Interface Characterization of the High-\textit{k} Gate Dielectric Pr$_2$O$_3$

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Pr$_2$O$_3$ is currently under consideration as a potential alternative gate dielectric candidate for sub-0.1 \textmu{}m Complementary Metal Oxide Semiconductor (CMOS) technology. For all thin gate dielectrics, the interface with silicon plays a key role, and in most cases is a dominant factor in determining overall electrical properties. We studied the Pr$_2$O$_3$/Si(001) interface by a non-destructive depth profiling using synchrotron radiation photo-electron spectroscopy and \textit{ab initio} calculations. Our results provide evidence that a chemical reactive interface exists consisting of a mixed Si-Pr oxide such as (Pr$_2$O$_3$)$_x$(SiO$_2$)$_{1-x}$, typically in non-stoichiometric composition. There is no formation of neither an interfacial SiO$_2$ nor interfacial silicide: all Si-Pr bonds are oxidized and all SiO$_4$ units dissolve in the Pr oxide. Interfacial silicates like (Pr$_2$O$_3$)$_x$(SiO$_2$)$_{1-x}$ are promising high-\textit{k} dielectric materials because they represent incremental modification of SiO$_2$ films by Pr ions so that the interface characteristics can be similar to Si-SiO$_2$ interface properties. Under ultrahigh vacuum conditions, silicide formation is observed when the silicate film is heated above 800°C. The praseodymium silicate system observed at the interface between Si(001) and Pr$_2$O$_3$ offers greater flexibility towards integration of Pr$_2$O$_3$ into future CMOS technologies.

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