New amorphous ultra-thin $Ti_xAl_{1-x}O_y$ alloy oxide layer for next generation of high-K gate dielectrics

Scientific Achievement

We have established an optimized process to produce $Ti_xAl_{1-x}O_y$ (TAO) stoichiometric layers. The process involves sputtered-deposition of thin TiAl alloy films followed by *in situ* oxidation at room temperature to produce TAO layers without developing a SiO_2 interfacial layer, which would greatly decrease the overall dielectric constant of a high-k/SiO_2 heterostructure. Studies show that the use of chemically active atomic oxygen provides sufficient activation energy to oxidize the Ti_xAl_{1-x} metallic layer into an amorphous alloyed oxide film while the oxidation barrier property of Ti_xAl_{1-x} prevents further diffusion of oxygen atoms to the film-Si interface, which inhibits the formation of an undesirable SiO_2 interfacial layer. Meanwhile, it is observed that the Al metal partially reduces the SiO_x existing at the TA/Si interface because of preferential bonding of O to Al, thus effectively reduces the unfavorable SiO_x layer. Electrical characterization of $Ti_xAl_yO_z$ layers shows that the 3 nm $Ti_{0.75}Al_{0.25}O_3$ layer exhibits a high capacitance density 7.7~8.3 $\mu F/cm^2$ (with a record thin *EOT* = 0.42 – 0.48 nm), mainly due to the suppression of SiO_x interfacial layer formation.

More recent work shows that the process established for production of TAO layers can be extended to the growth of MgO layer. The MgO film obtained has practically no SiO_x layer that is superior to the general process using reactive sputtering. The bilayerd films of TAO-MgO are synthesized on Si and will be investigated to manipulate the electric properties of TAO based CMOS.

Future work will include investigating the synthesis of the amorphous high-K dielecrtic layer using atomic layer deposition to achieve atomic scale control of film growth and interface formation.

Significance

We demonstrated that TAO alloy investigated here provides a novel material with the appropriate properties required for the next generation of nanoelectronics.

We demonstrated that $Ti_xAl_{1-x}O_y$ layers with < 0.5 nm equivalent oxide thickness can be achieved. Studies indicate that our unique 2-step process, a low temperature oxidation following room temperature sputter-deposition of TiAl layers, is critical to produce ultra-thin $Ti_xAl_{1-x}O_y$ layers on Si with sub-atomic or no SiO_x interface formation and achieve a high-performance TAO high-K dielectric layer for the next generation of nanoscale CMOS. Partial results of the work described above were published in *Appl. Phys. Lett.* **86**, 031902 (2005). Several invited talks have been given at national and international conferences.

Collaboration with Dr. Irene' group in UNC-Chapell Hill will be carried out to explore the density of trapping states and band gap of TAO films and TAO-MgO heterosturctures.

Performers

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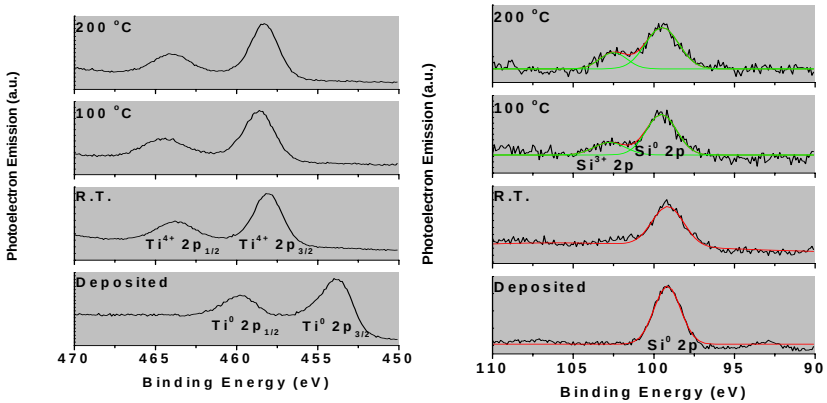
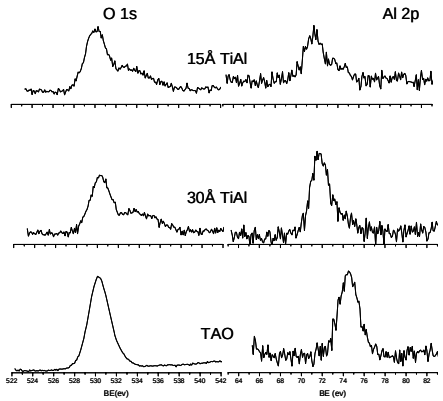
New amorphous ultra-thin TixAl1-xOy alloy oxide layers for next generation of high-K gate dielectrics

R.T. sputter-deposition of thin TiAl alloy films followed by *in situ* oxidation using atomic oxygen fully oxidizes TiAl and inhibits the formation of SiO_2 interface

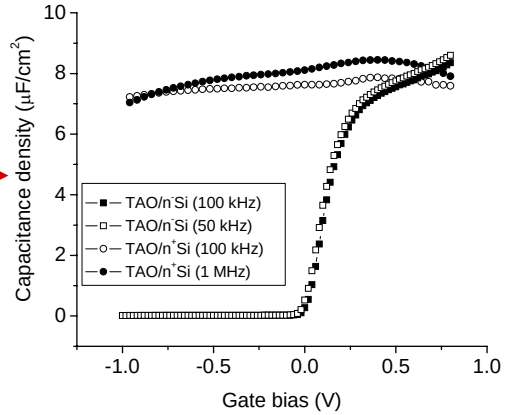


XPS analysis of TiAl films



Unique Thermodynamic and Kinetic Oxidation of TAO alloy assists the reduction of SiO_x layer

High accumulation capacitance densities (7.7 – 8.3 μF/cm^2), corresponding to an *EOT* less than 0.5 nm



Future Work

- **Optimize bandgap and density of trapping states at TAO-Si interface**
- **Investigate effects of introducing an atomically thin MgO (~1nm) layer into the TAO-Si structure on the overall electrical properties of a TAO-MgO films for high K dielectrics**
- **Investigate effect of compositional changes in the TAO layer**

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