°C for 1 h. The electrical stress response of the capacitors is investigated by monitoring the BD statistics of leakage current dependence on time. Constant voltage stress (CVS) with a negative bias on the top electrode (gate injection) is applied to study the TDDB characteristics. The applied voltage is kept constant and the change in the current density J is monitored as a function of the stress time, t_s. A breakdown event is defined as a sudden and distinct increase in the current; the t_s increases until the current exceeds 1 μA. Hard breakdown (HBD) is taken as a BD criterion. Every t_{bd} – BD data point at 63.2 % value (t_{63}) is obtained from Weibull distribution of 40 samples.

3. Results and Discussions

The time-to-breakdown t_{bd} is statistically distributed and is described by the Weibull distribution: $F(t) = 1\text{-}\exp(-t/t_{63})^{\beta}$, where F is the function of cumulative fraction of failed devices; t denotes the variable of time-to-breakdown; t_{63} is the characteristic time for 63.2 % of the devices to fail, β is the shape factor of Weibull distribution (Weibull slope). Plotting the Weibull function in the form W=ln[-ln(1-F(tbd))] vs. ln t_{bd} yields a straight line with a slope β, which entity is a measure for the BD behaviour. The dielectric quality reflects on the value of β: for nearly perfect SiO_2, $\beta > 1$ in the intrinsic region where the breakdown is an inherent property of SiO_2. The high-k dielectrics possess large density of electrically active defects which enhance the dielectric failure. In dependence on the nature of defects, their density and stress conditions including the measurement temperature, the slope of Weibull distribution could be lower or higher than 1.

3.1. Pure Ta2O5 films [19]

The capacitors are stressed at voltages between -3 and -3.5 V until BD, with 40 samples for each voltage, allowing for an accurate extraction of the statistical parameters, (for stress voltages more negative than about -3.7 V, the time-to-breakdown is extremely short and accurate characteristics can not be obtained); t_{bd} is defined as hard breakdown occurs. There

is a correlation between t_{bd} and leakage current J_0 in the initial samples: devices with low J_0 break later than those with high one. Fig. 1 shows the Weilbull distributions of capacitors under various V_s at room temperature. The distribution is with a slope of β at high percentiles higher than that at low ones. This is due to the coexistence of extrinsic and intrinsic modes: the tendency of β to be smaller at low percentiles is typically observed for the extrinsic/intrinsic BD modes. There is no visible dependence the steeper slope to be observed at higher V_s implying that the BD is not accelerated by V_s. The explanation could be sought in the presence of process-induced defects in Ta_2O_5 which hamper the manifestation of well pronounced stress-voltage dependence of β. In the short time range β is ~ 0.3, in the long time one the slope is steep, i.e. a separate detection of early and long-time BD is visible, and the region with very small Weibull slope proceeds to a higher-slope distribution. The early BDs are considered as a result of weak localized regions formed after critical number of traps. When discussing Weibull distribution of high-*k* stacks, a number of factors must be considered. The Weibull slopes are limited by the structure and chemical composition of both the interface layer and the bulk high-*k* layer. Therefore, the values of β should be defined by mechanisms of degradation of these two sublayers. The effect of interface layer is essential due to the high electric field across this layer. This layer is physically thinner than the Ta_2O_5 and is exposed to high electric field due to its lower dielectric constant. A part of the voltage drop across the interface region during the stress will drop across the Ta_2O_5 after interface degradation. Considering the double-layer structure of the high-*k* film the early breakdowns are assigned to extrinsic BDs, whereas *the breakdowns caused by the interface layer itself could be defined as intrinsic BDs*, since the presence of the interface layer is an inherent property of high-*k* stack. The defined by this way intrinsic BD explicitly includes the effect of interface layer and its BD. So all early breakdowns with t_{bd} from 10 to ~ 10^3 s, are related to extrinsic BDs and they characterize weak spots in the films. Their amount is small and the main fraction of failures are actually with t_{bd} ~ 10^3-5×10^4 s. The observed difference in β values for early and intrinsic BDs can not be due only to statistical effects and seems to be additionally related to the strong effect of interface lower-*k* layer at the Si which not only triggers BD but influences its Weibull distribution.

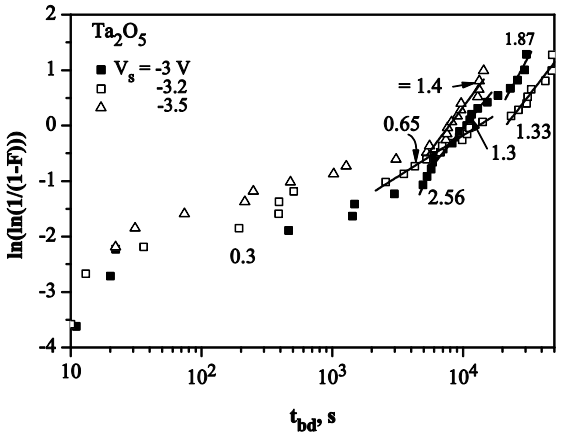

Fig. 1 TDDB Weibull distribution of Ta_2O_5 capacitors under different stress voltages. The values of Weibull slope are given

Ultimately, the low Weibull slope values typically observed in high-*k* stacks even in the regions considered as intrinsic BD, are assigned to low critical defect density needed to cause BDs. β value, however, has been involved to explain single SiO_2 layer BD rather than double-layer high-*k* stack. The observed quite lower values of β in the region of long t_{bd} for Ta_2O_5 than SiO_2 films with the same physical thickness means that the percolation model developed for SiO_2 does not seem to apply to Ta_2O_5 layers. So we can anticipate that β values even in this t_{bd} region correspond to the fact that the BD distribution is basically controlled by process-induced defects forming weak spots which are randomly distributed. From the other hand, if the BD is caused by stress-induced traps and the percolation model for SiO_2 is valid for high-*k* Ta_2O_5, β is proportional to the number of traps which form a conducting path. Thus, the lower β values of Ta_2O_5 mean lower number of stress-induced traps (as compared with SiO_2 with the same physical thickness) which constitute the BD [20]. This is only possible if the trap radius is significantly larger than in SiO_2. Thus, the use of percolation concept directly results in low critical trap density with very large trap radius at BD. Therefore, a reason for the relatively low Weibull slopes in the range of $t_{bd} \sim 10^4$ s could be a large effective radius of defects involved in BD events [21]. As is seen, the percolation approach for Ta_2O_5 stacks can be accepted only if we assume the small critical defect density at breakdown combined with large spacing between defects where tunneling of trapped electrons becomes probable, and this leads to a small Weibull slope. If we consider, however, EOT of Ta_2O_5 (2.2 nm) instead of its physical thickness, β values in the range of long t_{bd} ($> 2\times10^3$ s) are generally in accordance with those of ~ 2 nm SiO_2 layer ($\beta \sim 1$ [22]), and consequently the percolation model could be used for Ta_2O_5. To complete the discussion of TDDB characteristics we examine the curves whose t_{bd} is close to 10^4 s, (Fig. 2). If the percolation model is valid the curves should be shifted to the left with increasing $|V_s|$, i.e. V_s acts as an acceleration factor for BD. This is fulfilled for V_s = - 3.2 and -3.5 V. The position of the data for V_s = -3 V does not correspond to the percolation concept. This means that the mechanism of degradation in this case is quite specific and the extrinsic explanation seems reasonable. We speculate that the TDDB characteristics with $t_{bd} \sim 10^4$ s, at V_s = -3 V are attributed to the activation of pre-existing traps during the stress and these traps presumably dictate the current behaviour. The physical nature of the involved traps are oxygen vacancies (typically ob-

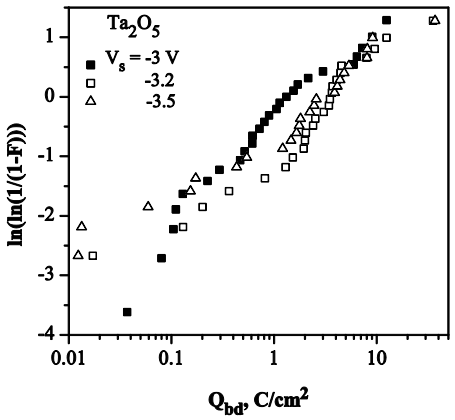

Fig. 2 Charge-to-breakdown distribution for Ta_2O_5 devices under CVS

served in Ta_2O_5) and gate-deposition induced defects during sputtering of W electrode. In opposite, new traps generation dominates at higher V_s, the dielectric quickly goes on to HBD, and V_s is an acceleration factor for BD. The generation of new defects (a formation of the percolation path) could additionally depend on the local field produced by the initial traps. Accordingly, this would affect the way of formation of the conductive path(s). So to all appearance both the pre-existing traps and the new traps generated affect the region with long t_{bd}: at V_s = -3 V dominate extrinsic failure modes and at -3.2; -3.5 V percolation concept appears to more accurately describe the results.

Charge to breakdown Q_{bd} is a more effective tool than t_{bd} for evaluating the generated defect density per injected electron. The Weibull distribution of Q_{bd} is shown in Fig. 3. The Q_{bd} is obtained by the integral of the leakage current over time ($Q_{bd} = \int_0^{t_{bd}} Jdt$), so all current bursts are considered. The Q_{bd} values are 1.3 C/cm^2 at 63.2 % failure of Ta_2O_5 for V_s= -3 V and comparable ones (3.6 C/cm^2) for the stress biases of -3.2 and -3.5 V, (63.2% are the percents corresponding to ln[-ln(1-F)] = 0). Accordingly, a higher Q_{bd} is obtained at larger stress voltages. The higher Q_{bd} means lower defect generation rate. The behaviour of Q_{bd} confirms that the mechanism of degradation for V_s = -3 V is different from that for -3.2 and -3.5 V. In the former case the trapping at pre-existing traps dominates, entails the appropriate conditions for BD, and the effect of V_s as a factor for generation of new traps can not be observed. There is no relative change of the current at BD which could constitute well defined Q_{bd}. In terms of t_{bd} this means that the time needed to create the local increase of current resulting in BD event has not a certain value. The reason is the dominant effect of weak spots. This makes the use of the current variation just before BD as a measure for evaluating the rate R_{gen} at which defects are generated and the defect density N_{bd} required to cause BD, strongly unreliable. The long BD times and the evidence of weak spots could be interpreted with an impact of both the process-induced defects and the interfacial layer on the BD behaviour. Therefore, the results demonstrate that *the picture for BD in Ta_2O_5-based capacitors is quite complicated. The origin of BD is not the same as that in single SiO_2* which is expectable, having in mind the double-layer structure of Ta_2O_5 films on Si. The role of weak spots is essential in BD behaviour, but

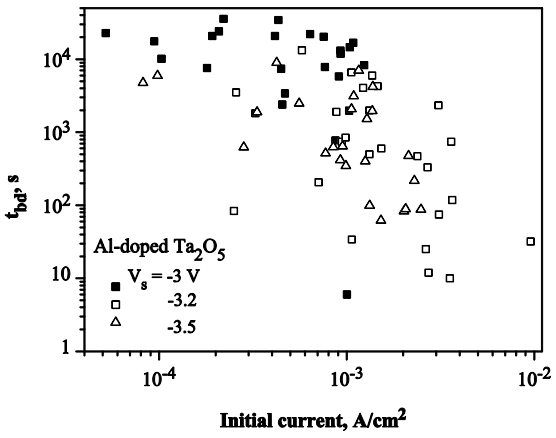

Fig. 3 t_{bd} vs. initial current in Al-doped Ta_2O_5 devices for different CVS levels

the other factors such as the quality of interface region and its thickness homogeneity could not be discarded as a contributing factor especially in the so called "intrinsic" BD.

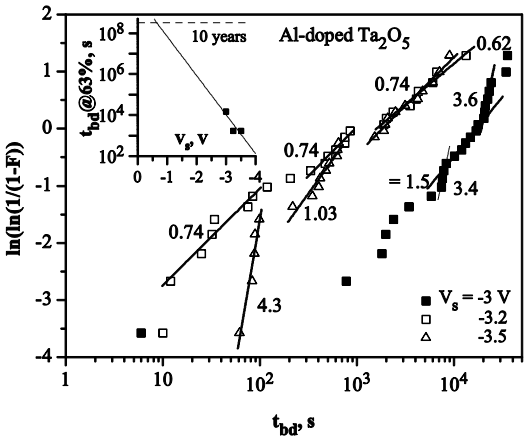

Fig. 4 Weibull distributions of t_{bd} at various stressing voltages for Al-doped Ta_2O_5 capacitors. The inset shows the t_{63} values vs. stress voltage

3.2. Al-doped Ta2O5 [19]

The BD occurs a little faster for the doped layers (EOT = 1.5 nm) as compared to the Ta_2O_5, i.e. it emerges that the presence of Al speeds up the breakdown. t_{bd} depends on both the bias stress and the initial current of capacitors (Fig. 3): t_{bd} is smaller at larger V_s and larger initial current. The observed multimodal BD distribution (Fig. 4) with varying slope for given V_s suggests the presence of extrinsic failure caused by processing defects. The slope of the curves for t_{bd} over ~ 10^3 s is due to intrinsic BD in terms of high-k stacks defined above. Quite high β values of doped films for t_{bd} ~ 10-10^3 s, (up to β = 4.3, against β ~ 0.3 for undoped films) indicate that Al effectively reduces some of the defects in Ta_2O_5. Nonuniform distribution of weak spots causes a variation in t_{bd} and leads to variation in Q_{bd} as well (Fig. 5). Q_{bd} at 63.2 % failure is 10.5 C/cm^2 when V_s = -3 V, and Q_{bd} values are equal (2.1 C/cm^2) after stressing with -3.2 and -3.5 V. Compared to the Ta_2O_5, the Q_{bd} values are quite larger in the former and smaller in the latter case, respectively.

The curve for V_s = -3 V for doped films shifts to the right resulting in a reasonable behaviour of Q_{bd} as a function of V_s, i.e. Q_{bd} is reduced at higher stress voltage which means higher defect generation rate at higher $|V_s|$ for the doped sample if the percolation model is valid. This behaviour is in contrast to the case of Ta_2O_5 and implies that Al significantly affects the defects defining the BD at V_s of -3 V. Compared with the Ta_2O_5 the Q_{bd} and TDDB characteristics for the doped samples are improved which means lower charge trapping. The maximum voltage to guarantee a 10 years lifetime is found to be -0.65 V for Al-doped Ta_2O_5 (inset of Fig. 4, t_{bd} values at 63.2% are plotted vs. V_s). It was not possible to extract accurately the operating voltage for 10 years lifetime for Ta_2O_5 due to the very small variation of t_{63} with V_s (Fig. 1). The doped capacitors are also better than Ta_2O_5 ones in life-time scaling due to the larger β value of the former.

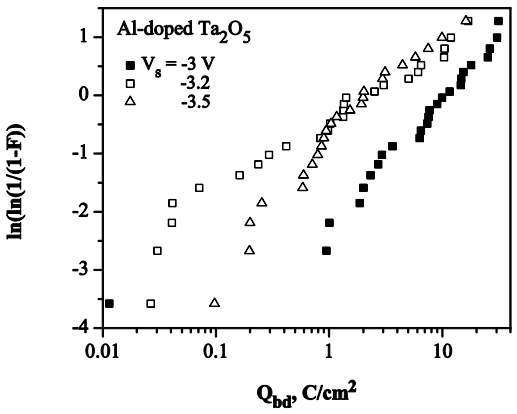

Fig. 5 Weibull distributions of Q_{bd} for Al-doped Ta_2O_5 under various V_s

All those results indicate that the BD in both *undoped and Al-doped Ta_2O_5 is affected by the process-induced defects and it cannot completely be explained only by the percolation model*. The presence of defects forms weak spots which dictate the BD. This is compounded by the double-layer structure of the high-*k* stack and the impact of the interface region. As a result, *the value of Weibull slope is a total product of these two effects and can not exhibit by default any clear trend*. When the effect of interfacial layer dominates over the effect of defects the BD is attributed to intrinsic BD of the stack. This also means that the dominant mechanism of degradation is embodied in the density of pre-existing defects in high-*k* dielectric. In this context two different mechanisms of BD emerge for pure and Al-doped Ta_2O_5: i) the pre-existing traps causing weak spots in undoped layers play a key role in electrical degradation; they mainly constitute the BD and extrinsic mechanism of degradation is prevalent, especially at low voltage; at high V_s, stress-generated new traps appear to initiate the BD. ii) Al doping reduces defects in Ta_2O_5 resulting in the domination of intrinsic failures in the breakdown statistics, and the mechanism of degradation is more adequate (but not completely!) to the percolation concept. The type of defects, however, are different in two type samples regarding their structural nature, amount and energy location, which factors reflect on the TDDB data and could explain the observed difference between undoped and doped Ta_2O_5. According to the TEM data, the weak spots are not local physical thinning of the dielectric, (pure and doped one). The SILC-measurements of W-gated Ta_2O_5 capacitors under CVS at gate injection have revealed that the processes of electron trapping at pre-existing traps and positive charge build-up are responsible for the SILC [23]; there was no evidence of stress-induced generation of new traps. Unlike the case of Ta_2O_5, the SILC in Al-doped Ta_2O_5 is a result of new traps generation [24]. The stress-generated traps act as stepping (transport) sites for injected electrons giving rise to SILC, (i.e. the electrons are trapped and released immediately thereafter). Therefore, considering the previous SILC measurements, it is reasonable to interpret the results in terms that *BD mechanism in pure and lightly Al-doped Ta_2O_5 is intimately related to both pre-existing traps and stress-induced new traps*. In the former case the impact of trapping at pre-existing traps is a little dominant and in the latter one new traps generation mainly defines the BD process. In this sense the BD degradation of doped films is dominated by the Al-induced modification of the Ta_2O_5 network. Regarding microstructural aspects of the traps, wide category of bond

defects (weakened and non-perfect Ta-, Si- and Al-related bonds) and oxygen vacancies represent precursors for BD defects. The bond-breaking is suggested as a general mechanism to describe the electrical breakdown behaviour.

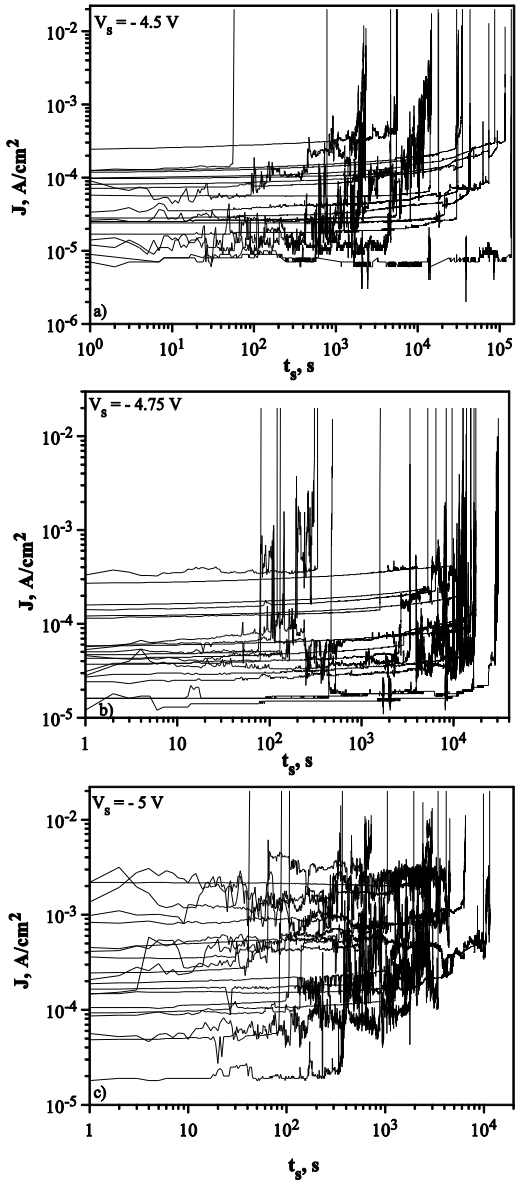

Fig. 6 TDDB characteristics of Hf-doped Ta_2O_5 stacks stressed at room temperature with V_s of - 4.5 (a); - 4.75 V (b); - 5 V (c)

3.3 Hf-doped Ta2O5 [25]

Fig. 6 shows the leakage current density-stress time (J-t_s) characteristics under various V_s at room temperature. The curves demonstrate relatively constant current up to BD, similarly to the case of pure and lightly Al-doped Ta_2O_5. With similar values of J_0, pure Ta_2O_5 stacks reveal shorter time-to-breakdown. The longer t_{bd} in the doped films may be attributed to the compensation of oxygen vacancies by Hf in Ta_2O_5 accompanied by the observed improvement of the stack parameters. The structural nature of the weak spots is regions with a concentration of bond defects (weakened and non-perfect Ta-; Si-; and Hf-related bonds).

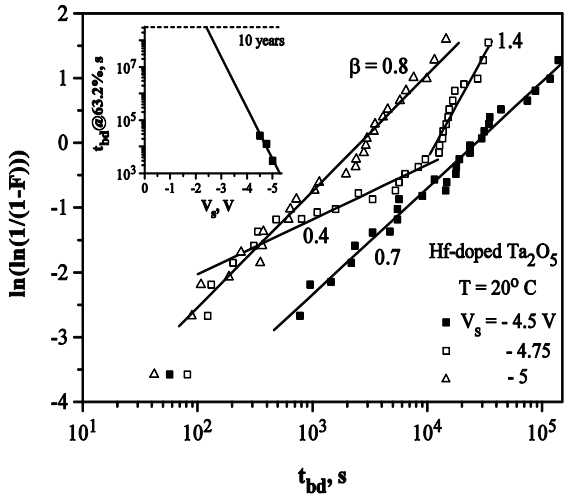

Fig. 7 Weibull plots of Hf-doped Ta_2O_5 under different V_s.
The inset shows t_{63} values vs. stress voltage

Weibull plots for various V_s are given in Fig.7. The distribution is with similar slopes for the lowest and the largest V_s. In the short time range (10^2-10^4 s) low β value (0.4) corresponds to the early BDs; the slope is steep (1.4) in the longer time range. Generally, the Weibull distribution of TDDB differs from that of Ta_2O_5 where very clear separation of early and long-time BDs was detected with different β values. The lack of well pronounced region of early breakdowns for the doped samples implies that they have less process-induced defects. Considering the bi-layer structure of the films and inevitable difficulties in correct estimation of the applied fields in the interface layer and in the high-k layer we again discuss the BD characteristics here in terms of ones controlled by applied voltage rather than the applied field. We will focus on the long-time BD (more than ~ 10^4 s) as the most relevant to the intrinsic electrical degradation of high-k films and where the influence of the interfacial region on the breakdown phenomenon is explicitly included. The detected lower β values (0.7-1.4) than the value for SiO_2 with the same physical thickness indicates that the percolation model does not seem to apply to Hf-doped Ta_2O_5 films, and the extrinsic explanation of HBD seems more likely. The percolation model can be accepted only if we assume low number of defects involved in BD with large spacing between defects where tunneling of trapped electrons becomes probable and causes low value of Weibull slope. (Note that the charge trapping could be everywhere in

the stack, i.e. in the bulk high-*k* as well as within the interface layer; the trapping in the interface layer could not only trigger breakdown of the stack but influences its Weibull distribution.) If we consider EOT of Hf-doped Ta_2O_5, however, instead of its physical thickness, β values in the range of $t_{bd} > 10^4$ s are in accordance with those of ~ 2 nm SiO_2 layer, and consequently the percolation model for the stressed Hf-doped stack can be used. An additional support for the percolation approach is the fact that the curves are shifted to the left with increasing $|V_s|$, i.e. the stressing voltage acts indeed as an acceleration factor for BD, and the generation of new defects affects the HBD (Fig. 7). This behavior of the Weibull distribution also indicates improved BD characteristics of the Hf-doped Ta_2O_5 with respect to undoped one. The maximum projected voltage for a 10 years lifetime is found to be -2.4 V, or equivalently 3 MV/cm, (inset of Fig. 7). This parameter is significantly larger than that of SiO_2 [26] and Al-doped Ta_2O_5 with the same EOT. Therefore, lifetime scaling of Hf-doped Ta_2O_5 is definitely better than both pure and Al-doped Ta_2O_5, and might be better than SiO_2 when compared the same EOT value.

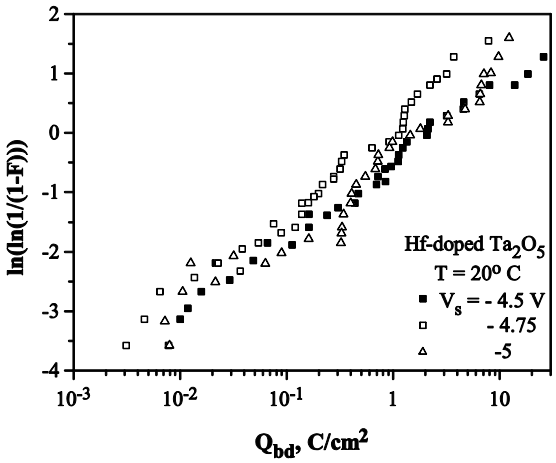

Fig. 8 Q_{bd} distribution for Hf-doped Ta_2O_5 under V_s from - 4.5 to - 5 V

The Weibull distribution of charge-to-breakdown is shown in Fig. 8. The curves corresponding to V_s = - 4.5 and - 4.75 V are as if in accordance with the percolation model (the curve with more negative Vs is shifted to the left). The curves for the lowest and highest $|V_s|$, however, are indistinguishable. Since the Q_{bd} variation does not appear to have a definite behavior as a function of V_s, it is not correct to consider V_s as an acceleration factor for breakdown. The trapping at pre-existing traps at V_s = - 5 V obviously dominates and the effect of V_s as a factor for generation of new traps can not completely be revealed. The observed phenomenon corresponds to the long-term t_{bd} where the role of interfacial region in the BD events is essential. Thus the effect of charge trapping in the interface layer itself could be dominant on the BD process. We found linear relationship between Q_{bd} and t_{bd} implying that the average leakage current at BD has narrow distribution and the distribution of t_{bd} is caused by large size defects. Similarly to the case of pure and Al-doped Ta_2O_5, SILC at breakdown for Hf-doped films can not be used as a measure of increasing defect density during stressing due to the strong effect of weak spots. As it

was reported earlier [6] electron trapping at pre-existing sites in high-*k* dielectrics can be the first stage of stress-induced trap generation process. The strong trapping phenomena, however, results in very complex relation between the BD and SILC, completely different from that for SiO_2. The evidence for the presence of weak spots in these experiments in combination with long t_{bd} indicates that both the process-induced defects and the interfacial layer affect HBD. The action of these factors leads to specific Weibull distribution and to unpredictable dependence of t_{bd} and Q_{bd} on V_s. The introduction of Hf into the matrix of Ta_2O_5 generates shallow traps which are responsible for the domination of the tunneling processes in the conductivity in Hf-doped Ta_2O_5 [13], [17]. These traps in contrast to the expectation do not speed up breakdown, and t_{bd} for the doped film is even larger than in the pure Ta_2O_5 under the same stressing voltages. Presumably, the presence of Hf into Ta_2O_5 ultimately improves the BD characteristics and modifies the dielectric BD mechanism(s) manifesting itself as differences in the breakdown statistics of undoped and doped films.

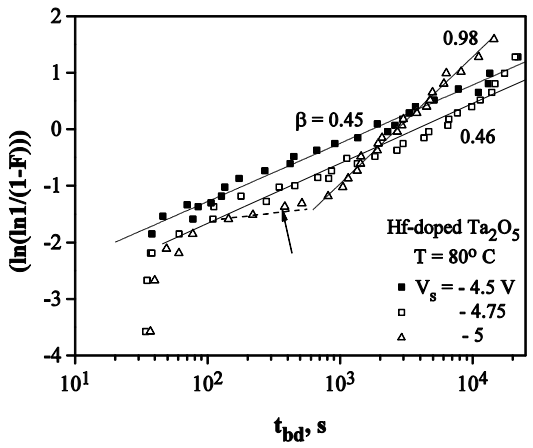

Fig. 9 TDDB Weibull distribution of Hf-doped Ta_2O_5 devices under various stress voltages at 80ºC

The high temperature stressing at 80°C modifies Weibull distribution to some extent - the breakdown occurs faster than that at room temperature, but there is no visible temperature dependence of the shape factor β (Fig.9). The combined effect of high T and stressing voltage on the Weibull slopes does not exhibit unambiguously trend; the percolation model for BD at 80°C is not applicable for all V_s. The effect of V_s at high temperature on the BD has no simple explanation, but nevertheless there are indications for TDDB reliability degradation: the stress at high temperature worsens the characteristics, stimulates charge trapping with evidence that large size defects dictate the breakdown; TDDB lifetime degrades, and it is not possible to extract the operating voltage for 10 years lifetime. The results indicate for some redistribution of defects at high temperature for both doped and undoped samples. For example, the presence of regions with different slopes at a certain Vs and a single plateau between them (Fig. 9, the region indicated by arrow) implies for the activation of different type traps and their dominance in the conductivity of Hf-doped films. The nature of defects is not the same for the pure and doped Ta_2O_5 which

manifests as differences in the corresponding Weibull distributions. The stressing at high temperatures weakens some bonds and results in enhanced trap generation. One can not also exclude the effect of hydrogen-related particles on the degradation at elevated temperatures. Hydrogen is ubiquitous in the high-*k* system and can be everywhere in the stack. During stressing at high temperature liberated protons at the interface with Si could be a key factor for enhanced charge trapping at strained bonds in the interface layer. Being liberated hydrogen readily diffuses in the high-*k* layer resulting in generation of positively charged centers or neutral trapping centers.

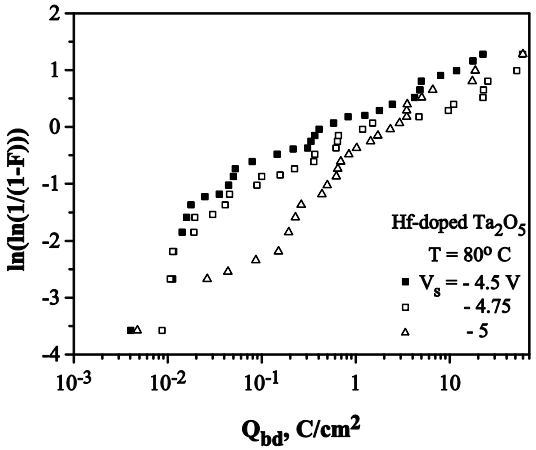

Fig. 10 Weibull distributions of Q_{bd} at 80ºC for Hf-doped Ta_2O_5 under different V_s

The charge to breakdown for the doped films at 80ºC does not reduce at large stress voltage and the Q_{bd} data can not be interpreted within the percolation model: instead, the Q_{bd} curves are shifted to the right with increasing $|V_s|$ (Fig. 10). The observed higher Q_{bd} at largest V_s generally means a lower defect generation rate. The shallow traps which are an attribute of Hf-doped Ta_2O_5 could be responsible for this phenomenon.

Referring to the conductivity and SILC measurements [5], [17], we note that distinctly different conduction mechanisms control the leakage current in pure and Hf-doped Ta_2O_5 which are defined by the traps participating in the current transport. The oxygen vacancies are the main defects in Ta_2O_5 which constitute the domination of Poole-Frenkel mechanism. The conduction in Hf-doped Ta_2O_5 is performed through shallow traps resulting in domination of tunneling processes in the conductivity. The consequence of the transport through shallow traps is considerably weaker T-dependence of the current. One possible scenario of the HBD mechanism in Hf-doped films includes breaking at strong stress of weakened from the charge trapping bonds; this results in new traps generation (i.e. percolation model is valid) which quickly leads to HBD. The broken bonds could be precursor breakdown defects. Unlike the case of Ta_2O_5 where the BD mechanism is dominated by the trapping at the pre-existing traps (deep traps attributed to oxygen vacancies; the vacancy can trap one or two electrons), new traps generation at strong stress becomes more effective for Hf-doped Ta_2O_5, and affects its final BD. The HBD in the doped Ta_2O_5 is presumably dictated by the Hf-induced shallow traps instead of deep oxygen vacancies.

This indicates that the Hf-induced modification of Ta_2O_5 network governs the TDDB behavior manifesting as stress-generation of new traps. These in-fabricated traps cause weak spots in the doped films and account for the early breakdowns. At high levels of stress, which are used to examine TDDB characteristics, the weakened by the trapping bonds break and play the role of a nucleation center for the generation of defect clusters that can form a conduction link through the dielectric until HBD occurs, i.e. stress-generated new traps process becomes significant and the mechanism of BD is more adequate to the percolation approach. In this context electron trapping at pre-existing traps is a concomitant process for BD. Therefore, *the BD mechanism in Hf-doped Ta_2O_5 stack is associated with both pre-existing shallow traps and stress-induced new traps.* In the final stage of BD the last process is dominant. These processes are compounded with the impact of the interface region and its breakdown. When the degradation of interface layer dominates over the effect of the initial defects in the high-*k* layer the BD is designed as an inherent property of high-*k* stack, i.e. as its intrinsic BD. In the term of t_{bd} this corresponds to long t_{bd} ($> 10^4$ s) where the high applied field on the interface region quickly provokes breakdown. So the combined effect of the initial defects, the stress-induced new traps and the effect of the interface region itself constitutes the Weibull distribution of dielectric BD in high-*k* systems.

4. CONCLUSION

The picture of the BD in Ta_2O_5-based films on Si is quite complicated and different than that of SiO_2 with the same physical thickness. The pre-existing traps which provoke weak spots with non-uniform distribution are responsible for the early BDs. Their effect is strong enough, even in the range of long time-to-breakdown where the impact of inevitable lower-*k* interface layer at Si can not be neglected. Since the presence of this layer is inherent property of high-*k* film on Si, it is reasonable to designate the failure of the interface layer as an intrinsic mode of the BD of high-*k* stack. Thus, the behaviour of Weibull distribution of time-to-breakdown for pure and doped Ta_2O_5 could be interpreted as coexistence of extrinsic and intrinsic BD modes. Both the pre-existing traps and the new traps generated affect the region with long time-to-breakdown. The domination of one of these competitive effects dictates the mechanism of degradation: the effect of process-induced defects dominates in Ta_2O_5 and the BD can not completely be explained by the percolation approach: the trapping at pre-existing traps facilitates the breakdown and the effect of stressing voltage as a factor for generation of new traps can not be well observed. The doping reduces defects in Ta_2O_5 which manifests in larger Weibull slopes and better TDDB characteristics of the doped samples: the generation of new traps prevails over the charge trapping and the mechanism of breakdown is more adequate to the percolation model. Accordingly, the BD degradation in doped Ta_2O_5 is dominated by the dopant-induced modification of Ta_2O_5 network indicating that the dopant element in high-*k* dielectrics could be a primary factor in reliability issues.

Lifetime scaling of the doped films is better than Ta_2O_5 and might be better than SiO_2 with the same equivalent oxide thickness. Trapping phenomena, however, are still observed in the doped films which complicate TDDB characteristics; in some cases the effect of stressing voltage as an acceleration factor for electrical degradation is obscure.

The influence of pre-existing traps is compounded with the effect of high applied field in the interface layer and of stress-induced new traps generation in the range of long-time-to-breakdown. The action of these factors leads to specific Weibull distribution of the high-*k* samples and to unpredictable dependence of time and charge to breakdown on the stressing voltage. *The peculiarities of the TDDB characteristics of the pure and doped Ta_2O_5 are assumed to be due to the inherently different process-induced defects* (deep levels attributed to oxygen vacancies in the former and shallow traps in the latter case). The trapping at pre-existing traps is the starting point for the electrical failure in both stacks. Further, the trapping at deep traps remains dominant for Ta_2O_5 up to final stage of breakdown. The HBD in the doped Ta_2O_5 is defined by the dopant-induced shallow traps: at strong stress the weakened by trapping bonds break and this vastly facilitates new traps generation, and the mechanism of degradation is more adequate to the percolation model. The stressing at high temperatures additionally weakens some bonds and enhances trap generation. When the interface region experience extremely high applied filed, the degradation of interface layer could prevail over the defect-related processes in the high-*k* layer. Therefore, *three competitive factors constitute the Weibull distribution of dielectric BD in high-k systems*: initial defects, stress-induced new traps and the degradation of the interface layer itself. The domination of one of them depends on the stress conditions, nature of pre-existing traps and the interface layer parameters. A subtle problem for high-*k* stacks is that the Weibull slope is a total product of these three entities and consequently it can not exhibit by default any clear trend and well pronounced relationship with stressing voltage and stressing temperature. This is indeed observed if one tries to find regularity in β variation with V_s and T. This implicitly suggests that the simple comparison only of Weibull slopes of high-*k* stack with the corresponding values of SiO_2 is not the proper approach to interpret the TDDB characteristics of high-*k* films and could result in inaccuracies in reliability prediction.

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