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Atomic Layer Deposition of Hafnium Oxide on Silicon – Application of Molecular Spectroscopy Techniques to Support Reactor Diagnostics and Models of Chemical Reaction Mechanisms

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Atomic layer deposition (ALD) employs alternating reactant exposures of two precursors which react on a surface sequentially to build thin films atomic layer by atomic layer. Ideally, it is an effective technique for the deposition of defect-free conformal thin films. The next generation of Si-based semiconductor devices is shrinking to a size where thin layers of SiO_2 no longer adequately provide the required electrical insulation needed for good device performance and ALD is a promising technique for providing the required insulation. This talk will review the chemistry and ALD process for the creation of thin HfO_2 films. Our group at NIST has been working on developing *in situ* diagnostics that could be applicable to industrial ALD processes by employing various molecular absorption spectroscopic techniques in the near- and mid-infrared. A NIST-designed reactor has been used for both gas-phase and surface diagnostics during ALD deposition. Techniques that will be reviewed have included Fourier-transform infrared (FTIR) spectroscopy and tunable laser diode wavelength modulation spectroscopy in the near-infrared, quantum cascade laser absorption spectroscopy at ~ 10 microns in the mid-infrared, and reflection-absorption IR spectroscopy (RAIRS). In addition, the group has been developing chemical-kinetic reaction mechanisms with the goal that these can be incorporated into computational fluid dynamics-based reactor-scale models. Initial measurements to validate these models with spatially- and temporally-resolved *in situ* measurements will be discussed.