

THERMALLY-OXIDIZED HfO₂ ON Se-PASSIVATED n-TYPE Si(100)

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Se passivation of Si(100) creates a surface which is free of dangling bonds. Electrically, the passivation may also result in a surface free of surface states. Fig. 1 shows the atomic structure of the Se-passivated Si(100) surface. It is interesting to examine the effect of Se passivation on the electrical properties of the high-k dielectric/Si(100) interface. In this paper, we report our results on interface engineering between HfO₂ and n-type Si(100) with Se passivation, in our effort to obtain a device-quality dielectric/Si interface for future Si CMOS nanoelectronics. Hf of ~40 Å was deposited on Se-passivated Si(100) by e-beam evaporation and then oxidized in O₃ or O₂ to form HfO₂ at temperatures from 300 to 600°C. I-V and C-V characterization was performed to examine the electrical properties of the HfO₂/Se/Si(100) interface. O₃ oxidation seems to over-oxidize into the n-type Si substrate, causing a large negative shift in flat-band voltage (Fig. 2). A structural model is proposed for the O₃-oxidized dielectric stack, in which the Se monolayer becomes a layer of positive charge sandwiched in the dielectric stack. Samples annealed in O₂ below ~350°C show much improved properties: an EOT which is the smallest in all the samples we have investigated so far, 31 Å (Fig. 3); a flat-band voltage which is close to the theoretical value; and a small leakage current which is orders of magnitude lower than the control samples (Fig. 4). In Fig. 3, the passivated samples always show smaller EOT than the control samples up to 600°C, although the difference in EOT decreases as the oxidation temperature increases. These results support our theory that over-oxidation sandwiches the Se monolayer as a layer of positive charge in the dielectric stack and demonstrate that Se passivation of Si(100) suppresses Si oxidation in O₂ up to 600°C.

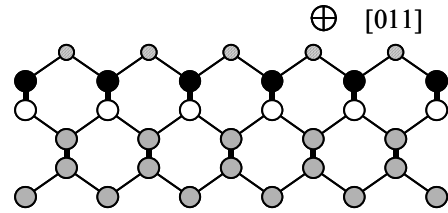


Fig. 1. Atomic structure of the Se-passivated Si(100) surface.

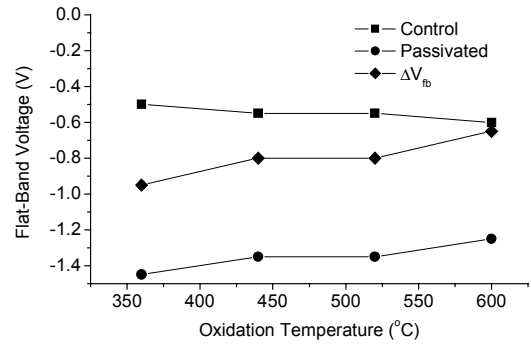


Fig. 2. Flat-band voltage, extracted from C-V, as a function of oxidation temperature for passivated and control samples oxidized in O₃.

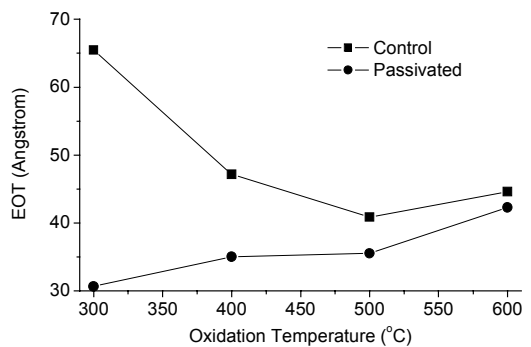


Fig. 3. EOT, extracted from C-V, as a function of oxidation temperature for passivated and control samples oxidized in O₂.

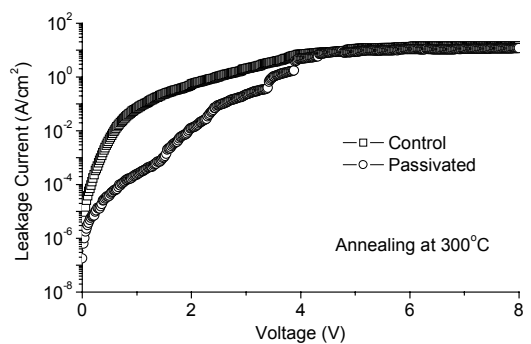


Fig. 4. Leakage current of passivated and control samples oxidized in O₂ for 15 min at 300°C.