Chemisorption Mechanisms of Aminosilane Precursors during ALD of SiO_2: *in situ* characterization and ab initio study

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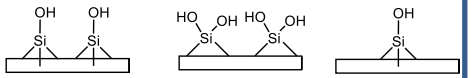
1. Background

- Surface reaction mechanism of ALD SiO_2 have been studied using DFT
- The study of effect of different hydroxyl group types to the chemisorption of Si precursor are still missing
- The comparative study of surface reaction mechanism predicted by DFT and experimental method are still rare.

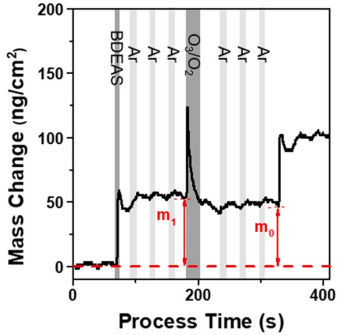
2. Methodology

- Experimental
  - *in situ* QCM and FTIR
- DFT calculation
  - Dmol3, Material Studio 7, Biovia, USA
  - Surface hydroxyls types



[Vicinal-OH] [Geminal-OH] [Isolated-OH]

3. In situ characterization (QCM)

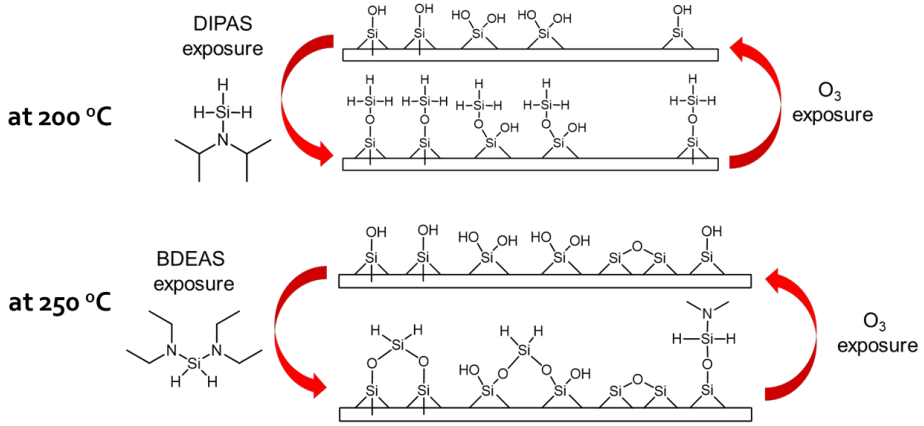


$$\frac{m_0}{m_1} = \frac{M(Deposited\ film)}{M(precursor) - nM(ligand)}$$

n = the number of released ligands

- DIPAS (200°C)
  - m_0/m_1 = 1.86-1.94 → n = 0.99
- BDEAS (250°C)
  - m_0/m_1 = 0.91 → n = 1.48

4. Surface reaction mechanism (DFT)



Number of released ligands

Aminosilane precursor	Calculated	In situ QCM
DIPAS (200°C)	1.0	0.99
BDEAS (250°C)	1.5	1.48