Mixing and Decomposition of Al_2O_3(2 nm)/HfO_2(2.5 nm) Stacks on Si Induced by Rapid Thermal Annealing

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In order to pursue with the down scaling of Si-based ultra-large scale integration (ULSI) technology, several materials holding dielectric constant higher than that of silicon oxide were proposed as gate dielectric replacements for metal-oxide-semiconductor field effect transistors (MOSFET). The appreciably large dielectric constant, as well as the low density of trapped charges and interfacial electronic states of HfO_2 films on Si has attracted much attention to this material. However, hafnium oxide films on Si crystallize at relatively low temperatures and do not form effective barriers to the migration of oxidant species and other impurities toward the interface with Si during subsequent post deposition thermal processing steps of ULSI technology. To overcome these difficulties, different Hf-based dielectrics have been proposed for gate dielectric applications, such as Hf silicates and aluminates. However, hafnium silicate films on Si undergo phase separation and crystallization during annealing while hafnium aluminate films on Si present high density of negative interfacial charge.

As an alternative, it has been proposed that these undesired characteristics can be minimized on well defined, nanoscopic Al_2O_3/HfO_2 stacks on Si, which have the good electrical characteristics of the HfO_2/Si interface and form effective diffusion barriers owing to the topmost Al_2O_3 layer. The integration of this kind of gate dielectric in ULSI technology relies, however, on the capability of the stack structure of maintaining its integrity after all thermal processing steps of device fabrication following gate dielectric deposition**.**

In this work the Al_2O_3/HfO_2/Si structures were prepared by atomic layer deposition and the atomic transport was accessed by profiling all elements in the system with subnanometric depth resolution, by means of medium and low energy ion scattering and by narrow resonant nuclear reaction profiling. Al migration toward the stack/Si interface, Al loss by desorption from the surface, and Hf transport across the Al_2O_3 film layer toward the outermost surface are observed. The loss of oxygen from the stack is also noticeable, most probably caused by compound dissociation and desorption of oxygen containing species. The observed presence of Hf at the outermost surface of the dielectric stack and of Al at the dielectric/Si interface can have detrimental consequences to the electrical properties of device.

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